ANNUAL REPORT

1996



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

Director: Prof. Norbert Kroó

Address: Budapest, Konkoly-Thege M. út 29-33, Hungary

Letters: H-1525 Budapest, P.O.B. 49

Phone: (36-1-) 395 9153 Fax: (36-1-) 395 9278 Telex: 22 47 22 kfki h

URL: http://www.kfki.hu/~szfkihp

ANNUAL REPORT 1996

Edited by L. Csillag, J. Kollár, G. Konczos, B. Selmeci

Closed on 1st December, 1996

Dear Reader,

I am glad to hand you over the third volume of the yearbook of the Research Institute for Solid State Physics of the Hungarian Academy of Sciences. Our aim has been to get you acquainted with some of the recent results of our Institute.

The staff of our departments continues to be involved to a large extent, in basic research in theoretical and experimental solid state physics, in materials sciences, in the interaction of light with matter and in laser physics. Part of our research is of applied character centered mainly around our activity in materials sciences and laser development and applications.

In spite of our mounting financial difficulties, I feel satisfied with our achievements. The level of our publication activity remained as before. The reflection of the scientific community has also been positive as seen e.g. from the results of the evaluation conducted by the Hungarian Academy of Sciences early this year since we came out from it as one of the highest ranked institute.

After a long period of reconstruction the Research Reactor is fully operative at our site. The utilisation of this gathered significant momentum. An increasing number of measurements have been carried out with domestic and international partners.

International co-operation has always been and continues to be a significant tool in our research. In addition to our traditional bilateral co-operation we are happy to report our increased presence in the research programmes of the European Union and NATO.

We have a continued interest in high education, mainly at the Eötvös Loránd University and at the Technical University Budapest, but in limited volume at other universities, too. In the frame of this activity, we operate a solid state physics and an optics laboratory for the praxis of undergraduate students in addition to regular and voluntary courses and doctoral research training.

May I hope that this booklet will be a useful tool to get acquainted with the work and achievements of our research teams.

Budapest 1 December, 1996.

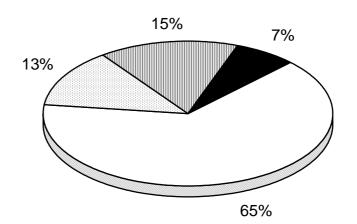
Norbert Kroó Director

Work at Kin

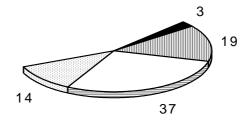
Key figures

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

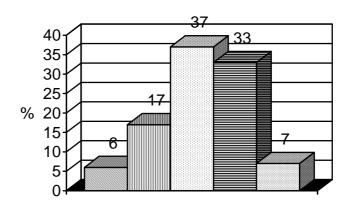
- a) by professions:
 - □scientists
 - engineers
 - technicians/assistants
 - administrators



- b) by scientific titles/degrees:
 - member of Hungarian Academy of Sciences
 - doctor of science (Dr. habil.)
 - □ candidate of science (Ph.D.)
 - ■university doctor

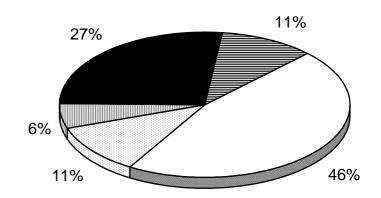


- c) by ages:
 - under 30 years
 - 30-40 years
 - 40-50 years
 - **■** 50-60 years
 - □ over 60 years



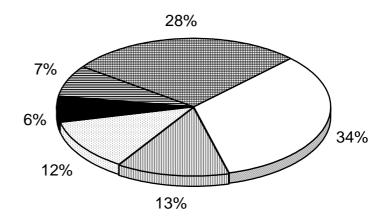
Financial management

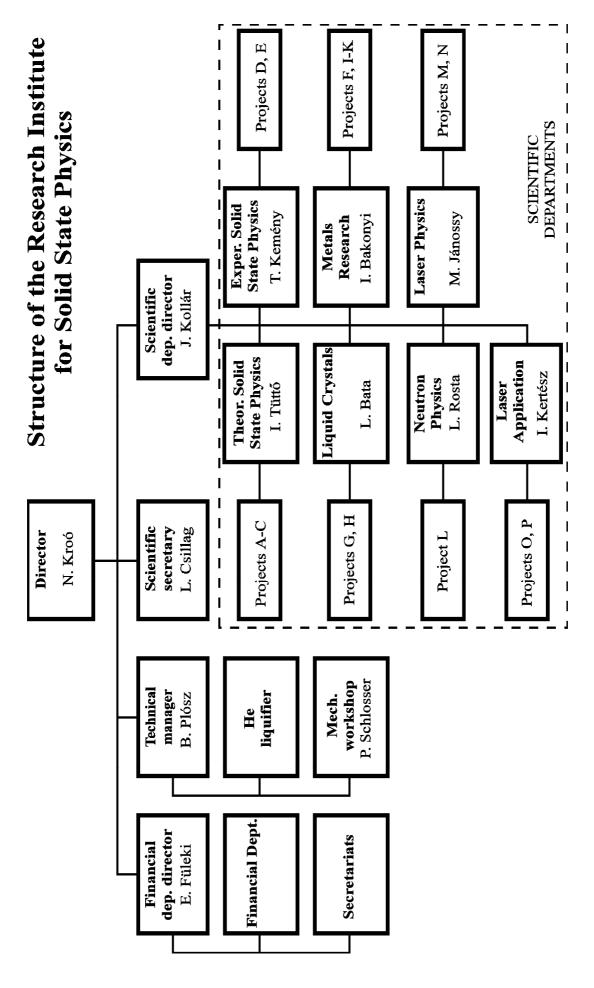
- a) Sources of operation costs:
 - ☐ MTA (Hungarian Academy of Sciences)
 - ☐ OTKA (Hungarian Scientific Research Fund)
 - ☐ foreign (international) grants
 - OMFB (National Committee for Technological Development)
 - others (incl. contracts)



b) Distribution of expenditures:

- □ wages and salaries
- overhead, labour (health service, etc.)
- overhead, other (energy, etc.)
- consumables
- others (incl. travel costs)
- **■** investments





A. STRONGLY CORRELATED SYSTEMS

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

Low dimensional magnetic models. — Recently several new materials have been discovered in which the localized magnetic moments are coupled in a way resembling ladders. The energy spectrum and the behaviour of these systems depends strongly on the value of the spin and the number of legs of the ladder. We studied the phase diagram of such ladder models using the density matrix renormalization group (DMRG). First in a rather technical work we have checked the accuracy of the DMRG procedure on the example of the Ising model in transverse field, as the simplest quantum mechanical spin problem, and have shown how the so-called truncation error is related to the real error in the energy values. With this background we have determined the phase diagram of a two leg ladder model including also plaquette couplings, and have found indication for the existence of several different massive phases.

One-dimensional fermionic models. — We investigated in detail the model defined through the relativistic limit of the one dimensional attractive Hubbard model. This model possesses both massive and massless dressed particles which are described just like the particles in the Hubbard chain, by Bethe-Ansatz type equations. We analysed the eigenstates of the system. We have found that the limiting model has higher symmetry than the original Hubbard chain; it acquires in addition also the chiral symmetry. We determined the scattering properties of the particles, and also the conformal properties of the field corresponding to the massless sector. All these results confirm, that the scaling limit of the Hubbard chain can be identified with the chiral invariant Gross-Neveu model.

Theory of dissipative motion of heavy particles. — We studied the low temperature behaviour of two level systems (TLS) interacting with the conduction electrons in amorphous metals. To approach the temperature region below the Kondo temperature we generalized the model to electron spin degeneracies: $N_f > 2$. The solution of the scaling equations written in N_f^2 order confirmed that the only stable fixed point of the system is equivalent to the Kondo-model of spin 1/2, moreover we found the limits of this equivalency. We also studied what conditions can make a commutative TLS model — not showing Kondo-effect in simple cases — to be non-commutative. The asymmetry of the electron band even in leading order, the splitting of the levels in higher orders result in logarithmic divergencies in the couplings, which were originally invariant in the scaling.

E-Mail:

Gábor Fáth fath@power.szfki.kfki.hu
Örs Legeza olegeza@power.szfki.kfki.hu
Karlo Penc penc@ power.szfki.kfki.hu
Jenõ Sólyom solyom@ power.szfki.kfki.hu
Károly Vladár vladar@ power.szfki.kfki.hu
Ferenc Woynarovich fw@ power.szfki.kfki.hu

⁺ Permanent position: Technical University of Budapest

Grants

OTKA¹ I/4 T4473. Low dimensional interacting electon systems and magnetic models

OTKA T 014443. Completely integrable 1-d systems

OTKA T 015870. Models of strongly correlated low-dimensional electron systems

OTKA T 017128. Theoretical study of dissipative motion of heavy particles

Publications⁺

Articles

- A.1. Ö. Legeza and G. Fáth: On the accuracy of the density matrix renormalization group method. Phys. Rev. **B53**, 14 349 (1996).
- A.2. F. Woynarovich: Massive particles in the relativistic limit of the non-half-filled 1D attractive Hubbard model. J. Phys. **A29**, L37 (1996).
- A.3. K. Penc, H. Shiba**, F. Mila* and T. Tsulagoshi*: Ferromagnetism in multiband Hubbard models: From weak to strong Coulomb repulsion. Phys. Rev. **B54**, 4056 (1996).
- A.4. K. Penc, K. Hallberg*, F. Mila* and H. Shiba*: Shadow band in the one-dimensional large U Hubbard model. Phys. Rev. Lett. **77**, 1390 (1996)
- A.5. Z. Domanski*, R. Lemanski* and G. Fáth: The asymmetric Hubbard model on a two-dimensional cluster. J. Phys.: Condens. Matter **8**, L261 (1996)
- A.6. O. Újsághy*, A. Zawadowski and B.L. Győrffy*: Spin-orbit induced magnetic anisotropy for impurities in metallic samples of reduced dimensions: Finite size dependence in the Kondo effect. Phys. Rev. Lett. **26**, 2378 (1996)
- A.7. G. Zaránd*, A. Zawadowski: Theory of two-level systems and their role in point contacts. Physica **B218**, 60-63, (1996).
- A.8. Ö. Legeza, G. Fáth and J. Sólyom: Phase diagram of magnetic ladders constructed from a composite-spin model. Phys. Rev. B **53**, (1966) (accepted for publication)
- A.9. F. Woynarovich and P. Forgács*: Scaling limit of the one-dimensional attractive Hubbard model: The half-filled band case. Nuclear Physics. (accepted for publication)
- A.10. 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. Physical Review Letters. (accepted for publication)

⁺ The *Annual Report* contains publications appeared or accepted by the publishers in the period 1 December 1995-30 November 1996

¹OTKA = Hungarian Scientific Research Fund

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

- A.11. W. Stephan* and K. Penc: Dynamical density-density correlations in onedimensional Mott insulators, cond-mat/9609231. Phys. Rev.B **54**, Dec15 (1996) (accepted for publication)
- A.12. T.P.Devereaux*, A.Virosztek, and A. Zawadowski: Multiband electronic Raman scattering in bilayer superconductors. Phys. Rev. B **54**, (1996) (accepted for publication)

Conference proceedings

- A.13. K. Penc, F. Mila* and H. Shiba*: Spectral function of One-Dimensional Strongly Correlated Electrons. In: *Proceedings of the Pacific Conference on Condensed Matter Theory*, Journal of the Korean Physical Society (Proc. Suppl.) **29**, S85-S91 (1996).
- A.14. O. Újsághy*, A. Zawadowski: Spin-orbit induced magnetic anisotropy for impurities in metallic samples: finite size dependence in the Kondo effect in mesoscopic samples. In: *Rencontres de Moriond*, January 20-27, 1996

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

Classical systems and phase transitions. — The Ising model (IM) and directed walk (DW) are among the most studied problems in lattice statistics. The IM is a standard model for magnetic or liquid-gas phase transitions whereas the DW is used to describe linear fluctuating objects such as directed polymers or interfaces in two-dimensional systems. We have observed a hitherto unnoticed connection between IM and DW in two-dimensional layered lattices. We have shown that the complete solution of the DW provides all the necessary information to obtain the thermodynamical properties and correlation functions of the IM. For self-similar (aperiodic, hierarchical) distribution of the couplings exact renormalisation-group study has given the result that the critical properties of IM and DW are governed by two different fixed points of the same RG transformation.

In non-equilibrium phase transitions of kinetic Ising models in one dimension a novel phase transition of the kink system was found earlier from an Ising-like absorbing state to an active state. At this transition point the critical properties of the underlying spin system have been investigated now by numerical simulations. Not only its dynamics was found to differ from that of the Glauber-Ising case but also its statics: some of the static exponents of the Ising model are influenced by the presence of the non-temperature driven phase transition, while Fisher's scaling law proved to remain valid.

An extension of expansion theorems for correlation functions at high temperatures and low fugacities in classical continuous systems interacting via an unstable interaction has been done. A toy model for crystallization has also been presented.

Classical and quantum chaos. — We have continued the investigation of transient chaos near the intermittent state of permanent chaos and have shown that the correlation functions exhibit unusual scaling properties.

We have studied properties of Bose-condensed gases in traps and determined, in the semi-classical region, the density-density correlation function measurable by inelastic light scattering.

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.

E-Mail:

Ferenc Iglói igloi@ power.szfki.kfki.hu András Sütő suto@ power.szfki.kfki.hu Nóra Menyhárd menyhard@ power.szfki.kfki.hu Péter Szépfalusy szepfalusy@ludens.elte.hu

⁺ Permanent position: Eötvös Loránd University, Budapest

Grants:

OTKA T12830 Critical behaviour of low-dimensional systems
OTKA T17493 Nonequilibrium phase transitions and chaotic phenomena
OTKA T14855 Phase transitions and spectral problem in quantum systems

Publications

Articles

- B.1. F. Iglói and L. Turban*: Common trends in the critical behaviour of Ising and directed walk models. Phys.Rev.Letters **77**,1206-1209 (1996)
- B.2. F. Iglói and P. Lajkó: On the critical temperature of non-periodic Ising models on hexagonal lattices, Z.Phys. **B99**, 281-283 (1996)
- B.3. F. Iglói and F. Szalma: Interface fluctuations on a hierarchical lattice. Phys. Rev. **E54**, 1106-1110 (1996)
- B.4. F. Iglói and P. Lajkó: Surface magnetisation and surface correlations in aperiodic Ising models. J. Phys. **A29**, 4803-4814 (1996)
- B.5. A. Sütő: Low density expansion for unstable interactions and a model of crystallization. J.Stat.Phys., **82**, 1541-1573(1996)
- B.6. L. Lustfeld* and P.Szépfalusy: Correlation functions on the border line of transient chaos. Phys.Rev. **E53**, 5882-5889 (1996).
- B.7. A. Csordás*, R.Graham* and P. Szépfalusy: Off-resonance light scattering from Bose condensates in traps. Phys.Rev. **A54**, R2543-2546 (1996)
- B.8. N. Menyhárd and G. Ódor*:Phase transitions and critical behavior in one-dimensional non-equilibrium kinetic Ising models with branching annihilating random walk. J.Phys.A. (accepted for publication)
- B.9. J.L. van Hemmen* and A. Sütő: AC-hampered tunnelling of the magnetisation. J. Phys.:Condensed Matter (accepted for publication)

C. ELECTRONIC STATES IN SOLIDS

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

We have developed a **full charge-density technique** to evaluate total energies from the output of self-consistent linear muffin-tin orbitals (LMTO) calculations in the atomic-sphere approximation (ASA). The Coulomb energy is calculated exactly from the complete, nonspherically symmetric charge density defined within nonoverlapping, space-filling Wigner-Seitz cells, the exchange-correlation energy is evaluated by means of the local density approximation or the generalized gradient approximation applied to the complete charge-density, and the ASA kinetic energy is corrected for the nonspherically symmetric charge-density by a gradient expansion. The technique retains most of the simplicity and the computational efficiency of the LMTO-ASA method, and calculations of atomic volumes and elastic constants of the 4d elements show that it has the accuracy of full-potential methods.

Using this technique we have carried out a calculation for the equilibrium atomic volumes of the α -phase light actinide metals using LDA and GGA exchange-correlation energy functional. The deviation between the experimental and GGA values is less than 1%. The comparison of the LDA and GGA results show 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 LDA is not able to describe properly the exchange-correlation effects, while the accuracy of the GGA is satisfactory for this system as well.

We studied the **magnetic properties of surfaces and interfaces** by performing fully-relativistic spin-polarized local spin density calculations. For Au covered Co monolayer on Au(111) - in very good agreement with experiments - we obtained the enhancement of perpendicular magnetic anisotropy as a function of the Au coverage. The relation between the orbital magnetic moment anisotropy and the band energy anisotropy was also studied and compared to the predictions of tight-binding model calculations.

An extensive study of the magnetic anisotropy energies (MAE) of the high-moment ferromagnetic phase of fcc Fe/Cu(001) over- and interlayers were carried out in terms of the fully relativistic spin-polarized Screened Korringa-Kohn-Rostoker method. Independently of the film thickness, for free surfaces the orientation of the magnetization was found to be in-plane, while for capped films a perpendicular magnetization is predicted up to a switching thickness of 5 Fe monolayers. Based on an analysis of layer-resolved anisotropy energies it was shown that the main contribution to the MAE arises from the Fe layer at the Fe/Cu interfaces. Particular features of the MAE's with respect to the number of cap layers as well as to the film thickness can be viewed in terms of the interfacial hybridization between Fe and Cu. By using the coherent-potential approximation the interdiffusion between the substrate and the magnetic film was found to reduce the MAE dramatically.

We have developed a theory of sound propagation in quasi one dimensional **charge**and **spin-density wave materials** based on an improved version of electron-phonon coupling, which enabled us to study the effect of the formation and sliding of the density wave condensate on the propagation of various sound modes. We have shown that only the transverse sound wave polarized parallel to the chains does couple to the moving condensate.

We extended our theoretical description of the electronic Raman scattering in **high temperature superconductors** to the case when several bands cross the Fermi level, which includes the bilayer cuprates. Although the Raman response in the A_{1g} channel is the sum of the single band contributions and a mixing term, we have shown that the latter is negligible for the materials in question.

One of the major outstanding problems of many-body theory is to find the simplest physically relevant lattice fermion model which shows **itinerant ferromagnetism** in an extended range of the parameters. We investigated two promising classes of models: single-orbital Hubbard models on non-Bravais lattices with triangular plaquettes, and generalized Anderson lattices. In either case, the stability of eventual ferromagnetic order is decided by the competition with strongly correlated non-magnetic states, such as the collective Kondo state. Following a recent suggestion by Müller—Hartmann, we studied the extent of the ferromagnetic phase of the triangular double chain, using exact diagonalization, and single-spin-flip variational trial states. We found that the saturated ferromagnetic state is robust, extending from the intermediate to the strong coupling regime, and over a wide range of band filling. In addition, we proved that Müller-Hartmann's `low-density scenario' does not work in three dimensions. Two dimensions is a marginal case, and we proposed certain criteria for ordering.

Previous research on band ferromagnetism, and on Kondo lattices, is now converging in the study of **correlated two-band models**, where a set of interacting electrons has to Kondo-compensate the localized spins of a different set of electrons. One of the simplest of such models is the Anderson-Hubbard lattice model. We generalized the Gutzwiller variational method to be able to treat this model, and derived the interaction dependence of the lattice Kondo energy . It is argued that the finding of a new Kondo scale should be useful in understanding the remarkable stability of ferromagnetism in Anderson-type lattice models .

In the **bilayer model of the high T** $_{c}$ **superconductors** we investigated the properties of the non-resonant Josephson coupling case. Assuming that the intralayer and the interlayer interactions are different, the effective interaction is stongly enhanced by the high energy parts of the spectrum, and the predictions of the bilayer model for s type superconductivity contradicts to the results of the Raman measurements.

E-Mail:

Patrik Fazekas pf@ power.szfki.kfki.hu
János Kollár jk@ power.szfki.kfki.hu
István Tüttő tutto@ power.szfki.kfki.hu
Balázs Újfalussy bu@ power.szfki.kfki.hu
Attila Virosztek viro@ power.szfki.kfki.hu
Levente Vitos lv@ power.szfki.kfki.hu

Grants

OTKA T016740 Electronic states in complex structures (solids, surfaces and interfaces)

OTKA T014201 Theory of phase diagrams of heavy fermion systems

OTKA T020030 Interacting electrons in low dimensions OTKA T019045 Collective excitations in unconventional superconductors

Publications

Articles

- C.1. B.Újfalussy, L. Szunyogh* and P. Weinberger*: Fully relativistic spin-polarized description of interface exchange coupling for Fe multilayers in Au(001). J. Magn. Magn. Mater. **156**, 255-256 (1996)
- C.2. L. Szunyogh*, B. Újfalussy, P. Weinberger*, and C. Sommers*: Fully relativistic spin-polarized description of magnetic interface coupling: Fe multilayers in Au(100). Phys. Rev. **B54**, 6430 (1996)
- C.3. B. Újfalussy, L. Szunyogh*, P. Bruno*, and P. Weinberger*: First-principles calculation of the anomalous perpendicular anisotropy in Co monolayer on Au(111). Phys. Rev. Lett., **77**, 1805 (1996)
- C.4. P. Weinberger*, P.M. Levy*, J. Banhart*, L. Szunyogh*, and B. Újfalussy: Band structure and electrical conductivity of disordered layered systems. J. Phys.: Condens. Matter **8**, 7677 (1996)
- C.5. B. Újfalussy, L. Szunyogh*, and P. Weinberger*: Magnetic anisotropy in Fe/Cu(001) over- and interlayers: the high-moment ferromagnetic phase. Phys. Rev. **B54**, 54 (1996)
- C.6. A. Virosztek and K. Maki*: Sound Propagation in Density Wave Conductors and the Effect of Long-range Coulomb Interaction. Phys. Rev. **B53**, 3741-3745 (1996)
- C.7. T.P. Devereaux*, A. Virosztek and A. Zawadowski: Multiband Electronic Raman Scattering in Bilayer Superconductors. Phys. Rev. **B54**, 12523-12534 (1996)
- C.8. K. Itai* and P. Fazekas: Interaction effect in the Kondo energy of the periodic Anderson-Hubbard model. Phys. Rev. **B54**, R752 (1996).
- C.9. P. Pieri*, S. Daul*, D. Baeriswyl*, M. Dzierzawa*, and P. Fazekas: Low density ferromagnetism in the Hubbard model, Phys. Rev. **B54**, 9250 (1996).
- C.10. L.Vitos, J.Kollár and H.L.Skriver*: Ab initio full charge density study of the atomic volume of a-phase Fr, Ra, Ac, Th, Pa, U, Np, and Pu. Phys. Rev. B (accepted for publication)
- C.11. J.Kollár, L.Vitos and H.L.Skriver*: The anomalous atomic volume of α-Pu. Phys.Rev. B (accepted for publication)
- C.12. L. Szunyogh*, B. Újfalussy, P. Bruno*, and P. Weinberger*: Anomalous perpendicular magnetic anisotropy in a Co monolayer on Au(111). J. Magn. Magn. Mater. (1996) (accepted for publication)

- C.13. P. Fazekas and K. Itai*: Collective Kondo effect in the Anderson-Hubbard lattice. Physica B (accepted for publication)
- C.14. S. Daul*, P. Pier*i, M. Dzierzawa*, D. Baeriswyl*, and P. Fazekas: Low density ferromagnetism in a one-dimensional Hubbard. Physica B (accepted for publication)
- C.15. P. Fazekas: Band ferromagnetism versus collective Kondo state in lattice fermion models. Phil. Mag. B (Proceedings volume of the Debrecen Graduate School on Strong Correlation, September 1996) (accepted for publication)

Conference proceedings

- C.16. L.Vitos, J.Kollár and H.L.Skriver*: Energetics of the light actinides in a full charge density scheme. In: *Stability of Materials*, *Nato ASI Series*, Eds. A.Gonis, P.E.A. Turchi and J.Kudrnovsky, Plenum Press, pp. 393-399, 1995
- C.17. J.Kollár, L.Vitos 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, (1996)
- C.18. B. Újfalussy, L. Szunyogh*, and P. Weinberger*: Alloying aspects of the magnetic ground state and anisotropy of Fe/Cu thin film overlayers. In: *Proc. of 1st International Alloy Conference (IAC-1)*, Athens, Greece, June 16--21, 1996 (accepted for publication)

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

Neutron scattering. — The short range order of amorphous Ni₈₃La₁₇ was examined by neutron and X-ray diffraction. The specimen was produced by ion-plasma sputtering. In this procedure the loss of material is very high, thus the preparation of Ni isotopic specimens was not reliable. Computer modelling — based on molecular dynamic technique and the Born-Green-Bogoljubov equation — was used to obtain the structural information from the two experimental total structure factors. All three partial pair correlation functions, atomic first neighbour distances, coordination numbers and angle distributions were derived.

Neutron diffraction study was performed on nanocrystalline Fe-Si and SiC systems. For the as-prepared Fe₈₂Si₁₈ sample ordered DO₃, whereas after 194 hours ball-milling metastable A2 structure was determined. A significant increase of the lattice parameter and the broadening of Bragg-reflections were measured due to the decreased grain size.

Dynamic neutron radiography was used to visualize the characteristic features of evaporation, condensation, fluid flow and clogging points in absorption-type refrigerators. Compression-type refrigerators filled up with environment friendly cooling agent were investigated. It was established that a layer of synthetic lubrication oil segregates on the surface of cooling material in the evaporator, and this hinders the cooling efficiency of the units. On the basis of results new constructions were developed by the manufacturers.

Nanocrystalline materials for soft magnetic applications. — A new class of the non-equilibrium materials with considerable practical importance is the nanocrystalline alloys. Besides the basic interest to study a new state of matter with a much enhanced surface to volume ratio, nanocrystalline materials with a typical 10 nm grain size show very good soft magnetic properties as the magnetocrystalline anisotropy is significantly reduced. In our group OTKA and Copernicus projects are aimed to study nanocrystalline materials produced by different routes as ball milling and crystallization of amorphous alloys. Since one of the commonly used class is the B and Cu alloyed Fe-Zr system, the crystallization of amorphous Fe_{100-x}Zr_x (7<x<12) alloys were studied by differential scanning calorimetry (DSC), Mössbauer spectroscopy and Curie point measurements. The partially crystallized samples contain besides bcc-Fe also an amorphous phase with Zr content near 17-20 at%. In the fully crystallized samples bcc-Fe and Fe₃Zr were found, the Fe₂Zr intermetallic phase of the ingots were not present.

The special influence of B and Cu additives to the crystallization of the FeZrCuB alloys was investigated by differential scanning calorimetry (DSC). The magnetic properties of toroidal cores made of melt spun Fe₉₀Zr₇B₂Cu₁ and Fe₈₆Zr₇B₆Cu₁ metallic glass ribbons were studied after being heat treated in the 550-750 ^OC temperature range. The pieces removed from these cores were investigated by high precision X-ray diffraction for lattice parameter studies, calorimetry and transmission electron microscopy. Mössbauer spectroscopic measurements of these samples were also extended to low temperature external magnetic field studies which made possible the separation of the contributions from different phases and reveal the magnetic

coupling between them. Initial magnetic permeability changes sharply during the nanocrystal formation. Mössbauer spectroscopy does not reveal any drastic change of the phase composition in the temperature range where a significant variation of the soft magnetic properties is observed. Modification of the exchange coupling between the grains formed at different temperatures might significantly contribute to the improvement of the magnetic properties.

To optimise the composition, the influence of different additions were also investigated. The role of nucleating additives (M=Cu, Ag, Au, Pd, Pt, Sb and Ga) in the formation of nanocrystalline structure and in the improvement of soft magnetic properties is investigated in $Fe_{86}Zr_7B_6M_1$ type alloys by calorimetric (DSC), thermomagnetic (initial permeability) and Mössbauer spectroscopic studies. It is found that the nucleating additives lower the temperature of the first crystallization step and improve the soft magnetic properties due to the refined nanostructure of the crystallization products. Other parts of this Copernicus program, namely the high heating rate studies, the electronic system development for the sensor application and the power loss measuring instrumentation is described in Section J.

Solid state reactions. — Evaporated multilayers and ball milled materials were studied. Detailed investigations were made on Fe-B samples and diffusion amorphization was observed in this system for nanostructured multilayers. Single phase amorphous alloy is formed in a limited concentration range around 40 at% boron in agreement with the predictions of free-energy diagrams. The properties of the interface region of the multilayers was studied by Mössbauer spectroscopy, X-ray diffraction and transmission electron microscopy. The interface region is amorphous and consumes 2 nm from the iron layer. The same hyperfine field distribution is observed within the amorphous interface when the individual layer thicknesses exceed the width of the interface. The width of this distribution is much larger than those measured in amorphous Fe-B alloys and the excess width is attributed to concentration distribution along the interface. On the contrary, the amorphous component in samples with smaller layer thicknesses is more homogenous as deduced from the hyperfine field distributions and the hyperfine parameters depend on the ratio of the iron and boron layer thicknesses. Solid state amorphization during the sample deposition is assumed to account for this behavior.

Mechanical alloying could produce homogenous amorphous alloy in a narrower composition range than diffusion amorphization while the attrition of the intermetallic compounds, FeB and Fe₂B, did not produce amorphous material of the same composition. The amorphous alloy formed under mechanical alloying was shown to change gradually in composition and homogenity during the milling process. The role of controlled atmosphere and contamination from the milling tools was studied in the formation of the observed phases and concentrations.

External magnetic field Mössbauer studies. — Measurements were carried out in the 4.2-300 K temperature range up till 7 T external magnetic field. The Mössbauer spectroscopic measurements were supported by magnetic measurements, part of which was carried out in cooperation with the ATOMKI in Debrecen and also by X-ray diffraction which was partly made at the Solid State Research Department of the Roland Eötvös University, Budapest.. Besides the prevously mentioned nanocrystalline studies the following other problems were investigated:

i. It was verified for ball milled nanocrystalline Fe (samples produced by the Solid State Physics Department of the KLTE, Debrecen) that changes of the shape

- distribution of the particles in the milling process significantly influences the local magnetic properties studied by external magnetic field Mössbauer spectroscopy.
- ii. Amorphous Fe_2Zr alloy was produced by ball milling the corresponding intermetallic compound. The magnetic properties of the amorphous alloy which is paramagnetic even at 4.2 K is basically different fom those of the intermetallic compound with 630 °C ferromagnetic Curie temperature. The study of the magnetic properties of the Fe atoms in different local environments is a part of the Korean Hungarian cooperation which is aimed to investigate the amorphous and nanocrystalline Fe-Zr-N system.
- iii. The magnetic behaviour of the melt spun amorphous Fe-Y alloys with 15-60 at% Y were studied. The spin-glass and re-entrant properties are the consequence of the percolation of the non magnetic atoms. Besides the non magnetic Y, they also include the Fe environments above the critical nearest neighbour Y number. We have studied the concentration, temperature and magnetic field dependence together with the appearance of the relaxation behaviour.
- iv. The unusual temperature dependence of the susceptibility of the FeSi compound motivated the study of its Mössbauer spectrum up to 7T external magnetic field. The investigation is a joint work with the Kamerlingh Onnes Laboratorium, Leiden and is aimed to investigate the strong electron correlations characteristic to narrow band gap nonmagnetic semiconductors.

E-Mail:

Sára Judit Balogh
Dénes Kaptás
Tamás Kemény
László Kiss
György Mészáros
Bernadette Sas
Erzsébet Sváb
Imre Vincze
baloghj@power.szfki.kfki.hu
kaptas@ power.szfki.kfki.hu
kemeny@ power.szfki.kfki.hu
kissl@ power.szfki.kfki.hu
sas@ power.szfki.kfki.hu
svab@ power.szfki.kfki.hu

Grants

Copernicus COP 753 Manufacture, structure and properties of amorphous and nanocrystalline materials

OTKA T 017456 The spin glass behaviour and its relation to the magnetic properties of nanostructures

OTKA T 020624 Photon- and electron-spectroscopic study of the interfaces of layer structures

OTKA T 020962 Formation and magnetic properties of granular structures

OTKA I/7 T 017129 Metastable systems investigated by neutron scattering

AKP96-137/6² Mössbauer spectroscopy of nanostructures and strongly correlated electron systems

²Hungarian Academy of Sciences Research Project

_

Publications

Articles

- D.1. E. Sváb, F. Hajdu, Gy. Mészáros: Semi-empirical fitting of partial pair correlation functions of amorphous alloys. Z. Naturforsch. 50a, 1205-1210 (1995)
- D.2. E. Sváb, Gy. Mészáros, F. Deák: Neutron powder diffractometer at the Budapest research reactor. Materials Science Forum, **228-231**, 247-252 (1996)
- D.3. M.Balaskó*, E. Sváb: Dynamic neutron radiography instrumentation and applications in Central Europe. Nuclear Instruments and Methods in Physics Research **A377**, 140-143 (1996)
- D.4. L.F. Kiss, G. Huhn*, T. Kemény, J. Balogh and D. Kaptás: Magnetic properties of Fe-Zr metastable phases. Journal of Magnetism and Magnetic Materials **160**, 229-232 (1996)
- D.5 A. Böhönyei, L.F. Kiss, A. Lovas: Reversible relaxation spectra of (Fe-)Ni-P metallic glasses. J. Non-Cryst. Sol. 192&193, 424-427 (1995)
- D.6. M. Balaskó*, E.Sváb, I.Vida*, I.Szikra*: Neutron radiography visualization of internal processes in refrigerators. Physica B (accepted for publication)
- D.7. M.I. Mendelev*, S.N. Ishmaev*, F. Hajdu, Gy. Mészáros, E. Sváb: Short range order in Ni₈₃La₁₇ metallic glass. Physica B (accepted for publication)
- D.8. I. Bakonyi, V. Skumryev*, R. Reisser*, G. Hilscher*, L.K. Varga, L.F. Kiss, H. Kronmüller* and R. Kirchheim*, Preparation, structure and physical properties of Fe-, Co- and Ni-rich melt-quenched ribbons containing Zr or Hf. Z. für Metallkunde (accepted for publication)

Conference proceedings

- D.9. S.N.Ishmaev*, E. Sváb, O.B. Tarasova*, L.S. Smirnov*: Short range order in amorphous alloys of the Ti-Zr system. In: *Proc. 8th World Conference on Titanium: Science and Technology*, Birmingham, Ed. P. Danckwerts, Institute of Materials, London, 1996, **Vol.3**, pp.2228-2235
- D.10. M.Balaskó*, E. Sváb: Industrial applications of dynamic radiography in Hungary. In: *Proc. International Conference Inservice Inspection*, Pula, Croatia, Ed. V. Krstelj, Croatian Soc. for NDT, 1996, pp. 9-17
- D.11. M.Balaskó*, E. Sváb, G. Endrõczi*: Combined dynamic neutron radiography and vibration diagnostics for industrial applications. In: *Proc. 5th World Conference on Neutron Radiography*, Berlin, 1996 (accepted for publication)
- D.12 L.F.Kiss, D.Kaptás and N.Hegman*: Absence of field cooling effect on the hysteresis loop in amorphous Fe₉₃Zr₇, NATO Advanced Studies Series, Ed. G.C.Hadjipanayis, Magnetic Hysteresis in Novel Magnetic Materials (accepted for publication)

- D.13 T.Kemény, L.K.Varga, L.F.Kiss, J.Balogh, A.Lovas, L.Tóth* and I.Vincze, The nanocrystal formation in Fe-Zr-B-Cu amorphous alloys. In: 9th International Conference of Rapidly Quenched and Metastable Materials, Bratislava, 1996 (accepted for publication)
- D.14 L.K.Varga, A.Lovas, L.Pogány, L.F.Kiss, J.Balogh and T.Kemény, The role of nucleating element additives in the crystallization and soft magnetic properties of Fe-Zr-B based amorphous alloys. Ibid. (accepted for publication)
- D.15 R.J.Cooper*, J.Balogh, N.Cowlam* and T.Kemény, A study of amorphisation in Fe-B multilayers by neutron reflectometry. Ibid. (accepted for publication)
- D.16 A.Böhönyey*, G.Huhn*, L.F.Kiss and L.Pogány, Composition dependence of reversible structural relaxation in Fe-Ni-P metallic glasses. Ibid. (accepted for publication)
- D.17 W.Hofstetter*, H.Sassik*, R.Grössinger*, R.Trausmuth*, G.Vértesy* and L.F.Kiss, Determination of the onset of crystallisation of amorphous materials using different methods. Ibid. (accepted for publication)

Others

D.18 M.Balaskó*, E. Sváb, J. Rant*: Hydrogen partial pressure in aggresive cooling agents studied by neutron radiography: In: *Proc. of 5th World Conference on Neutron Radiography*, Berlin, 1996, p.34 (abstract)

See also: J15, J16, J11, L15

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 two years the A_1C_{60} type compounds became the center of interest.

 A_1C_{60} compounds. In the A_1C_{60} system (A=K,Rb,Cs) several different phases were found as a function of temperature. These phases show unexpected structural and transport properties. They have a rock salt structure at high temperature (400 K) and they are conductors. Slowly cooling them to room temperature they transform to an orthorhombic phase which is a crystalline polymer. When these compounds, instead of slow cooling, quenched to low temperatures, a monoclinic phase develops. In this metastable phase the C₆₀ molecules are connected in pairs: a dimer state is formed. Using extensive Rietveld mapping in the C₆₀ angular orientation space we determined the precise orientation and bonding configuration of the C₆₀ molecules. In contrast to expectations found in the literature the bonding between C₆₀ molecules are through a single bond unlike the four membered ring configuration of the polymer. Beside the structure of the several phases appearing in the A₁C₆₀ system we determined the stability regions of the different phases. We found that at low temperatures where the polymer is the stable form, the phase separated intermediat state of K₁C₆₀ has significantly higher Gibbs free energy. We also investigated the kinetics of the phase transitions. Differential scanning calorimetry measurements revealed that the polymerization takes place with 2D growth process coupled to phase separation which in turn is a slow 3D diffusion controlled process.

X-ray resonant scattering — Scattering of hard x-ray or gamma-ray photons on atomic nuclei have a significant cross section when the energy of the photon is the same as the difference between two energy levels of the nucleus. This resonant scattering is closely related to the Mössbauer effect. Resonant scattering experiments in the time window can be done by using pulsed synchrotron radiation.

X-ray resonant forward scattering of synchrotron radiation on ¹⁵¹Eu. Synchrotrons — unlike Mössbauer sources — emit x-rays in a wide energy range. A successful resonant scattering experiment requires the very good monochromatization (in the meV range) of the synchrotron radiation. In collaboration with the European Synchrotron Radiation Facility (Grenoble) and the Institute of Experimental Physics of the University of Hamburg, we have designed and built a silicon single crystal x-ray monochromator working at the 21.5 keV energy of the Mössbauer transition of the ¹⁵¹Eu nucleus. We were the first to detect delayed x-ray photons scattered by a sample containing europium. We have also recorded the oscillatory time dependence ("quantum beats") of the scattered intensity.

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. We have recorded the hologram of a SrTiO₃ single crystal and successfully reconstructed the three dimensional order of Sr atoms.

Nucleation theory. — The applicability of our phenomenological diffuse interface theory (DIT) for vapor condensation has been investigated in the case of non-polar, polar and metal substances. It was demonstrated that for non-polar, weakly polar and metal vapors the DIT predictions are in a remarkably better agreement with the experiments than the classical theory. The fundamentals of the DIT were studied in the framework of the van der Waals/Cahn-Hilliard (vdW/CH) and the state-of-the-art density functional theory (DFT) of Oxtoby. The vdW/ CH analysis suggests that the assumptions of the DIT all reasonable. The DFT calculations contradict this. The origin of the discrepancy is the inaccurate density profile predicted by the DFT which stems from the simplified molecular interaction (Yukawa) assumed. Cluster dynamics calculation were performed to describe the time-dependence of crystal nucleation in the framework of the DIT. It has been shown that for vapor condensation and crystal nucleation the predictions of the DIT are in a comparable or better agreement with the experiments than those of the modern density functional theories.

E-Mail:

Gábor Bortel gb@power.szfki.kfki.hu
Gyula Faigel gf@ power.szfki.kfki.hu
László Gránásy grana@ power.szfki.kfki.hu
Katalin Kamarás kamaras@ power.szfki.kfki.hu
Gábor Oszlányi go@ power.szfki.kfki.hu
Sándor Pekker power.szfki.kfki.hu
Miklós Tegze mt@ power.szfki.kfki.hu
Tamás Pusztai pusztai@power.szfki.kfki.hu

Grants

OTKA T016057 Preparation and structural, optical and thermal studies of fullerenes and related materials

OTKA T017485 Theoretical investigation of nucleation processes

OTKA T019139 The study of polymer fullerides and other crystalline C_{60} compounds

AKP 96 225 /12 Atomic resolution holography using nuclear gamma decay

EC Copernicus CIPA-CT93-0032 Technology and optical properties of high temperature superconductors

U.S.-Hungarian Joint Fund 225 Single crystal C₆₀ spectroscopy

U.S.-Hungarian Joint Fund 271 Optical properties of high-T_c crystals

U.S.-Hungarian Joint Fund 431 Structural study of C₆₀ compounds

Publications

Articles

- E1. L. Gránásy, T. Kemény, G. Oszlányi, G. Bortel, G. Faigel, M. Tegze, S. Pekker, L. Forró* and A. Jánossy*: Enthalpies of phase transformation in the alkali fulleride RbC₆₀. Solid State Commun. **97**, 573-578 (1996).
- E2. M. Tegze and Gy. Faigel: X-ray holography with atomic resolution. Nature, **380**, 49-51 (1996).
- E3. G. Bortel, G. Oszlányi, G. Faigel, M. Tegze, T. Pusztai and S. Pekker: Comparison of powder and single crystal data of $C_{60}(C_{14}H_{10}O_2)$ an oxygen containing anthracene derivative of C_{60} . Mater. Sci. Forum, **228-231**, 879 (1996).
- E4. T. Pusztai, G. Bortel, G. Faigel, G.Oszlányi, M. Tegze, P.W. Stephens* and L. Forró*: Structure refinements of alkali fullerides. Mater. Sci. Forum, **228-231**, 683 (1996).
- E5. G. Oszlányi, G. Bortel, G. Faigel, L. Gránásy, G.M. Bendele*, P.W. Stephens*, L.Forró*: Single C-C bond in (C₆₀)₂-². Phys. Rev. **B54**, 11849 (1996)
- E6. L. Gránásy: Diffuse interface model of volume nucleation in glasses. Thermochim. Acta **280-281**, 83-100 (1996)
- E7. L. Gránásy: Diffuse interface approach to crystal nucleation. Key Engineering Materials **215-216**, 451-458 (1996)
- E8. L. Gránásy, S. Pekker, L. Forró*: Thermodynamics of polymorphism in AC₆₀ (A=K, Rb, Cs) alkali fullerides. Phys. Rev. **B53**, 5059-5062 (1996)
- E9. L. Gránásy: Diffuse interface theory for homogeneous vapor condensation. J. Chem. Phys. **104**, 5188-5198 (1996)
- E10. L. Gránásy: Fundamentals of the diffuse interface theory. J. Phys. Chem. **100** 10768-10770 (1996).
- E11. L. Gránásy, S. Pekker, O. Chauvet*, L. Forró*: Phase selection and transformation kinetics in KC₆₀. Phys. Rev. **B54**, 11865-11868 (1996).
- E12. L. Gránásy, T. Pusztai, E. Hartmann*: Diffuse interface model of nucleation. J. Cryst. Growth **167**, 756-765 (1996)
- E13. L. Biró*, S. Pekker, E. Balázs*: KC₆₀ investigated by Scanning Tunneling Microscopy. Synthetic Metals, **77**, 123-126 (1996)
- E14. M. Carrard*, L. Forró*, L. Mihály*, S. Pekker: Morphology of (KC₆₀)n Polymeric Fibers. Synthetic Metals, **80**, 29-34 (1996)

- E15. D. Koller*, M.C. Martin*, L. Mihály*, G. Mihály*, G. Oszlányi, G. Baumgartner*, L. Forró*: Energy gap in superconducting fullerides: optical and tunneling studies. Phys. Rev. Lett. **77** Issue 19, (1996).
- E16. L. Gránásy, S. Pekker, L. Forró*: Thermodynamics of A₁C₆₀ (A=K, Rb, Cs) alkali fullerides. Fullerene Sci. Techn (accepted for publication)
- E17. G. Bortel, S. Pekker, L. Gránásy, G. Faigel G. Oszlányi: Molecular and crystal structure of the AC₆₀ (A=K, Rb) dimer phase, J. Phys. Chem. Solids (accepted for publication)
- E18. O. Leupold*, J. Pollmann.* E. Gerdau*, H.D. Rüter*, G. Faigel, M. Tegze, G. Bortel, R. Rüffer*, A.I. Chumakov*, A.Q.R. Baron*: Nuclear Resonance Scattering of Synchrotron Radiation at the 21.5 keV Resonance of ¹⁵¹Eu. Europhys. Lett. (accepted for publication)
- E19. L. Gránásy: Diffuse interface model of crystal nucleation. J. Non-Cryst. Solids (accepted for publication)
- E20. L. Gránásy, T. Pusztai:Comment on "Crystallization kinetics" and "Nucleation and growth transformation kinetics". Phys. Rev. B (accepted for publication)
- E21. K. Kamarás, D.B. Tanner*, L. Forró*: Experimental investigation of symmetry reduction and electron molecular vibration coupling in various RbC₆₀ phases. Fullerene Sci. and Techn. (accepted for publication)

Conference proceedings

- E22. G. Oszlányi, G. Bortel, G. Faigel, L. Gránásy, P.W. Stephens*, G. M. Bendele*, L. Forró*: Single C-C bond in KC₆₀ and RbC₆₀. In: *Fullerenes and Fullerene Nanostructures*, Eds. H. Kuzmany, J. Fink, M. Mehring, S. Roth, World Scientific Singapore, 1996, pp.354-358.
- E23. L. Gránásy, M. Tegze, S. Pekker, L. Forró*: Thermodynamics of phase transformations in the A_1C_{60} (A=K, Rb, Cs) alkali fullerides. Ibid. pp. 97-101.
- E24. S. Pekker M. Carrard*, L. Forró*, L. Mihály*,: Formation and Morphology of (KC₆₀)_n Polymer Fibers. Ibid. pp.110-114.
- E25. A. Jánossy*, S. Pekker, G. Oszlányi, L. Korecz*, L. Forró*: Conducting fulleride polymers. In: *Springer Proc. in Physics*, Eds. K. Kjimura, S. Kuroda. Vol. 81, pp.163-171 (1996).
- E26. L. Gránásy, S. Pekker, L. Forró*: Thermodynamic aspects of phase transformations in the A₁C₆₀ (A=K, Rb, Cs) alkali fullerides. In: *Proc. of Advances in the Chemistry and Physics of Fullerenes and Related Materials*, Vol. 3, eds. K.M. Kadish and R.S. Ruoff (The Electrochemical Society, Pennington, 1996) pp. 1080-1092.
- E27. S. Pekker, L. Gránásy, G. Oszlányi, G. Bortel, G. Faigel, M. Tegze, O. Chauvet*, L. Forró*, P.W. Stephens*, A. Jánossy: Polymorphism of fulleride ions in A₁C₆₀ (A=K, Rb, Cs) salts. Ibid. Vol.2 pp.245-258.

Others

- E28. M. Tegze and G. Faigel: X-ray holography with atomic resolution. IUCR Congress 1996, Seattle USA. (abstract)
- E29. G. Faigel, G. Bortel, L. Gránásy, G. Oszlányi, S. Pekker, T. Pusztai $\,M$.Tegze Stable and metastable phases in the A_1C_{60} system (A=K, Rb, Cs). Ibid. (abstract)
- E30. G. Faigel and M. Tegze, Atomic resolution x-ray holography. EPS 10 Trends in Physics 1996, Sevilla, Spain. (abstract)

F. CHARGE- AND SPIN-DENSITY WAVES

G. Kriza and G. Mihály⁺

Fluctuations in low-dimensional systems. — Thermal fluctuations in low-dimensional systems have more profound consequences than in three dimensions: They may dominate the properties of the system over a large part of the phase diagram. We have investigated the consequences of fluctuations of the order parameter of collective electronic states — spin-density wave and superconductor —in low-dimensional organic conductors by a large variety of transport and magnetic measurements.

Spin-density wave fluctuations. The itinerant antiferromagnetic state called spindensity wave (SDW) is one of the typical ground states of quasi-one-dimensional metals. The NMR spin-lattice relaxation in these systems have been shown to be dominated by the fluctuations of the phase of the SDW order parameter. By a systematic comparison of the NMR relaxation and dielectric relaxation as a function of temperature, magnetic field, defect concentration, we have shown that the anomalously high dilectric constant in these materials has the same origin as the NMR relaxation, i.e., it arises from the phase excitation of the SDW. We have also pointed out that a peak in the temperature dependence of the NMR relaxation — previously thought to signal a phase transition — originates from a dynamic crossover in the SDW phase fluctuations.

Two-dimensional superconduting fluctuations. — It is known that the highly anisotropic, quasi-two-dimensional Cu-O-based superconductors show no sharp phase transition in a magnetic field. Instead, there is a crossover from the high-temperature Gaussian fluctuations of the superconducting order parameter to the low-temperature "vortex liquid" state characterized by the fluctuating Abrikosov vortices. We have investigated the same phenomenon in the two-dimensional organic superconductor $(ET)_2Cu[N(CN)_2]Br$ by measuring the dynamic and static magnetization over a broad range of temperature and magnetic field. Because of the lower critical temperature and thus lower critical magnetic field of this system, a significantly larger part of the phase diagram is accessible experimentally than in Cu-O-based superconductors. We have shown the existence of the vortex liquid state down to 3% of the critical temperature. We have found that the so-called irreversibility line that delimits the vortex liquid state follows an exponential temperature dependence over the entire temperature range investigated.

E-Mail:

György Kriza kriza@power.szfki.kfki.hu

Grants

OTKA T7277 Dielectric properties of coherent density waves

NSF-Hungarian Acad. Sci. Travel Grant: Effect of Disorder on the Spin-Density Wave Excitations

Bilateral Cooperation Fund provided by the NWO of the Netherlands: Electronic Correlations in Alkali Metal Fullerides

⁺ Permanent position: Technical University Budapest

Publications

Articles

- F.1. R. Gaál,* G. Fülöp,* G. Szeghy,* G. Kriza, and G. Mihály: Phase diagram of the quasi-two-dimensional organic superconductor (ET)₂Cu[N(CN)₂]Br. Physica B (accepted for publication).
- F.2. S. E. Brown,* W. G. Clark,* and G. Kriza: Relation between the dielectric constant and nuclear spin-lattice relaxation by phase fluctuation of a ponned spin-density wave. Phys. Rev. B (accepted for publication).

Conference proceeding

- F.3. L. Balicas,* G. Kriza, and F.I.B. Williams,* Positive and Negative Quantum Hall Plateaus in (TMTSF)₂PF₆. In: *Proceeding of the International Conference on Physical Phenomena in High Magnetic Field*, Tallahassee, Florida, 1995 (World Scientific, Singapore, 1996), p.256.
- F.4. G. Mihály: Photoinduced properties of CDW materials. In: *Physics and Chemistry of Low Dimensional Organic Conductors*, NATO ASI Series B Vol. 354, p.443 (Plenum, New York, 1996).

G. LIQUID CRYSTAL RESEARCH

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

Study of ferroelectric liquid crystals. — We started to study new types of ferroelectric liquid crystals: chiral disc and bowl shaped columnar liquid crystals and special smectic A materials formed by achiral banana shaped molecules. The piezoelectric properties of chiral tilted columnar phases were measured. It was observed that the piezoelectric responses of such materials is much weaker than that of chiral smectic liquid crystals with the same symmetry. Based on the measurements we propose a model for the switching dynamics. We found evidences that columnar liquid crystals of bowl shaped molecules are ferroelectric and measured the polarisation of such phases. We observed the electro-optical effects associated with the switching of the polarisation of a ferroelectric smectic phase composed by achiral banana shaped molecules.

Phase diagrams and electro-optical properties of novel ferroelectric mixtures were studied. Binary and ternary mixtures were prepared, based on three members of the homologous series of 4-n-alkoxyphenyl esters of the 4'-n-alkoxybenzoic acids and on homologues series of 4-n-alkoxyphenyl 4'-n-alkoxy benzoates. Three structurally different chiral compounds and chiral additive of (S)-(1-methylheptyl)-1,1'-4'-1" - terphenyl-1,4"-dicarboxylate were used to make novel ternary and four component mixtures with chiral smectic C phase. The phase diagrams of two -, three -, and four -component mixtures are presented and the corresponding physical properties are discussed. Spontaneous polarisation values up to 200 nC/cm² were found and two distinct modes of electro-optical switching, associated with different stages of helix distortion were observed.

Liquid crystal composite systems consisting of cholesteric liquid crystals in which small amount of reactive monomer was dispersed and polymerized by UV light was studied. The process yielded a dramatic change of the phase sequence. By thin film chromatography and IR measurements we showed that the process resulted in a new material which is responsible for the dramatic change.

We made small angle neutron scattering studies to study the structure of silica particles dispersed in smectic liquid crystals.

E-Mail:

Nándor Éber eber@power.szfki.kfki.hu Katalin Fodor-Csorba fodor@ power.szfki.kfki.hu Antal Jákli jakli@ power.szfki.kfki.hu Anikó Vajda: vajda@power.szfki.kfki.hu

Grants

OTKA T-016152 Liquid crystal research

OTKA T 7409 Physical investigation of liquid crystal - polymer composites OMFB GB 75/96 Synthesis and characterisation of novel ferroelectric liquid

crystals for display applications

Publications

Articles:

- G.1. A. Jákli, S. Markscheffel* and A. Saupe*: Helix deformation and bistable switching of ferroelectric liquid crystals. Journal of Applied Physics **79**, 1891 (1996)
- G.2. E. Dietzmann*, W. Weissflog*, S. Markscheffel*, A. Jákli, D. Lose*, S. Diele*: Perfluorinated swallow tailed compound: In search for achiral ferroelectric phases. *Ferroelectrics*, **180**, 341 (1996)
- G.3. A. Jákli and A. Saupe*: Field induced thickness variations of ferroelectric liquid crystal films. Phys. Rev. **E53**, R5580, (1996)
- G.4. S.Markscheffel*, A. Jákli and A. Saupe*: Dielectric properties of ferroelectric liquid crystals. Ferroelectrics **180**, 59 (1996)
- G.5. Bata L., Éber N , Jákli A: Ferroelektromos folyadékkristályok (Ferroelectric Liquid Crystals, in Hungarian). Fizikai Szemle **XLVI**, 59-63 (1996)
- G.6. N. Éber, L. Bata: Folyadékkristályok az optoelektronikában (Liquid crystals in the optoelectronics, in Hungarian). Ibid. **XLVI**, 117-126 (1996)
- G.7. Fodorné Csorba K, Bata L., Vajda A.: Folyadékkristályok szerkezete és tulajdonságai (Structure and properties of liquid crystals, in Hungarian). Magyar Kémiai Folyóirat, **102**, 125-142 (1996)
- G.8. A. Jákli: Electrically induced vibrations and flows in ferroelectric liquid crystals. Mol. Cryst. Liq. Cryst. (accepted for publication)
- G.9. A. Jákli, Gy. Káli, L. Rosta: Structure of silica aggregates in liquid crystal matrix. Physica B (accepted for publication)
- G.10. Jákli A, Bata L: Folyadékkristály polimerek és folyadékkristály polimer kompozit rendszerek (Liquid crystal polymers and liquid crystal polymer composites, in Hungarian). Fizikai Szemle (accepted for publication)
- G.11. Bata L, Éber N., Fodorné Csorba K., Vajda A.: Új folyadékkristályok a kutatás és gyakorlat számára I (New liquid crystals for research and applications I, in Hungarian). Magyar Kémikusok Lapja (accepted for publication)
- G.12. Bata L, Éber N., Fodorné Csorba K., Vajda A.: Új folyadékkristályok a kutatás és gyakorlat számára II (New liquid crystals for research and applications II, in Hungarian). Ibid. (accepted for publication)
- G.13. Éber N., Bata L.: Folyadékkristályok a modern technikában (Liquid crystals in modern technics, in Hungarian). Ibid. (accepted for publication)
- G.14. D.Z. Obadovic*, L. Bata, K. Fodor-Csorba, A. Vajda and T. Tóth Katona: X-ray Diffraction study of some liquid crystals of S*_A type. Review of Research, Physics Series, Faculty of Sciences, Novi Sad (accepted for publication)

- G.15. A. Vajda, K. Fodor-Csorba, L. Bata, T. Paksi*, Zs. Kakas*, I. Jánossy and J.Hajtó: Phase diagrams and electro-optical properties of novel ferroelectric mixtures. Mol.Cryst.Liq.Cryst. (accepted for publication)
- G.16.D. Catalano*, E. Ciampi*, K. Fodor-Csorba, C. Forte*, M. Geppi*, D. Imbardelli*: A ²H NMR study of orientational order, phase transitions and dynamics in a liquid crystalline compound. Liquid Crystals (accepted for publication)

Conference proceeding

G.17. A. Jákli: Piezoelectricity and ferroelectricity of columnar liquid crystals. In: *Proceedings of 4th Indian National Seminar on Liquid Crystals*, Patiala, (accepted for publication)

Book chapter

G.18. K Fodor-Csorba: Chapter 23, Pesticides. In: *Handbook of Thin Layer Chromatography*, Eds. J.Sherma, B. Fried, Marcel Dekker, New York-Basel, 1996, pp. 753-817

Others

- G.19. A. Jákli, A. Saupe*, G. Scherowsky*, X. H. Chen*: Ferroelectric columnar mesophases of pyramidic discotic liquid crystals, *16th ILCC*, Kent (June 26, 1996) abstract C2. O03
- G.20. L. Bata, K. Fodor-Csorba, S. Holly*, A. Jákli, Gy. Káli, T. Paksi*, L. Rosta and A. Vajda: Infrared and neutron spectroscopy of liquid crystal composites. Ibid. abstract B1.005
- G.21.M. Giocondo*, A. Jákli, A. Saupe*: Tilted smectic layers on homeotropically treated plates of a SmC* liquid crystal, Ibid. abstract D1P.26 (P-169)
- G.22. K. Fodor-Csorba, G. Galli*, A. Vajda, E. Gács-Baitz*, K. Újszászy*, L. Bata: Synthesis and properties of chiral liquid crystalline terepthalic acid derivatives. Ibid. abstract D3P.10
- G.23.Gy.Török, K.Fodor-Csorba, L.Rosta: Elastic and quasielastic neutron scattering on liquid crystal. Ibid. abstract B3P.19
- G.24. A. Jákli: Piezoelectricity and ferroelectricity of columnar liquid crystals. (Invited talk). *4th National Indian Seminar on Liquid Crystals*, Patiala, Nov. 1-3, 1996, Abstract Nº.1.
- G.25. A. Vajda, K. Fodor-Csorba, L. Bata, T. Paksi*, Zs. Kakas*, I. Jánossy, J. Hajtó: Phase diagrams and electro-optical properties of novel ferroelectric mixtures. *Int. Symp. on Liquid Crystals and Supramolecular Order*, Bangalore, India, (January 3-5, 1996) Abstract p.10

See also: H.4., H.14., H.15., H.17.

H. INSTABILITIES AND NONLINEAR PHENOMENA IN LIQUID CRYSTALS

Á. Buka, T. Börzsönyi, I. Jánossy, T. Tóth Katona

Pattern forming instabilities. - The response of a homeotropic nematic liquid crystal layer to low-frequency oscillatory rectilinear shear (Couette flow) was investigated experimentally and theoretically below the onset of instability. The cell was placed between crossed polarizers and light transmission was studied using parallel light beam. The transmitted ligh intensity was calculated for different cell thicknesses, oscillation frequencies, and amplitudes using the nematodynamic equations. In a (relatively) high-frequency and in the small-amplitude limit a fully analytical description is possible, otherwise numerical treatment is needed. The experimental results are in good quantitative agreement with theory. For sufficiently large shear rates a transition to a stationary roll pattern was observed.

Nonequilibrium *growth of the smectic B* phase into the supercooled nematic was further studied. In addition to the effect of the anisotropic surface tension the influence of the heat diffusion anisotropy was also included. A nontrivial angular dependence between the growth velocity and the principal axes of the diffusion tensor was found experimentally and verified with phase field simulations.

The influence of the thermal ageing of the substance was studied experimentally on the morphology of the phase boundary. The recorded effects are interpreted as a result of molecular, conformational changes.

A special attention was paid to the study of quasi-equilibrium, compact interfaces at small undercoolings. The first destabilization of the faceted and non-faceted fronts was recorded and compared with theory.

The formation, structure and dynamics of point defects in *electrically induced roll* patterns was experimentally investigated and compared for normal rolls and travelling waves in planar cells and "abnormal" rolls in homeotropic geometry. Results are compared with Ginzburg-Landau theory which conveniently describes defect dynamics and their interaction in terms of amplitude and phase of the structure.

Non-linear optics. - We began to study light-induced conformational changes of azocompounds, dissolved in a nematic liquid crystal. The conformational transitions were induced with an Ar laser beam, at different wavelengths and the resulting transmittance changes of the cell were detected with a weak probe beam at the excitation wavelength. Different combinations of the polarization direction of the pump and probe beams were investigated. The results could be interpreted in terms of a dynamic eqilibrium between light-induced *trans-cis* and *cis-trans* transitions of the azo dyes. We showed that the dichroism of both the trans and the cis form can be deducted from the data. Preliminary results on a di-azo dye indicates the strong reduction of the dichroism during the formation of the *cis* isomers.

E-Mail:

Tamás Börzsönyi btamas@power.szfki.kfki.hu Ágnes Buka ab@ power.szfki.kfki.hu István Jánossy janossy@ power.szfki.kfki.hu Tibor Tóth Katona katona@ power.szfki.kfki.hu

Grants:

OTKA T-014957 Structure formation in non equilibrium, complex systems Volkswagen Foundation (German-Hungarian bilateral): Pattern formation in liquid crystals

EC Research Network: Pattern formation, noise and spatio-temporal chaos

Publications

Articles

- H1. T. Tóth Katona, T. Börzsönyi, Z. Varadi, J. Szabon, Á. Buka, R. Gonzalez-Cinca*, L. Ramirez-Piscina*, J. Casademunt* and A. Hernandez-Machado*: Pattern formation during mesophase growth in a homologous series. *Phys. Rev.* **E54**, 1574-1583 (1996)
- H2. R. Gonzalez-Cinca*, L. Ramirez-Piscina*, J. Casademunt*, A. Hernandez-Machado*, L. Kramer*, T. Tóth Katona, T. Börzsönyi and Á. Buka: Phase-field simulations and experiments of faceted growth in liquid crystals. *Physica* **D99** (1996) (accepted for publication)
- H3. Á. Buka, T. Tóth Katona, T. Börzsönyi and P. Tóth: Mintázatképző instabilitások folyadékkristályokban (Pattern forming instabilities in liquid crystals, in Hungarian). *Fizikai Szemle* (accepted for publication)
- H4. M. Treiber*, N. Éber, Á. Buka and L. Kramer*: Travelling waves in electroconvection of the nematic Phase 5: A test of the weak electrolyte model. *Journal de Physique* (accepted for publication)
- H5. T. Börzsönyi, A.P. Krekhov*, Á. Buka and L. Kramer*: Response of a homeotropic nematic liquid crystal to rectilinear oscillatory shear. *Journal de Physique* (accepted for publication)
- H6. T. Börzsönyi and Á. Buka: Flow aligning homeotropic nematic liquid crystal under low frequency oscillatory shear. *Material Science Forum* (accepted for publication)

Conference proceeding

H7. I. Jánossy: Optical effects in dye-doped liquid crystals. In: *Photoactive Organic Materials*, Ed: F.Kajzar et.al. NATO ASI Series, (Kluwer Academic Publishers Dordrecht), pp.477-486 (1996).

Book chapters

- H8. L. Kramer* and Á. Buka: Introduction to pattern formation in nonequilibrium systems. In: *Pattern Fformation in Liquid Crystals*, Eds. L. Kramer and Á. Buka, Springer Verlag, New York, (1996) pp.1-13.
- H9. Á. Buka: Viscous fingering. Ibid. pp.291-305.

Others

- H10. Á. Buka and L.Kramer* (editors): Pattern Formation in Liquid Crystals. Springer-Verlag, New York (1996)
- H11. T. Tóth Katona, R. Gonzalez-Cinca*, T. Börzsönyi and Á.Buka: Comparison of experimental and phase field model results on the growth of nematic-smectic-B interface. In: *16th International Liquid Crystal Conference*, Kent, (June 25, 1996) Abstract A1.O04
- H12. T. Börzsönyi, A. Krekhov*, Á. Buka and L. Kramer*: Shear induced instabilities in nematics. Ibid. Abstract D3.009
- H13. J.M. Gilli*, S. Thiberge*, C. Chevallard*, Á. Buka and L. Kramer*: Metastable neel wall parallel to glass plates in nematic liquid crystals. Ibid. Abstract D2P.40
- H14. T. Tóth Katona, N. Éber and Á. Buka: Patterns on the nematic-smectic-B interface of binary mixtures and the influence of the thermally forced ageing in one-component substances. Ibid. Abstract D4P.42
- H15. Á. Buka, N. Éber, L. Kramer* and M. Treiber*: Properties of travelling waves in the electroconvection of a nematic. Ibid. D4P.50
- H16. P. Tóth*, A. Rossberg*, L. Kramer* and Á. Buka: Order-chaos transition in electroconvection in homeotropic nematics. Ibid. Abstract D4P.52
- H19. D.Z. Obadovic*, L. Bata, T. Tóth Katona and K. Fodor-Csorba: Structural properties of liquid crystal mixtures based on the homologous series of alkoxyphenyl alkoxy benzoates. Ibid. Abstract B3P.08

See also: G.14, G.15, G.25

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 systems PMR spectrum width and second moments, hydrogen content, spin-lattice and spin-spin relaxation times were measured on *binary Zr-Ni* and *ternary Zr-Ni-Cu* amorphous alloys of different Zr and hydrogen content. The temperature interval in which the measurements were done covers the range from liquid helium to about 350 K. The alloys were prepared by melt spinning from high purity metals after electron beam melting, the non-crystalline state was checked by X-ray diffraction. The samples were charged with hydrogen from the gas phase at low pressures near ambient temperature.

As the main results are concerned, on the basis of the interpretation of spin-spin relaxation existing in the high temperature range the activation energy and correlation time of hydrogen diffusion could be determined as a function of Zr, Cu and hydrogen content: all these factors effect mainly the correlation time and not the activation energy contrary to the generally used models. From the measured second moments using a local structural model an inhomogeneous hydrogen distribution could be concluded.

Transition metal complexes. — Continuing the study of transition metal complexes ${}^{1}H$ 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 at two frequencies. The characteristics of the intramolecular motions of the propyl group (the correlation times and activation energies, respectively) were re-evaluated. For both complexes the same dynamics was found, which was expected because of the isomorphic structure of the two complexes. In addition, clear signs of presence of high-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. The mechanism of the paramagnetic relaxation was found to be of rapid diffusion type. Similar measurements were started on $[Fe(Rtz)_{6}](BF_{4})_{2}$ (Rtz = 1-n-alkyl-1H-tetrazole) and $[Fe(1,10-phenanthroline)_{2}(NCS)_{2}]$ complexes.

Nanocrystalline and other metastable metallic phases. — A detailed study of the low-temperature electrical resistivity on electrodeposited nanocrystalline (nc) Ni foils produced under a variety of preparation conditions was performed in order to correlate the residual resistivity with the grain size that was determined from TEM and XRD measurements. For a single-phase nc-HfNi₅ alloy ribbon of the composition Hf₁₁Ni₈₉ produced by melt quenching with a grain size of about 10 nm, a magnetization study revealed the presence of a minority magnetic phase. The presence of this phase probably enriched in Ni could not be revealed even by a HR-TEM study and, therefore, it was concluded that the excess Ni is segregated to the grain boundaries. For meltquenched (Zr-Hf)₉₀(Fe,Co,Ni)₁₀ type metastable (amorphous, nc and b.c.c. supersaturated solid solution) alloys, the density was measured and from these data, the composition dependence of the average atomic volume V was analysed around 90 at.% Fe, Co and Ni content in order to determine the atomic volumes of both early and late transition metal components. For the amorphous Zr-Fe system, V_{Fe} was found to be close to the critical atomic volume of fcc-Fe below and above which a low-spin and a high-spin state, respectively, of Fe atoms has been previously predicted theoretically

and observed experimentally as well. Due to a fluctuation of V_{Fe} in the amorphous alloys, a fluctuation of the Fe magnetic moment from site to site can be expected. This fact may bear some significance for the peculiar magnetic behaviour reported for Zr-Fe metallic glasses around 90 at.% Fe.

Metallic multilayers. — Electrodeposited Ni-Cu alloys and Ni-Cu/Cu multilayers were produced from a sulfate bath by direct-current (d.c.) plating and pulse-plating, respectively. The total thickness of the deposits was typically 5 µm and they were removed from their substrates. For the d.c. plated Ni-Cu alloys, the deposition rate and the alloy composition was established as a function of the deposition current density. The electrical resistivity and the thermopower measured at room temperature in zero external magnetic field for these Ni-Cu electrodeposits as well as their Curie temperature were in good agreement with relevant data reported for metallurgically processed Ni-Cu alloys. The same parameters were investigated also for the pulse plated Ni₈₁Cu₁₉/Cu multilayers as a function of the constituent magnetic and nonmagnetic layer thicknesses. Anisotropic magnetoresistance (AMR) was found for the homogeneous Ni-Cu deposits whereas giant magnetoresistance (GMR) was observed in the multilayers for which a systematic variation of the relative importance of the AMR and GMR contributions with layer thicknesses was established. GMR was observed in pulse-plated Ni₈₁Cu₁₉/Cu multilayers with a maximum GMR value of about 2% for Ni-Cu layer thicknesses around 2 to 3 nm. A columnar growth of the multilayers was detected by transmission electron microscopy. The column width (grain size) was the largest for multilayers with the maximum GMR. It could also be established that the multilayer planes are often inclined at an angle, which depends on the chemical modulation wavelength, with respect to the substrate plane. This definitely gives rise to a current-perpendicular-to-plane contribution to the GMR, offering a plausible explanation for the location of the maximum of the GMR vs thickness curve. The lattice constant mismatch between the Ni-Cu and Cu layers gives rise to considerable stresses which are relaxed, besides the formation of twinning and dislocation structures, also by an induced periodic lattice distortion (structural modulation).

E-Mail:

Imre Bakonyi bakonyi@ power.szfki.kfki.hu Csaba Hargitai: hacsa@power.szfki.kfki.hu György Lasanda lasi@ power.szfki.kfki.hu Kálmán Tompa tompa@ power.szfki.kfki.hu József Tóth tothj@ power.szfki.kfki.hu

Grants

OTKA T015649 Giant magnetotransport phenomena in nanophase metals OTKA T016670 NMR relaxation and local properties in solids OMFB-British Council Joint project No. 15: Electrodeposited thin films CNRS-HAS Joint research project No. 3064: Microstructure, magnetic properties and magnetoresistance of magnetic metallic multilayers and alloy films

Publications

Articles

- I.1. I. Bakonyi, E. Tóth-Kádár and R. Kirchheim*: Preparation, structure and physical properties of Fe-, Co- and Ni-rich melt-quenched ribbons containing Zr or Hf. Part II: Electrical transport properties. *Z. Metallkde*. **86**, 784-793 (1995)
- I.2. G. Lasanda, K. Tompa, C. Hargitai, P. Bánki, I. Bakonyi: Proton nuclear magnetic resonance and H-site occupancy in Zr_{0.5}Ni_{0.5-y}Cu_yH_x metallic glasses. *J. All. Comp.* 231, 325-329 (1995)
- I.3 K. Tompa, P. Bánki, G. Lasanda, L.K. Varga: Susceptibility and proton line shift of Zr_{0.33}Ni_{0.67}-H_x amorphous alloys. *J. All. Comp.* **231**, 330-333 (1995)
- I.4. J. Tóth, K. Tompa, A. Lovas, P. Bánki: High temperature hydrogen diffusion in Zr_{0.33}Ni_{0.67}-H_x amorphous alloys. *J. All. Comp.* **231**, 334-336 (1995)
- I. Bakonyi, E. Tóth-Kádár, T. Becsei, J. Tóth, T. Tarnóczi, Á. Cziráki*, I. Gerõcs*, G. Nabiyouni*, W. Schwarzacher*: Giant magnetoresistance in self-supporting electrodeposited Ni-Cu/Cu multilayers. *J. Magn. Magn. Mater.* 156, 347-349 (1996)
- I.6. I. Bakonyi, E. Tóth-Kádár, L. Pogány, Á. Cziráki*, I. Gerõcs*, K. Varga-Josepovits*, B. Arnold* and K. Wetzig*: Preparation and characterization of DC-plated nanocrystalline nickel electrodeposits. *Surf. Coat. Technol.* **78**, 124-136 (1996)
- I.7. M. Bokor, T. Marek, K. Tompa: Solid-state NMR of 1-propyltetrazole complexes of iron(II) and zinc(II). ¹H spin-lattice relaxation time. *J. Magn. Res. A* **122**, 157-164 (1996)
- I.8. K. Tompa, P. Bánki, C. Hargitai, G. Lasanda, L.K. Varga: PMR measurements on (Ni_{1-x}Cu_x)_{0.5}Zr_{0.5}-H_y amorphous alloys. *J. All. Comp.* **232**, 84-89 (1996)
- I.9. I. Bakonyi, É. Kisdi-Koszó*, Z. Altounian*: Atomic volumes and magnetic properties of melt-quenched (Zr,Hf)₁₀(Fe,Co,Ni)₉₀ type metastable alloys. *Mater. Sci. Eng. A* (accepted for publication)
- I.10. M. Bokor, T. Marek, K. Süvegh*, K. Tompa, A. Vértes*: Positron annihilation study of Fe²⁺and Zn²⁺ complexes. J. Radioanal. Nucl. Chem. (accepted for publication)
- I.11. M. Bokor, T. Marek, K. Tompa, A. Vértes*: Solid-state ¹H NMR in 1-propyl-1H-tetrazole complexes of iron(II) and zinc(II). *J. Mol. Struct.* (accepted for publication)
- I.12. Z.F. Dong*, K. Lu*, R. Lück*, I. Bakonyi, Z.Q. Hu*: Structural identification of a melt-spun Hf-Ni nanocrystalline alloy. *Nanostruct. Mater.* (accepted for publication)

- I.13. C. Hargitai: Hydrogen in amorphous Ni_{1-x}Zr_x alloys: short range order in a glassy lattice gas. *Mater. Sci. Eng. A* (accepted for publication)
- I.14. K. Tompa, P. Bánki, C. Hargitai, G. Lasanda, A. Lovas, L.K. Varga: High temperature ¹H spin-spin relaxation in Zr-Ni-Cu-H amorphous alloys. *J. All. Comp.* (accepted for publication)
- I.15. J. Tóth, I. Bakonyi, K. Tompa: Hydrogen-induced resistivity increase in amorphous and metastable crystalline (Fe,Co,Ni)-Zr ribbons. *J. All. Comp.* (accepted for publication)
- I.16. E. Tóth-Kádár, I. Bakonyi, L. Pogány, Á. Cziráki*: Microstructure and electrical transport properties of pulse-plated nanocrystalline nickel electrodeposits. *Surf. Coat. Technol.* (accepted for publication)

Conference proceedings:

- I.17. Á. Cziráki*, B. Fogarassy*, L.K. Varga, I. Bakonyi, A. Lovas, K. Tompa, P. Kessler*, H. Lichte*: Structural changes in a hydrogenated amorphous Zr₃₃Ni₆₇ alloy. In: *Proc. 4th European Conf. on Advanced Materials and Processes (EUROMAT)* Venice (1995), Associazione Italiana di Metallurgia (1995), Symp. F, pp. 293-296
- I.18. I. Bakonyi, E. Tóth-Kádár, J. Tóth, T. Tarnóczi, Á. Cziráki*: Microstructure, electrical transport and magnetic studies of electrodeposited nanocrystalline Ni, Co and Cu metals. In: *Processing and Properties of Nanocrystalline Materials*. Eds. C. Suryanarayana, J. Singh and F.H. Froes (The Minerals, Metals & Materials Society, Warrendale, Pa., U.S.A., 1996), pp. 465-476.
- I.19. M. Bokor, T. Marek, A. Vértes*, K. Tompa: 1H solid state NMR in Fe(II) and Zn(II) complexes. In: *Extended Abstracts of 28th Congress AMPERE* (Canterbury, 1996). M.E. Smith and J.H. Strange (eds.), pp. 292-293.
- I.20. G. Lasanda, P. Bánki, C. Hargitai, A. Lovas, K. Tompa, É. Zsoldos*: PMR line-shapes and second moments in Zr-Ni-Cu-H amorphous alloys. Ibid, pp. 250-251.

Others

- I.21. Á. Dávid*, D. Greskovits*, Gy. Lasanda, K. Tompa: Granulátumok nedvességtartalmának gyártásközi vizsgálata NMR-módszerrel (NMR study of the humidity content of granular materials during production, in Hungarian). Congressus Pharmaceuticus Hungaricus X. (Budapest, 1996). Gyógyszerészet (Journal of the Hungarian Pharmaceutical Society), p. 23 (1996) (abstract)
- I.22. L.F. Kiss, L.K. Varga, I. Bakonyi: Magnetic properties of melt-quenched Nirich amorphous and bcc Zr-Ni alloys. J. Appl. Phys. 79, 5811 (1996) (abstract)

See also: D.8, J.2, J.4, J.12, J.19, J.20, J. 23, O.7

J. METALLURGY AND MAGNETISM

A. Lovas, J. Garaguly, P. Kamasa, G. Konczos, L. Pogány, T. Tarnóczi, I. Varga, L.K. Varga

The cyclic hydrogen charging and discharging process has been studied on amorphous Ni_{67-x}Cu_xZr₃₃ glassy alloys by using in-situ resistivity measurements. The resistance change is correlated with the directly measured H-content obtained by weight measurements and with the results obtained from chromatography. A large difference was found between the time scales belonging to the first charging run and the subsequent ones, and also between the charging times of samples with or without a surface pre-treatment. This indicates the simultaneous presence of surface and bulk processes in the activation mechanism of H-absorption. A fraction of H-atoms is dissolved irreversibly at room temperature, causing an increase in the resistivity of the absorbing alloy. Simultaneously with the evolution of the H-trapping sites, a progressive chemical reordering and micro-phase separation take place in the amorphous samples investigated as revealed by TEM studies.

Preparation and investigation of ceramic-reinforced amorphous composites. —

The correlation between the abrasive ability of the ceramic-reinforced amorphous metal matrix composites and the adhesion energy between the amorphous matrix and ceramic particles was investigated. The wear properties of the composite ribbons were investigated. The tests proved that composite ribbons with WC particles have higher abrasive ability compared to those with SiC particles of the same size. The sessile drop method was used to measure contact angles and adhesion energies of a Fe₄₀Ni₄₀Si₆B₁₄ liquid alloy at 1300 K on ceramic samples made of SiC and WC. The adhesion energy between the Fe₄₀Ni₄₀Si₆B₁₄ liquid (and solid, amorphous) matrix and WC particles is about 5 times higher than between the same matrix and SiC paticles. Therefore, a higher abrasive ability of ribbons with WC particles and a higher adhesion energy between the matrix and WC is experimentally found. The correlation between these two properties was explained.

Study of nanocrystalline soft-magnetic alloys. — We have continued the systematic thermomagnetic study of soft magnetic properties of nanocrystalline materials obtained from amorphous precursors by heat treatment. This year, we have focused on the temperature dependence of magnetization and initial permeability. In order to suppress further transformation of the metastable phases during heating, a measuring system with high heating rate was developed based on indirect joule heating of milligram samples in a miniaturized Pt furnace. Linear heating rates can be obtained up to 10 K/s but measurements in nonlinear mode can be extended up to 100 K/s. The technical saturation as a function of temperature reveals a composite consisting of a retained amorphous phase with a broad distribution of the Curie temperature (T_c) around that of the as-quenched state and a metastable bcc phase with reduced T_c compared to the equilibrium bcc phase obtainable after the second crystallization stage. Similar T_c values can be deduced from initial permeability versus temperature spectra obtained on toroidal samples heated in a He-protected furnace with 10 K/min up to 720 °C. In addition, the temperature dependence of initial permeability proved to be a sensitive tool for the study of exchange coupling between the nanograins through the retained amorphous phase.

As part of the Copernicus program, we have started application-oriented researches which will be finalized next year. A flux-gate magnetometer has been constructed

using an original electronic design. The sensitivity is 1 nT by using a soft magnetic amorphous ribbon. The work is aimed to develop the nanocrystalline sensor which will provide enhanced sensitivity in a wide temperature range. A special instrumentation has been built to measure power loss between 10 Hz and 100 kHz. The attainable induction level reaches technical saturation up to 10 kHz while at 100 kHz an excitation up to 0.5 T is possible.

E-Mail

Antal Lovas lovas@power.szfki.kfki.hu
József Garaguly garaguly@power.szfki.kfki.hu
Pawel Kamasa kamasa@power.szfki.kfki.hu
Géza Konczos konczos@power.szfki.kfki.hu
József Pádár padar@ power.szfki.kfki.hu
Lajos Pogány pogany@ power.szfki.kfki.hu
Lajos K. Varga varga@power.szfki.kfki.hu

Grants

OTKA T4219 Role of exchange interaction in the relaxation of metallic glasses OTKA T020891 Study of intracellular element distribution in soil

microorganisms

Magnetech Ungarn (Gyöngyös): Contract for optimization of heat treatment of

FINEMET type alloys

GE-TUNGSRAM: Contract for materials research by SEM AEKI³: Contract for materials research by SEM

Publications

Articles

J.1. A. Lovas, L.F. Kiss, F. Sommer*: Hardness and thermal stability of Fe-Crmetalloid glasses. *J. Non-Cryst. Solids* **192&193**, 608-611(1995)

- J.2. L.K. Varga, A. Lovas, K. Tompa, M. Latroche*, A. Percheron-Guegan*: Electrochemical pressure-composition isotherms for amorphous Ni_{1-x}Zr_x alloys. *J. All. Comp.* **231**, 321-324 (1995)
- J.3. A. Audouard*, J. Dural*, M. Toulemonde*, A. Lovas, G. Szenes*, L. Thomé*: Electronic slowing down-induced dimensional changes in amorphous Fe₈₅B₁₅. *Nucl. Instrum. Meth. B* **107**, 185-188 (1996)
- J.4. L. Pogány, C. Hargitai, I. Varga: Arrangement for the investigation of domain behaviour under low-frequency magnetic field. *J. Magn. Magn. Mater.* **160**, 189-190 (1996)
- J.5. A. Sólyom*, P. Marko*, G. Konczos: Rapidly quenched Fe-Si-Sb and Fe-Si-Co alloys. *acta phys. slov.* **46**, 125-128 (1996)

³AEKI: Research Institute for Atomic Energy, Budapest

- J.6. L.K. Varga, É. Kisdi-Koszó*, V. Ström*, K.V. Rao*: Thermomagnetic study of nanophases in Fe-based soft magnetic materials. J. Magn. Magn. Mater. 159, L321-L323 (1996)
- J.7. R. Varga*, P. Vojtaník*, M. Zatroch*, A. Lovas, É. Kisdi-Koszó*: Magnetic relaxation spectra of amorphous FeCrB alloy. *acta phys. slov.* **46**, 129-132 (1996)
- J.8. J. Zbroszczyk*, L.K. Varga, J. Olszewski*, W. Ciurzynska*, B. Wyslocki*, S. Szymura*, M. Hasiak*, G. Haneczok*: After-effect and microstructure of nanocrystalline alloys with different as-quenched disorder. *J. Magn. Magn. Mater.* **160**, 279-280 (1996)
- J.9. L.K. Varga, K. Tompa, A. Lovas, J.M. Joubert*, A. Percheron-Guegan*: Maximum hydrogen storage capacity of amorphous Ni_{1-x}Zr_x alloys. *Int. J. Hydrogen Energy* **21**, 927-930 (1996)
- J.10. J. Tóth, J. Garaguly, K. Tompa, A. Lovas, L.K. Varga: Hydrogen uptake monitored by resistance change in amorphous Ni₃₃Zr₆₇ alloy. *Int. J. Hydrogen Energy* **21**, 1039-1040 (1996)
- J.11. A. Audouard*, J. Dural*, M. Toulemonde*, A. Lovas, G. Szenes*, L. Thomé*: Growth phenomenon in amorphous solids irradiated with GeV heavy ions: Electronic-energy-loss dependence of the initial growth rate. *Phys. Rev.* **B54**, 15690-15694 (1996)
- J.12 W. Ciurzynska*, J. Zbroszczyk*, W.J. Olszewski*, M. Hasiak*, L.K. Varga: Microstructure and magnetic relaxation in amorphous and nanocrystalline Fe-Zr-B alloys. *Mater. Sci. Eng. A* (accepted for publication)
- J.13. J. Garaguly, A. Lovas, Á. Cziráki*, M. Reibold*, J. Takács*, K. Wetzig*: Reversible and irreversible hydrogen absorption in Ni_{67-x}Cu_xZr₃₃ glasses monitored by in situ resistivity measurements. *Mater. Sci. Eng. A* (accepted for publication)
- J.14. J. Garaguly, A. Lovas, K. Tompa, J. Takács*: Electrical resistivity change during hydrogen charging and discharging in Ni_{67-x}Cu_xZr₃₃ glassy alloys. *J. All. Comp.* (accepted for publication)
- J.15. P. Kamasa, L.K. Varga, É. Kisdi-Koszó*, J. Vandlik*: Complex testing system for ferromagnetic materials based on ac susceptibility mesurement. *Mater. Sci. Eng. A* (accepted for publication)
- J.16. G. Kaptay*, P. Bárczy*, F. Szigeti*, A. Lovas, Z. Gácsi*, L. Bolyán*: Interface phenomena in processing of ceramic-reinforced amorphous metal matrix composites. *J. Non-Cryst. Sol.* (accepted for publication)
- J.17. G. Kaptay*, A. Lovas, F. Szigeti*, P. Bárczy*, L. Bolyán*: Correlation between the abrasive ability of the ceramic reinforced amorphous metal matrix composites and the adhesion energy between the amorphous matrix and the ceramic particles. *Mater. Sci. Eng. A* (accepted for publication)

- J.18. T. Katona*, M. Varga*, A. Molnár*, A. Lovas: Effect of hydrogen treatment on the structure and surface properties of Cu-Zr and Cu-Ti alloys. *Mater. Sci. Eng. A* (accepted for publication)
- J.19. É. Kisdi-Koszó*, L.F. Kiss, L.K. Varga, P. Kamasa, P. Duhaj*: T_c measurement of metastable alloys using high heating rate. *Mater. Sci. Eng. A* (accepted for publication)
- J.20. A. Lovas, L.F. Kiss, F. Sommer*, É. Zsoldos*: Comparison of the thermomagnetic and thermal effects during devitrification of glassy Fe-TM-Metalloid alloys. *Mater. Sci. Eng. A* (accepted for publication)
- J.21. P. Vojtaník*, R. Varga*, J. Kravčák*, A. Lovas: Magnetic after-effect in amorphous $Fe_{85-x}Cr_xB_{15}$ (x=0,2,3,5,7) alloys. *Mater. Sci. Eng. A* (accepted for publication)

Conference proceedings

- J.22. P. Kamasa: The digital phase detection in cw NMR broad-line spectroscopy. In: *Proc. XXVIIIth Polish Seminar on NMR* (Cracow, 1995). Institute of Nuclear Physics (Cracow, 1996), Report Nr. 1717/PL, pp. 320-322.
- J.23. L. Pogány, Do Than Son, I. Varga, C. Hargitai, Z. Fülöp*: Measurement of magnetisation inside of a soft magnetic material and modelling the magnetic contrast on the surface by Monte Carlo method. In: *Digests of the Fourth Japan-Hungary Joint Seminar* (Fukuyama, Japan, 1996), pp. 25-26.

Other

- J.24. J. Pádár, L. Pogány, B. Biró*, I. Vörös*, J. Molnár*: Element content of endomycorrhizal spores in Zn enriched soil measured by electron probe microanalysis. In: *Program and Abstracts of COST Workshop on "Abiotic Stress Alleviation by Arbuscular Mycorrhizal Fungi"* (19-21 Sept. 1996, Budapest) (abstract)
- See also: D.5, D.8, D.13, D.14, D.16, I.3, I.4, I.5, I.6, I.8, I.14, I.16, I.17, I.18, I.20, I.22

K. NON-DESTRUCTIVE EVALUATION

F. Tóth

Magnetic flux leakage inspection system for testing storage tanks. — The working time of liquid storage tanks may span several decades. The tendency for corrosion of the tank floor plates varies considerably and will depend upon the stored product, upon the climatic conditions and the tank base.

Magnetic flux leakage inspection technique have been widely used in the oil field inspection industry for the examination of pipe, tubing and casings, but it is only in the last years that it has been applied to above-ground storage tank floors as well.

For detecting wall thickness, general areas of corrosion and rust on the underside of storage tanks a Magnetic Flux Leakage Inspection System has been developed. The tank floor tester has a magnetic bridge to magnetize the plate near saturation and surface side sensor system detects magnetic leakage fields diverted by anomalies in the part being inspected. Two compact handlebar mounted chassis contain the entire electronic controls, display, data collecting unit and power supply.

During inspection, the on-board computer converts the leakage field state into estimated wall loss by comparison with a correlation curve produced with data from calibration plate. This information is presented on a sixteen-channel display, and is converted into digital information and stored by the computer providing permanent records of the floor plate condition.

All information can be transferred to a host computer for producing color-coded diagrams of the total floor, individual plates or individual tracks within a plate. Maximum resolution obtainable is $15x15 \text{ mm}^2$. Maximum data facility: 25 m diameter tank floor.

Test plate thicknesses can vary from 6 mm to 15 mm. Reliable detectibility of corrosion pitting of 40% is achieved. With good top surface conditions it is possible to detect 20% underside corrosion pitting on 6 mm plate.

Structural integrity of service aged pipeline steel which was operated at high pressure and temperature have been investigated by magnetic hysteresis measuring method. It was found that Barkhausen emission, permeability and coercivity have been correlated with the microstructure, corrosion and stress state of material and these parameters can be used to monitor the progress of fatigue damage for nondestructive evaluation.

Grants

OMFB No. 94-97-47-0698 Micromagnetic non-destructive testing equipment for measuring internal stresses and fatigue

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 condensed matter research by neutron scattering was basically provided on the experimental facilities of the 10 MW Budapest Research Reactor and some special experiments were performed at other European neutron source laboratories (HMI Berlin, FLNP Dubna, LLB Saclay).

The small angle neutron scattering device (SANS) "Yellow Submarine" installed at the end position of the neutron guide No.2. was in full time operation in the whole 1996 year in the framework of the international user programme, according to the recommendation of the International Scientific Advisory Council at the Budapest Neutron Centre. From a double over subscription of the beam time 42 proposals were accepted, stemming from 12 foreign institutions and from 7 different Hungarian university or research centre laboratories. Only six experiments were performed for satisfying the purely in-house scientists' request. Two measurements were dedicated for methodical purposes aiming the improvement of the luminosity of the SANS instrument.

Scientific activity. — The major achievements of the SANS programme are listed below.

Phase transitions in the quenched iron salt aqueous solution has been investigated. It was shown that the previously observed by the use of Mössbauer effect phase transitions are evidently connected with the arising and disappearing of microinhomogenities with characteristic size of about 200 Å.

Silicon single crystal surface due to the ion bombarding forms a well defined brush structure, i.e. the ion bombarding treatment cuts the surface into parallel strings of thin silicon tubes, which is proved by measuring of the scattering density distribution.

Mixed micelles at high surfactant concentration form tubes and even planar shaped layer structures. These systems are closely related to the artificial and natural membranes. Measurements carried out on these systems answered many open questions connected with the structure forming forces and phase transitions arising under the influence of the temperature and/or ionic forces.

Porous materials have important meaning for technology, basically powder metallurgy. The technology of the production of tungsten wires was studied and the development of the size distribution of the pores, i.e. the increase of the density and at the same time the improvement of the mechanical properties of tungsten products were followed using samples which were taken from the different steps of the manufacturing procedure. Porosity appears also during the irradiation of constructive elements of any systems which are operating under radioactive condition.

The influence of the *radiation damage* on the structure of the metals, especially welded parts of reactor vessels and the so called self curing effects were investigated. This study is potentially important for designing of fusion reactor containers and the target materials of the spallation neutron sources too. Mechanically produced damage are equally important and so they were also studied.

Gels, organic and inorganic ones display *fractal structure*. These systems are on one hand extremely important, e.g. the so called supergels, or silica gel, and on the other hand they structure is very complicated as well. The isotope replacement was widely used in order to obtain some unique details of the gel structures and the gel structure formation.

Thanks to the two dimensional neutron detector samples possessing of *anisotropical structure* are rewarding topic of the SANS investigations. Among others, the structural behaviour of the oriented liquid crystals and ferrofluids were also studied. The latter material is very promising in industry, in chemistry and even in biomedicine. The option of easy restructuring of this systems by the use of external magnetic fields allows to carry out scattering experiments using polarised neutrons and by this approach a new way of observation of phase transitions and inter-particle interactions gets open. The results of observations allows deliberately manipulate with the structure and application use of the ferrofluid based materials.

The **three-axis spectrometer** on the curved neutron guide No.2 was used essentially for high resolution structural investigations (e.g. determination of the FeAl₂O₄ structure) and quasielastic scattering experiments. These latter measurements on 7BEF5 and EBBA liquid crystal materials revealed the segmental diffusion of the molecular parts in solid and liquid crystalline phases. In an other quasielastic scattering experiment on PANA supergels the non-monotonous dependence of the diffusion coefficient on momentum transfer was observed. This leads to the conclusion on the existence of a phase separation phenomenon and two different type of water absorption in these gels.

Combined polarised neutron small angle scattering (on the Budapest SANS instrument) and neutron spin echo measurements (on the instrument jointly operated with the Laboratoire Leon Brillouin in Saclay) were carried out on $Zn_{X}Mn_{1-X}Fe_{2}O_{4}$ based ferrofluids above and below the critical temperature. A drastic change in the diffusion process was observed due to the switching on/off the magnetic interaction by temperature and/or external magnetic field variation.

In the Cold Neutron Source project a considerable progress was made in 1996. The Technical Design and Safety Analysis Report has been completed in collaboration with the PNPI (Gatchina, Russia) development team and under project management of the ETV-ERÕTERV as General Designer. The Technical Documentation was accepted by an internal jury and submitted to the National Nuclear Safety Authority. The installation of the liquid hydrogen cold moderator into the research reactor became realistic and most probable within the next two years due to the consolidated funding scheme. The EU COPERNICUS proposal submitted and accepted in 1996 covering the costs of the cryogenic equipment plays crucial role and together with other grants (IAEA, OTKA) makes feasible the cold source implementation. The construction phase was started with the planned breakdown and scheduling of the tasks.

E-Mail:

Sándor Borbély borbely@power.szfki.kfki.hu
Tamás Grósz grosz@ power.szfki.kfki.hu
János Jani janij@ power.szfki.kfki.hu
Pál Jóvári jovari@power.szfki.kfki.hu
György Káli kali@ power.szfki.kfki.hu
László Kõszegi koszegi@ power.szfki.kfki.hu

László Rosta rosta@power.szfki.kfki.hu Gyula Török torok@ power.szfki.kfki.hu

László Cser cser@iif.kfki.hu

Grants

OTKA T 4490 Complex investigation of hydrophobic effects in aqueous solutions

OTKA T 16943 Decomposition of liquid crystal based binary systems

OTKA T 17016 Ordering phenomena in interface and surface thin layers

EU Network: WENNET Neutron scattering in molecular systems

EU PECO Use of neutron source facilities at LLB Saclay

Publications

Articles

- L.1. M. de Jong*, L. Kõszegi, J. Sietsma*, M.Th. Rekveldt*, A.van den Beukel*: A neutron depolarization study of stress-annealed amorphous Fe₄₀Ni₄₀B₂₀. J.Magn.Magn.Mater.**152**, 326-340 (1996)
- L.2. M. Prem*, O. Blaschko*, L. Rosta: Structure functions in decomposing Cu-Rh systems. Phys. Rev. B (accepted for publication)
- L.3. G. Kádár*, G. Káli, Cs. Dücső*, É.B. Vázsonyi*: Small angle neutron scattering in porous silicon. Physica B (accepted for publication)
- L.4. L. Cser, T. Grósz, G. Jancsó*, G. Káli: The nature of the interaction of tetramethylurea in various solvents. Physica B (accepted for publication)
- L.5. S. Ansell*, L. Cser, T. Grósz, G. Jancsó*, P. Jóvári, A. Soper*:Solute-solute correlation in aqueous solution of tetramethylurea. Physica B (accepted for publication)
- L.6. L. Almásy, L. Cser, I. Dézsi*, G. Káli: Small angle neutron scattering (SANS) study of frozen solutions. Physica B (accepted for publication)
- L.7. T. Grósz, V.A. Mityukhlayev*, L. Rosta, A.P. Serebrov*, A.A. Zaharov*: Liquid hydrogen cold moderator optimisation at the Budapest Research Reactor. Physica B (accepted for publication)
- L.8. R. Mezei*, K. Sinkó*, L. Cser, G. Káli, P. Fratzl*: Small angle scattering experiments on inorganic gels. Physica B (accepted for publication)
- L.9. V.T. Lebedev*, G.P. Gordeev*, L.A. Axelrod*, I.M. Lazebnik*, Gy. Török, L.Cser, L.Rosta: Polarised neutron scattering from the surface and bulk of a magnetic fluid. Physica B (accepted for publication)
- L.10. L. Rosta, T. Belgya*, L. Cser, T. Grósz, Gy. Kaszás*, G. Molnár*, Zs. Révai*, Gy. Török: Neutron guide system at the Budapest Research Reactor. Physica B (accepted for publication)
- L.11. L. Rosta, A. Jákli, G. Káli,: Structure of silica particle aggregates in liquid crystal matrix. Physica B (accepted for publication)

Others

- L.12. L. Almásy, C. Maier*, G. Pépy*: High resolution studies of physico-chemical systems with a special, RITA, 3 axis spectrometer. In: *Conference Programme and Abstracts of the 1st European Conference on Neutron Scattering*, Interlaken, Switzerland, 1996, p.219
- L.13. L. Cser, T. Grósz, G. Jancsó*: Small angle neutron scattering on systems with monomer-dimer equillibrium. Ibid. p.230
- L.14. L. Rosta: Neutron Beam Facilities at the 10MW Budapest Research Reactor. Ibid. p.212
- L.15. L. Rosta, M. Balaskó*, S. Borbély, L. Cser, T. Grósz, Gy. Káli, L. Kõszegi, G. Molnár*, E. Sváb, Gy. Török: Applied research with neutron beams at the Budapest Neutron Centre. Ibid. p.69
- L.16. A.L. Buyanov*, L. Cser, G.A. Evmenenko*, G. Káli, V.T. Lebedev*, G. Török: Neutron scattering investigation of supergels. Ibid. p. 47
- L.17. G. Pépy*, L. Almásy, C. Maier*: Etudes structurelles a haut resolution sur des systemes physicochimiques. In: *5eme Journées de Diffusion Neutronique*, Ambleteuse, France, 1996, PC1. (abstract)
- L.18. L. Rosta: Equipment et possibilités de recherche neutronique au Reacteur de Budapest. (Neutron scattering equipments and research facilities at the Budapest Reactor) Ibid. Ins7 (abstract)
- L.19. V.T. Lebedev*, G.P. Gordeev*, L.A. Axelrod*, I.M. Lazebnik*, Gy. Török, L. Cser, L. Rosta: Scan on Magnetic Fluid by Polarised Neutrons. PNPI Report, Gatchina, Russia, SS-9 No. 2101 (1995)
- L.20. V.T. Lebedev*, G.P. Gordeev*, B.P. Toperverg*, Gy. Török, L. Cser, L. Rosta, T. Rekveldt*: Magnetic Tomography on Ferrofluids. Ibid. No. 2102 (1996)
- L.21. L. Cser, T. Grósz, P. Jóvári, A.K. Soper*: Solute-solute correlations in aqueous solutions of tetramethylurea. *ISIS Experimental Report*, Rutherford Appleton Laboratory, Chilton, GB, 1996, p. A240

See also G.7, G.19, G.24

M. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, Cs. Tóth, S. Varró

Femtosecond duration extremely strong, nonperturbativ electron emission induced by intense free-electron laser pulses at far infrared wavelengths. — We revealed that extreme strong photoelectron emission can be induced using of hundred femtosecond duration intense pulses of a free electron lasers at far IR ($\lambda \sim 12~\mu m$) wavelength region. The emitted electron yield is anomalously (\sim hundred order times) higher than predicted by the idealized QED theories. Under the influence of our results theoreticiens elaborated various new numerical and analytical theories to describe the strong laser induced photon-electron interactions in real solids at the long wavelength non-perturbative regime. On the other hand, the effect in question offers the realization of new, extreme strong ultrafast electron sources for the practice.

Realistic theories also describe the wavelength dependence of the laser induced harmonic production in metals observed by us recently with femtosecond Titan Sapphire laser pulses.

Laser accelerators and X-ray generators based on multiphoton processes. — We performed new calculations on the quantum electrodynamical characteristics of laser-electron-accelerators(up to GeV energies) and intense Röntgen-generators (of terawatt intensities) based on the scattering and simultaneous absorption processes. The results show in addition that this special multiphoton process may explain the spectral characteristics of the energetic cosmic rays.

Theoretical studies on the interaction of strong laser fields with matter. — We constructed a model to describe higher harmonic generation at metal surfaces by powerful femtosecond laser pulses. Our resuls are in quite good agreement with recent experimental data. We also studied the effect of target dressing for small-angle electon scattering on atoms in the presence of a bichromatic laser field. We were able to prove that the relative phase of the two components of the field can play a considerable role in determining scattering cross-sections.

Holography at VUV/XUV laser wavelengths. — We developed a suitable method to determine the spatial coherence length of VUV/XUV laser sources by analysing the fringe visibility of simple holograms of test object. Organic films as photosensitive materials and atomic force microscope as read-out device were used for coherent (holography) and incoherent (contact print) imaging. These studies give information on the holographic images of biological objects.

E-Mail:

Győző Farkas farkas@power.szfki.kfki.hu Csaba Tóth ct@ power.szfki.kfki.hu Sándor Varró vs@ power.szfki.kfki.hu

Grants

OTKA I/4 4471 Electron emission processes induced by the simultaneous presence

of two intense laser fields of various frequencies

- OTKA I/7 T16014 Experimental and theoretical investigation of new fundamental physical processes (laser-matter interactions) induced by laser beams of superintense (10¹⁵ 10²⁰ W/cm²) laser systems.
- 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.

Publications

Articles:

- M.1. Gy. Farkas, Cs. Tóth, K. Neuman*, R.W. Falcone*, F.K. Tittel*:Wavelength dependence of the efficiency of harmonic generation at metal surfaces induced by 35 femtosecond Ti:Sapphire laser pulses. Opt. Comm. **132**, 289(1996)
- M.2. F.F. Körmendi*, Gy. Farkas: Soft X-ray generation by multiphoton scattering of a laser beam from fast free electrons. Phys.Rev. A **53**, R637(1996)
- M.3 S. Varró and F. Ehlotzky*: Higher harmonic generation at metal surfaces by femtosecond laser pulses. Phys.Rev. **A54**, 3245(1996)
- M.4. F.F. Körmendi^{*,} Gy. Farkas: Laser driven free electron accelerators. Phys.Rev.Lett. (1996). (accepted for publication)
- M.5. F.F. Körmendi*, Gy. Farkas: Laser accelerators and x-ray generators based on multiphoton processes. Laser Physics. (accepted for publication)
- M.6. Gy. Farkas, Cs. Tóth, A. Kõházi-Kis*, P. Agostini*, G. Petite*, P. Martin*, J.M. Berset*, J.M. Ortega*: Strong, thermoemission-free, electron emission from a gold surface under free-electron laser irradiation at 4-12 μm. Phys. Rev. Lett. (1996). (accepted for publication)
- M.7. I.E. Ferincz*, Cs. Toth, J.F. Young*: Resist characteristics of polymethylmetacrylate at vacuum ultraviolet wavelengths for high resolution imaging. Appl. Opt. (1996). (accepted for publication)
- M.8. S. Varró and F. Ehlotzky*: Effect of target dressing for electron scattering in a bichromatic laser field. J.Phys.A. (accepted for publication)

Conference proceedings

- M.9. Gy. Farkas, Cs. Toth, K.C. Neuman*, R.W. Falcone*, F.K. Tittel*: Spectral dependence of harmonic generation efficiency at metal surfaces. In: *Proceedings of the Quantum Electronics and Laser Science Conference*, *QELS '96*, *Anaheim*, *CA*, June 2-7, 1996, pp. 29-30
- M10. Cs. Toth, I.E. Ferincz*, J.F. Young*: Study of the spatial coherence of the VUV Xe²⁺ Auger laser by holographic imaging. In: *Proceedings of the 9th Annual Meeting of IEEE Lasers and Electro-Optics Society, LEOS'96*, Boston, MA, November 18-21, 1996, pp. 304-305

Others

- M.11. Gy. Farkas: Strong femtosecond duration electron emission from a gold surface induced by femtosecond infrared pulses of a free-electron laser. (Invited). In: Conf. Digest of the XVIII. International Free Electron Laser Conference, Rome, 29 Aug. 1 Sept., 1996. p.29
- M.12. Gy. Farkas, Cs. Toth, K.C. Neuman*, R.W. Falcone*, F.K. Tittel*: Spectral dependence of harmonic generation efficiency at metal surfaces. In: *Conf. Digest of the Quantum Electronics and Laser Science Conference, QELS '96, Anaheim, CA, June 2-7, 1996 Paper JTuA2*, p. 29
- M.13. Cs. Toth, I.E. Ferincz*, J.F. Young*: Study of the spatial coherence of the VUV Xe²⁺ Auger laser by holographic imaging. In: *Conf. Digest of the 9th Annual Meeting of LEOS '96, Boston, MA, November 18-21, 1996 Paper ThE4*, p. 63
- M.14. Gy. Farkas, Cs. Tóth, A. Kõházi-Kis, P. Agostini*, G. Petite*, J.M. Berset*, J.M. Ortega*: Strong, thermoemission-free, electron emission of a gold surface under free electron irradiation at 4-12 μm. In: *7th International Conference on Multiphoton Processes*, 30 Sept.-4 Oct. 1996, Garmisch-Partenkirchen. Book of Abstracts, Nº B22
- M.15. F.F. Körmendi*, Gy. Farkas: Multiphoton relativistic electron interaction processes: Acceleration to multi-GeV energies and production of Terawatt/cm² X-ray intensities. Ibid. Nº B33
- M.16. S. Varró, F. Ehlotzky*: Effect of target dressing in free-free transitions in a bichromatic laser field. Ibid. No A102
- M.17. S. Varró, F. Ehlotzky*: Higher harmonics generation at metal surfaces by powerful femtosecond laser pulses. Ibid. Nº B63

N. LASER PHYSICS

<u>M. Jánossy</u>, P. Apai, T. Bereczki, L. Csillag, Z. Donkó, Sz. Forizs, Á. Hoffmann, Z.Gy. Horváth, Zs. Lenkefi, P. Mezei, K. Rózsa, L. Szalai, K. Szőcs, Zs. Szentirmay

Experiments and modelling on segmented hollow cathode discharges. — We have continued our earlier investigations on the segmented hollow cathode discharge (SHC) which has been proved to be the most efficient source for the excitation of cathode sputtered metal ion lasers. We have carried out experiments to obtain the spatial distribution of the gain in the cross section of the SHC. We have shown that with decreasing pressure the maximum gain is on the axis of the discharge. At higher pressures the gain has two maxima. These two peaks are moving towards each other with increasing current. We also measured the gain on the 780.8 nm Cu-II transition. We found 140 %/m gain, which is the highest gain obtained so far in this class of lasers. Our estimated gain on the 154 nm VUV transition (which has a common upper level with that of the 780.8 nm transition) is approximately 3 %/m. With this gain, continuos VUV laser operation may be possible.

We have developed Monte Carlo simulation of the electrons' motion in the SHC. We have shown that there is a high number of high-energy electrons absorbed by the anode electrodes. This effect accounts for the increased voltage of the SHC. In spite of the relatively high pressure (10-20 mbar), a significant part of the electrons oscillates between the opposing cathode surfaces. We have explained the effect of the longitudinal magnetic field on the electrical characteristics of the discharge. This modelling study helps in the understanding of the experimentally observed behaviour of the discharge and may be used for the optimisation of discharge arrangements by computer experiments.

He-Zn hollow cathode laser. — The He-Zn hollow cathode laser operates at several Zn ion lines falling in the visible part of the spectrum. Investigations were performed on the excitation mechanism of the strong 492.4 nm and 491.2 nm laser transitions. Two different mechanism were suggested earlier for excitation of the upper laser levels. From the observation of laser oscillation in the afterglow and high laser intensities at large partial pressures of admixed Ar and Kr it could be concluded that the dominant process is charge transfer excitation by He ions followed by collisions with low energy electrons. The other process, direct electron excitation from the Zn ion ground state has different features, this makes it unlikely that it plays any significant role.

Electrolyte cathode atmospheric glow discharge (ELCAD). — The intensity of spectral lines emitted by the ELCAD was investigated as a function of air pressure, pH value of electrolyte and discharge current in order to understand the processes of spectral line emission. Only the atomic lines of metals dissolved in the electrolyte occurred in the spectrum, except the Mg-II 279.6 nm and the Ca-II 393.4 nm ionic lines. These spectral lines could be observed only if the air pressure was higher than 600 mbar and their intensity increased steeply with increasing pressure in the pressure range of 600-1200 mbar. Furthermore, the line intensities were found to increase also with decreasing pH (i.e. with decreasing cathode fall). The intensities reduced to zero at about 20-30 mA and this current threshold seems to be independent of the air pressure. The results are explained on the basis of a recombination model: the positive metal ions produced by cathode sputtering can only reach the negative glow if they recombine in the cathode dark space. After this, the neutral metal atoms can diffuse

into the negative glow, where they are excited by electron impact. The obtained increase of the intensities with increasing air pressure can be explained by the simultaneous increasing rate of recombination. The pressure dependence of the intensities calculated by this model are in excellent agreement with the experimental data. This model predicts the appearance of an intensity maximum at higher air pressures: it occurs, when the increasing rate of recombination can not compensate the decreasing rate of electron impact excitation. The threshold for the appearance of spectral lines as a function of air pressure and pH indicate the necessary condition of a small enough electron energy for recombination. The current threshold can be attributed to ceasing of cathode sputtering. The reason, that the ionic metal lines, except the mentioned Ca and Mg ionic lines, could not be observed in the spectrum, is due to the outer electronic shell of the single ions of the metals is closed, similarly to that of the rare gases. Because of this, the energy necessary for excitation is too high compared with the average electron energy of the plasma.

Surface roughness study of gold films on LiF deposits. — Attenuated total reflection and rear-side light emission were measured on 50 nm thick gold films evaporated on glass substrates preliminary covered with LiF sublayers of 0–500 nm thickness. The dielectric function of the metal film was determined in dependence of the fluoride thickness. Roughness spectra were calculated from the angular distribution of the emission intensity and from the images of an atomic force microscope (AFM). The optically determined roughness amplitudes were found to be proportional to the fluoride thickness up to 350 nm. The comparison of experimental corrugation parameters determined from the optical data and by AFM gave an unexpected result namely that waviness of LiF sublayers is responsible for the observed anomalies and not the grain structure.

Research on multidimensional lasers. — The "natural" laser processes may appear both in the cellular size microscopic world (laser paints) or in cosmic size plasma spheres, clouds (laser stars), representing the two extreme categories of multidimensional lasers. There are spectroscopic indications already, verifying the possible existence of these non-artificial lasers. Experimental model simulation of spontaneous and amplified light, emitted from differently shaped light sources are in progress. On the basis of our experience on the realisation of the first planar (Halo) lasers, we are working on the prediction of the spatial distribution of the supposed non-spontaneous (ASE or laser) radiation components of possible cosmic laser objects.

The special optical, spectroscopic and fluorescence imaging instrumentation, developed for the experimental investigation of the mentioned research program, was successfully used in other different scientific fields, in co-operation with the Institute of Biophysics of the Semmelweis Medical University, the National Institute of Oncology and the Institute of Lymnology of H.A.S. In the photodinamic diagnose of cancer, we demonstrated the benefits of incoherent fluorescence excitation in contrast to laser illumination. The deepness dependence of penetrated solar UV light intensity was measured by our experimental instrument in several Hungarian lakes, resulting important data for the estimation of real, natural conditions of light dependent, photobiology based underwater life.

E-Mail:

Pál Apai apai@power.szfki.kfki.hu Ákos Hoffmann hoffmann@power.szfki.kfki.hu Mihály Jánossy mjanossy@power.szfki.kfki.hu

karcsi@sunserv.kfki.hu Károly Rózsa László Szalai lszalai@sunserv.kfki.hu Zsolt Lenkefi lenkefi@power.szfki.kfki.hu Pál Mezei mezeipal@power.szfki.kfki.hu szenti@power.szfki.kfki.hu Zsolt Szentirmay Zoltán Donkó donko@sunserv.kfki.hu Zoltan Gyorgy Horvath horvath@power.szfki.kfki.hu Katalin Szocs szocs@power.szfki.kfki.hu bereczki@power.szfki.kfki.hu Tibor J. Bereczki Szabolcs Forizs forizs@power.szfki.kfki.hu

Grants:

OTKA T4227 Excitation mechanisms in hollow cathode lasers

OTKA T014909 Lasers in hollow cathode discharges

OTKA F015502 Basic processes of glow discharge in the cathode region

OTKA T-016075 Surface plasmon studies

OTKA T-014850 Electrolyte cathode atmospheric glow discharge

OTKA T-017293 Multidimensional lasers

Publications

Articles

- N.1. R.C. Tobin*, K.A. Peard*, B. Leigh*, G. Bode*, K. Rózsa, Z. Donkó and L. Szalai: Novel low-temperature pulsed metal-vapour lasers The high-voltage hollow-cathode metal ion laser. In: *Pulsed Metal Vapour Lasers* (ed. C.E.Little and N.V.Sabotinov) (Kluwer Academic Publishers: Dordrecht, Netherlands) pp. 189-194 (1996)
- N.2. Z. Donkó, K. Rózsa and R.C. Tobin*: Monte Carlo analysis of the electrons' motion in a segmented hollow cathode discharge. *Journal of Physics D: Applied Physics* **29**, 105-114 (1996)
- N.3. Z. Donkó and L. Szalai: Chaotic current oscillations with broadband 1/f^{\text{o}} spectrum in a glow discharge plasma. *Chaos, Solitons & Fractals* **7**, 777-783 (1996)
- N.4. Z. Donkó, P. Apai, L. Szalai, K. Rózsa and R.C. Tobin*: The segmented hollow cathode discharge: a pumping source for UV metal ion lasers. *IEEE Transactions on Plasma Science* **24**, 33-34 (1996)
- N.5. T. Cserfalvi*, P. Mezei: Operating mechanism of the electrolyte cathode atmospheric glow discharge. Fresenius Journal of Analitycal Chemistry **355**, 813-819 (1996)

- N.6. A. Hoffmann, N. Kroó, Z. Lenkefi and Z. Szentirmay: A high precision ATR study of surface plasmon mediated reflectance in noble metal films. Surf. Sci. **352–354**, 1043–1046 (1996).
- N.7. M. Danailov*, T. Gasmi*, P. Apai: Transient refraction index changes in UV-exposed optical fibres. Electronics Letters **32**, 482-483 (1996)
- N.8. A. Hoffmann, N. Kroó, Z. Lenkefi and Z. Szentirmay: Optical determination on surface roughness parameters of gold films by ATR reflectometry. Surf. Sci. (accepted for publication)

Conference proceedings

- N.9. T. Adamowicz*, Z. Donkó, W. Kwasniewski*, L. Szalai and K. Rózsa: Comparison of IR gain in He-Cu ion lasers with different hollow cathode geometries. In: *Proc. of V. Symp. on Ion Beam Techniques*, 21-23 March 1996, Szklarska Poreba, Poland (in Polish) (1996)
- N.10. A. Hoffmann, N. Kroó, Z. Lenkefi and Z. Szentirmay: The effect of surface roughness on the ATR spectra of gold films. In: *Proc. of ECOSS 16 (European Conference on Surface Science)* Genova (Italy), September 1996. FrMP103.
- N.11. A. Hoffmann, N. Kroó, Z. Lenkefi and Z. Szentirmay: An ATR study of the thickness dependence of the dielectric function of gold and silver thin films. In: *Proc. of ISSE'96 (19th International Spring Seminar on Electronics Technology)* Göd (Hungary), May 1996. pp. 192–197.
- N.12. A. Hoffmann, N. Kroó, Z. Lenkefi and Z. Szentirmay: The influence of roughness on the surface plasmon decay length. In: *Proc. of EPS 10 Trends in Physics (10th General Conference of the European Physical Society)* Sevilla (Spain), September 1996.
- N.13. A. Hoffmann, N. Kroó, Z. Lenkefi and Z. Szentirmay: Studies of surface plasmon oscillations on LiF roughened metal surfaces. In: *Proc. of EPS 15* (15th General Conference of the Condensed Matter Division) Baveno-Stresa (Italy), April 1996.
- N.14. K. Szõcs, K.Barna*, J. Fidy*, D. Gal*, Z. Gy. Horváth, T. J. Bereczki: Photodynamic diagnosis of tumours by 5-aminoleulinicacid induced protoporphyrin IX fluorescence, excited either by a coherent and an incoherent light source. In *ICP* '96. *Proc. of the 12th International Congress on Photobiology*, Sept. 1-6 Vienna, Austria, 1996, p. 317
- N.15. T.J. Bereczki, Z.Gy. Horváth: Fluctuation of the laser speckle on in vivo tissues. In: *Laser in Medicine*, Eds. W. Waidelich, G. Staehler, R.Waidelich, Springer, 1996, pp. 467-472
- N.16. K. Szõcs, K. Barna*, J. Fidy*, D. Gal*, Z.Gy. Horváth, T.J. Bereczki: Photodinamic diagnosis of tumours. In: Proc. of *V. Semmelweis Science Fair*, Sept. 26-27, 1996, Medical Science Monitor, Vol. 2. Supplement 3, pp 16-18 (1996)

Others

- N.17. Z. Donkó and L. Szalai: Period doubling and chaos in a modulated subnormal glow discharge. KFKI Report-1996-03/D pp. 1-11 (1996)
- N.18. R.C. Tobin*, B. Leigh*, F.E. Robilliard*, J. Schulze*, K. Rózsa and Z. Donkó: Atom and ion concentrations in a high-voltage hollow-cathode metal ion laser. *9th Gaseous Electronic Meeting (GEM)*, January 29-31, 1996, Flinders University, Adelaide, SA, Australia (1996) (abstract)
- N.19.R.C. Tobin*, B. Leigh*, K. Rózsa, Z. Donkó, L. Szalai and J. Schulze*: The segmented hollow-cathode ultraviolet laser. *International Quantum Electronics Conference (IQEC)*, July 14-19, 1996, Sydney, Australia (1996) (Abstract)
- N.20. T. Adamowicz*, Z. Donkó, W. Kwasniewski*, L. Szalai and K. Rózsa: Spatially resolved gain in segmented hollow cathode He-Cu discharges. *ESACAMPIG XIII Conference*, August 27-30, 1996, Poprad, Slovakia (1996) (abstract)
- N.21. K.Rózsa, L.Szalai and Z.Donkó: Oscillations in a low current argon glow discharge. Ibid. (abstract)
- N.22. Z. Donkó, T. Šimko and K. Rózsa: Monte Carlo model of an obstructed glow discharge in hydrogen. Ibid. (abstract)
- N.23. K. Rózsa, Z. Donkó, L. Szalai, T. Adamowicz* and R.C. Tobin*: UV lasers in highly efficient hollow cathode discharges. Joint Polish-German Conference on Modern Optics, September 23-28, 1996, Jaszowiec, Poland (1996). (abstract)
- N.24. A. Demidovich*, A. Shkaderevich*, M.B. Danailov*, P. Apai, T. Gasmi*, V. Gribkovski*, A. Kuzmin*, R. Ryabtsev*, L. Batay*: Comparison of CW lasing operation of Nd:YAG, Nd:KGW and Nd:BEL with laser diode pumping. CLEO/EUROPE-EQEC'96, Hamburg, CWF42 (abstract)
- N.25. K. Scmotzerné Barna*, K. Szõcs, T. Tóth*, D. Gal*, O. Csuka*: Különbözõ típusú fényérzékenyítő vegyületek összehasonlítása a fotodinamikus terápia hatékonysága alapján (Comparison of different photosensitize compounds on the basis of effect of photodynamic therapy, in Hungarian). Magyar Kemoterápiai Társaság XI. Konferenciája, Debrecen, 1996. jun. 4-6.(abstract)

O. LASER APPLICATION

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

Solid state laser development. — In the frame of a TD&QM EU Phare Programme "Q-switched Nd:YAG laser for High Quality Material Processing" was built. The system incorporates a special supply which is capable for continuous and pulsed operation up to 2 x 6 kW or 2 x 30 kW-peak respectively, our novel piezo driven Fabry-Perot Q-switch with intelligent control and two laser heads in series capable for 500 W average output power. The laser will be used in the job shop of the LASRAM Ltd., Budapest.

As an introduction two special experiments were carried out - in cooperation with the General Physics Institute, Moscow — for laser diode pumping of Er,Yb:glass and Nd:YAG crystall-slab. The InGaAs laser diode pumped Er,Yb:glass converted the 0,93 μ m wavelength to 1,54 μ m. The Nd:YAG crystall-slab was pumped by a 10 W diode array proving that the used sandwich geometry will be good also for YAG-Nd:glass composition, promising record output parameters.

Optical measuring techniques based on light scattering and interference. — Optical ray tracing program was applied for the definition and specification of the sensing volume of a new type of portable airborne particle counter. Experiments were carried out for the definition of the sensor utilising semiconductor laser light source and detector instead of He-Ne gas laser and photomultiplier tube. Preliminary calibration measurements showed improved performance with respect to earlier designs.

Sound frequency band vibrations of submicron amplitude scale in rigid mechanical structures were registered in experiments utilising the previously developed LIMAS system. The generating source of these were not established. Estimates suggest that the surrounding acoustic noise level might be the source.

Computer algorithm was developed for the determination of particle size in photon correlation velocimetry experiments. It was proved that the FFT histogram of the autocorrelation function of the scattered intensity corresponding to single particle transit contains the size information. The expectation value of the ratio of contents of two specific channels of the FFT histogram is monotonous function of particle size. 3D computer plots of the dependence of this ratio on particle size and velocity were created. Other measurement parameters like sampling time, fringe visibility and distance were taken into account as parameters. Computational results showed reasonable agreement with previously taken measurements made with polystyrene latex balls of known size.

Monte-Carlo simulation program was developed for the study of calibration procedures encountered in the practice of airborne particle counters. The program takes into account all major parameters - refractive index, laser line width, scattering geometry, detector noise, background stray light level, illumination homogeneity, particle size distribution and concentration - influencing light amplitude distribution in calibration experiments using spherical particles. As a result all kinds of calibration procedures can be simulated and the operator dependent arbitrary factors excluded.

The concentration and size distribution of aerosols released in simulated LWR accident - in air ingress experiment were investigated by laser particle counter and by scanning electron microscopy. An intensive aerosol stream was observed in the temperature region 700-1600 $^{\rm o}$ C. The consistency of the results obtained by different measurements demonstrate the convenience of the particular methods applied. In the size distribution of the aerosol particles released from heated LWR fuel roads two ranges with different slopes were observed. The intersection of this ranges is around 2 μ m.

Calculations were carried out in modelling of the determination of size distribution of liquid-borne particles using a time of flight method. The results of the calculation were compared with the results of pulse-height method, used previously.

Theoretical considerations were carried out in planning of the future experiments with squeezed light.

In November (1996) the III. Hungarian Aerosol Conference was organised by us and the proceedings of this conference was edited.

Amorphous thin layers. — Current project "Diamond-like" hydrogenated amorphous carbon (a-C:H). The two crystalline inorganic modifications of carbon, diamond and fully three-dimensionally interconnected sd³ hybridized carbon atoms is hard, electrically insulating and transparent graphite with layered structure of sp hybridized carbon atoms is soft, electrically conducted and no transparent. The amorphous carbon modifications bridge over the entire spectra of physical properties between diamond and graphite. Variability of properties enriches if hydrogen is added to amorphous carbon. Among these the highly efficient light emission in the visible range and low-field electron emission should be emphasized. Fundamental investigation of correlation between structure and physical properties of different amorphous carbon modifications is the main and rapidly developing direction of amorphous semiconductor research.

Our research in the field of amorphous carbon was developed to question of how the photoluminescence and its efficiency depend on optical gap and on the density of localized and tail states of a-C:H. For this purpose we have prepared a-C:H samples with different structure by glow discharge method. Band gap, localized and tail states of carbon samples determined by optical end electric measurements were related to carbon - carbon and carbon - hydrogen bonding properties extracted from NMR and Raman results. Luminescence features of these well characterized samples were studied in a wide emission and excitation energy range. The main conclusions are as follows: i) excited states of highly localized π electrons are responsible for effective luminescence; ii) by weakening of p electron localization parallel with decreasing of band gap the luminescence efficiency is quenching.

Photoluminescence and photoconductivity are related to each other by recombination of photoexcited carriers. Amorphous carbon was thought to be no photosensitive material. Our investigations prove photoconduction effect of a-C:H and show two peaks in its excitation energy dependence.

E-Mail:

Aladár Czitrovszky czi@power.szfki.kfki.hu Péter Jani jani@ power.szfki.kfki.hu Árpád Kiss kissa@ power.szfki.kfki.hu Margit Koós koos@ power.szfki.kfki.hu
György Messing messing@ power.szfki.kfki.hu
István Pócsik pocsik@ power.szfki.kfki.hu
Iván Kertész kertesz@sunserv.kfki.hu
Béla Plósz plosz@sunserv.kfki.hu

Grants:

OTKA 20202 Development of fundamental experiments with squeezed light OTKA T 017371 Diamond-like amorphous carbon; atomic bonds, nanostructure and macroscopic properties

OMFB-Technoorg 1018/95 Development of a new liquid-borne particle counter OMFB 47-0980 Development of a portable airborne particle counter

Publications

Articles

- O.1. P. Jani, A. Czitrovszky: Sound and vibrations on submicron amplitude scale in rigid mechanical structures, In: *Simulation and Experiment in Laser Metrology*, Akademie Verlag, Berlin, Volume **2** pp. 269-275 (1996)
- O.2. P. Jani, A. Nagy, A. Czitrovszky: Aerosol particle size determination using a photon correlation laser Doppler anemometer. J. Aerosol Sci., **27**, 531-532 (1996)
- O.3. A. Czitrovszky, J. Frecska*, P. Jani, L. Matus*, A. Nagy: Size distribution of aerosol released from heated fuel rods. J. Aerosol Science, **27**, 467-468 (1996)..
- O.4. A. Czitrovszky, P.L.Csonka*, P. Jani, Á. Ringelhann*, J. Bobvos*: Comparison of different measurement methods of airborne dust pollution within the city of Budapest. J. Aerosol Science, **27**, 19-20 (1996)
- O.5. A. Czitrovszky, P.L. Csonka*, P. Jani, Á. Ringelhann*, J. Bobvos*: Experimental investigation of altitude dependence of size distribution and concentration of dust particles within the city of Budapest. J. Aerosol Science, 27, 117-118 (1996)
- O.6. I. Pócsik and M. Koós: Spectral inhomogeneity a key issue for understanding relaxation in amorphous matter. J. Non-Cryst. Solids **198-200**,774-777 (1996)
- O.7. I. Pócsik, M. Koós, S.H. Moustafa, Gy. Lasanda, P. Bánki, K. Tompa: Temperature dependence of ¹H-NMR relaxation in hydrogenated amorphous carbon samples series. J. Non-Cryst. Solids **198-200**,632-635 (1996).
- O.8. I. Pócsik, M. Koós, S.H. Moustafa, J. A. Andor*, O. Berkesi, M. Hundhausen*: Comparative Raman studies if hydrogenated amorphous carbon films by using infrared and visible laser extinctions. Microchimica Acta (1996) (accepted for publication)

O.9. M.C. Iovu*, E. P. Kolomeiko*, M. Koós and I. Pócsik: Photosensitivity of a-C:H/p-Si heterojunction (in Russian). Pisma Zhurn. Techn. Fiz. (1996) (accepted for publication)

Conference proceedings

- O.10. A. Czitrovszky, P.L. Csonka*, P. Jani, Á. Ringelhann*, J. Bobvos*: Complex measurement of airborne dust pollution within the city of Budapest. In: *Laser methods for biomedical Applications*, Ed. by A.M. Prohorov, SPIE, vol. **2965**, (1996).
- O.11. P. Jani, A. Nagy, A. Czitrovszky: Particle size measurement with a photon correlation LDA system. In: *Proc. AAAR 15th Annual Conference*, Orlando, Florida, *1996*, p.237.
- O.12. A. Czitrovszky, P. Csonka*, P. Jani, Á. Ringelhann*, J.Bobvos*: Measurement of airborne dust pollution within the city of Budapest. In: *Proc. AAAR 15th Annual Conference*, Orlando, Florida, *1996*, p.210.
- O.13.P. Jani, A. Nagy: Monte-Carlo modelling in calibration of laser particle counters. In: *Proceedings of III. Hungarian Aerosol Conference*, Budapest, 1996, pp. 81-84
- O.14. P. Jani, A. Nagy, A. Czitrovszky: Determination of the size of aerosol particles using LDA system. Ibid. pp. 77-80
- O.15. A. Czitrovszky, P. Jani: Application of the instrumentation developed for sizing of micron and sub-micron particles. Ibid. pp. 71-75
- O.16. M. Koós, I. Pócsik, and O. Berkesi*: Analysis of disordered peak in Raman spectrum of hydrogenated amorphous carbon. In: *Extended abstracts of the NATO ASI on Amorphous Insulators & Semiconductors*, Sozopol, Bulgaria, May 26 June 8, 1996, p. 40
- O17. I. Pócsik, M. Koós, R. Blink*, D. Arcon*, P. Cevc*, Z. Trontejl* and J. Jeglic*: Ferromagnetic behaviour, spin-glass phenomena in hydrogenated amorphous carbon. Ibid., p.49
- O.18.M. Koós and I. Pócsik: Photoluminescence in hydrogenated amorphous carbon. In: *Proc. of NRW on Physics and Application of Non-Crystalline Semiconductors in Optoelectronics*, Chisinau, Moldova, Oct. 15-17, 1996 (accepted for publication)

P. OPTICAL THIN FILMS

K. Ferencz, 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 i.) Gires-Tournois type dispersive dielectric mirrors for mode-locked Cr:LiSGaF and Yb:glass lasers, and ii) chirped mirrors for Ti:sapphire lasers and its second harmonics. 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. Similar 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, which represents the shortest man-made electro-magnetic wavepackets up to date.

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. We found that the GDD of the laser active materials strongly depends on doping concentations.

High efficiency phase conjugation of broadband laser pulses in BaTiO₃. — Phase conjugation of spectrally broad laser pulses was demonstrated by spectrally dispersing the pulses in a photorefractive BaTiO₃ crystal in cooperation with ICTP Trieste, Italy. Because of the relatively high phase conjugated reflectivity obtained, application of this novel phenomenon for ultrafast pulse shaping and ultrafast measurement techniques seems to be feasible in the near future.

Other developments on optical coatings. — Low loss dielectric mirrors have been developed for a hollow cathode copper laser. The mirrors have been successfully tested by our colleagues at the Department of Laser Physics (K. Rózsa et. al.). Using our mirrors they could make the laser operate at a wavelength as short as 260 nm.

Optical waveguides deposited on optical gratings were developed for optical sensors used for medical applications.

E-Mail:

Kárpát Ferencz kf@power.szfki.kfki.hu Róbert Szipõcs rsz@ power.szfki.kfki.hu

Grant

OTKA T-020568 Dispersive dielectric mirrors for femtosecond laser systems.

OTKA CW-015285 Dispersion measurement on optical thin film structures and other optical elements using white light interferometry.

Publications

Articles

- P.1. I.T. Sorokina*, E. Sorokin*, E. Wintner*, A. Cassanho*, H.P.Jenssen*, R. Szipõcs: Prismless passively mode-locked Cr:LiSGaF laser. Opt. Lett. **21**, 1165-1167 (1996)
- P.2. L. Xu*, Ch. Spielmann*, F. Krausz*, R. Szipõcs: Ultrabroadband ring oscillator for sub-10-fs generation. Opt. Lett. **21**, 1259-1261 (1996)
- P.3. Ch. Spielmann*, S. Sartania*, F. Krausz*, R. Szipõcs, K. Ferencz, M. Nisoli*, Sandro S. Silvestri*, O. Svelto*: Generation of intense sub-5-fs light pulses: A tool for controlling atomic processes on the time scale of the light oscillation period. Nature (accepted for publication)

Conference Proceedings

P.4. L. Xu*, Ch. Spielmann*, F. Krausz*, R. Szipõcs, Ultrabroadband ring oscillator for short pulse generation, In: *Proc. Ultrafast Phenomenon '96*, USA

Others

- P.5. I.T. Sorokina*, E. Sorokin*, E. Wintner*, A. Cassanho*, H.P. Jenssen*, R. Szipõcs: 47 fs pulse generation from a prismless self-mode-locked Cr:LiSGaF laser. In: *Technical Digest of the Advanced Solid State Lasers Conference*, San Francisco, Optical Society of America, Washington, D.C. (1996)
- P.6. Ch. Spielmann*, L. Xu*, F. Krausz*, R. Szipõcs: Sub-10-fs Ti:sapphire lasers. In: *Technical Digest of the Conference on Lasers and Electro-Optics 1996*, Anaheim, CA, USA, paper CME3 (1996)
- P.7. A. Stingl*, Ch. Spielmann*, F. Krausz*, R. Szipõcs: Compact high-repetititon-rate femtosecond lasers using chirped mirrors. Ibid. paper CMK7 (1996)
- P.8. I.T. Sorokina*, E. Sorokin*, E. Wintner*, A. Cassanho*, H.P. Jenssen*, R.Szipõcs: Prismless Kerr-lens mode-locked femtosecond Cr:LiSGaF laser. In: *Technical Digest of the Conference on Lasers and Electro-Optics Europe* 1996, Hamburg, Germany, Optical Society of America, Washington, D.C. paper CWA1 (1996)
- P.9. Ch. Spielmann*, L. Xu*, F. Krausz*, R. Szipõcs: Ultrabroad-band sub-10-fs Ti:sapphire ring oscillator. Ibid. paper CFF2 (1996)
- P.10. A. Stingl*, Ch. Spielmann*, F. Krausz*, R. Szipõcs: Compact high repetition-rate sub-100-fs lasers. Ibid. paper CFF5 (1996)
- P.11. E.J. Mayer*, J. Möbius*, W.W. Rühle*, R. Szipõcs: Ultra-broadband mirrors for femtosecond lasers. Ibid. paper CPD2.6 (1996)
- P.12. R. Szipõcs: Theory and experiment with chirped mirrors for dispersion compensation. *Technical Digest of the European Quantum Electronics*

- Conference 1996, Hamburg, Germany, Optical Society of America, Washington, D.C., paper QThI4 (1996)
- P.13. Ch.Spielmann*, M.Lenzner*, F. Krausz*, R. Szipõcs, K.Ferencz: Chirped dielectric mirrors improve Ti:sapphire lasers. Laser Focus World **31**, 55-60 (1995)

EDUCATION

Graduate and postgraduate courses, 1996

- Statistical physics (F. Iglói, JATE⁴)
- Electrodynamics II (F. Iglói, JATE)
- Advanced solid state physics I (J. Sólyom, ELTE⁵)
- Advanced solid state physics II (J. Sólyom, ELTE)
- Electrodynamics (F. Woynarovich, ELTE)
- Solid state physics I. (A. Virosztek, BME⁶)
- Solid state physics II. (A. Virosztek, BME)
- Magnetism II (P. Fazekas, ELTE)
- The physics of magnetic materials (P. Fazekas, BME)
- Spectral theory of Schrödinger equation (A. Sütő, ELTE)
- Many body problem I (I. Tüttő, BME)
- Many body problem II (I. Tüttő, ELTE)
- Superconductivity (I. Tüttõ, ELTE)
- Solid state physics (I. Tüttő, BME)
- Solid state research (I. Vincze, ELTE)
- Amorphous and crystalline materials (J. Gyulai*, E. Hartmann* and T. Kemény, BME)
- Modern experimental methods in solid state physics (G. Faigel, ELTE, BME)
- Experimental methods in materials science (G. Faigel, G. Oszlányi, BME)
- Group theoretical methods in solid state physics (K. Kamarás and G. Kriza, ELTE)
- Beyond the crystalline state (A. Jákli, BME)
- Physics of liquid crystals and polymers (Á.Buka, ELTE)
- Non-conventional materials (Á.Buka, BME)
- Interaction of condensed matter and light, (I.Jánossy, JATE)
- Advanced material technologies (G. Konczos, ELTE, BME)
- From metals to ceramics (A. Lovas, BME)
- Modern physical methods in medical diagnostics (K. Tompa, ELTE)
- Experimental methods in solid state physics (Z. Szentirmay, ELTE)
- Nonlinear processes in intensive laser fields (S. Varró, JATE)

⁴JATE: Attila József University, Szeged

⁵ELTE: Loránd Eötvös University, Budapest,

⁶BME: Technical University of Budapest

Beam technologies (I. Kertész, N. Kroó, BME)

Laboratory practice and seminars

- Statistical physics seminar (A. Sütő, ELTE)
- Seminar for materials science (G. Lendvai* and I. Vincze, ELTE)
- Seminar for solid state physics and materials science (L. Sasvári and I. Vincze, ELTE)
- Basic experimental physics (L. Gránásy, BME)
- Experiments on liquid crystals (Á.Buka, ELTE)
- Advanced solid state physics (G. Kriza, G. Mihály, ELTE, BME)
- NMR spectroscopy (K. Tompa)
- Electrodynamics seminar (G. Kriza, BME)
- Laser optical measurements (T. Bereczki, K. Szõcs, BME)
- Experimental neutron physics (S. Borbély, L. Rosta, BME)

Diploma works

- P. Varga (BME): Resistivity and Hall-effect in superconducting cuprates (consultant: A. Virosztek)
- Sz. Varga (JATE): Isostructural phase transitions (consultant: F. Iglói)
- Cs. Bosnyák (ELTE): Electronic structure of metal surfaces (consultant: J. Kollár)
- V. Sándor (ELTE): d-type superconductivity (consultant: I. Tüttő)
- V. Csapó (ELTE): Superconductivity in SDW materials (consultant: I. Tüttõ)
- A. Király (ELTE): Alignment of columnar liquid crystals (consultant: A. Jákli)
- P.Tóth (ELTE/Bayreuth): Electroconvection in homeotropic nematic liquid crystals (consultant: Á.Buka)
- E. Szabó (ELTE): Study of ferroelectric liquid crystal mixtures (consultant: K. Fodor-Csorba)
- T. Becsei (ELTE): Giant magnetoresistance in Ni-Cu/Cu multilayers (consultant: I. Bakonyi)
- B. Pula (ELTE): Investigation of low-temperature electrical transport properties of nanocrystalline metals (consultant: I. Bakonyi)
- Do Thanh Son (BME): Backscattered electron signal control by computer (consultant: L. Pogány)
- B. Alföldi (ELTE): Multicomponent spin-spin relaxation and consequences in tomography (consultant: K. Tompa)

Ph. D. students

P. Lajko: Statistical physics of non-periodic Ising models (Supervisor: F. Iglói)

- F. Szalma: Statistical physics of interfaces on lattices (Supervisor: F. Iglói)
- Ö. Legeza: Ground state and excitations in ladder like magnetic systems (supervisor: J. Sólyom)
- L. Vitos: The full charge density method (Supervisor: J. Kollár)
- 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)
- T. Pusztai (ELTE): X-ray diffraction study of fullerene compounds (consultant: G. Faigel)
- 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)
- 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)
- Said H. Moustafa: Amorphous carbon thin layers; structure and macroscopic physicals properties (supervisor: M. Koós)
- L. Szalai: Investigation of hollow cathode metal ion lasers (Supervisors: K. Rózsa and Z. Donkó)

Dissertations

- L.K. Varga: Conduction band s and d electrons in amorphous transition-metalmetalloid alloys (Candidate of Physical Science, Hungarian Academy of Sciences)
- L. Pogány: Materials research by SEM (Candidate of Technical Science, Hungarian Academy of Sciences)
- E. Tóth-Kádár: Electrochemical preparation of metals and alloys with unique properties and structure (Ph.D., JATE)

- P. Kamasa: Design and development of a method for sensitivity enhancement of broad-line NMR spectrometer using digital phase sensitive detection (Ph.D., A. Mickiewicz University, Poznan, Poland)
- Gy. Török: Neutron diffraction structure determination of MBBA and EBBA liquid crystalline materials using Rietveld method (Candidate of Physical Science, Hungarian Academy of Sciences)
- Z. Donkó: Modeling of the cathode region of glow discharges (Candidate of Physical Science, Hungarian Academy of Sciences)

TABLE of CONTENTS

PREFACE	1
KEY FIGURES	2
A. STRONGLY CORRELATED SYSTEMS	5
B. COMPLEX SYSTEMS	8
C. ELECTRONIC STATES IN SOLIDS	10
D. NON-EQUILIBRIUM ALLOYS	14
E. X-RAY DIFFRACTION	19
F. CHARGE- AND SPIN-DENSITY WAVES	24
G. LIQUID CRYSTAL RESEARCH	26
H. INSTABILITIES AND NONLINEAR PHENOMENA IN LIQUID CRYSTALS	29
I. METAL PHYSICS	32
J. METALLURGY AND MAGNETISM	36
K. NON-DESTRUCTIVE EVALUATION	40
L. NEUTRON SCATTERING IN CONDENSED MATTER	41
M. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER	45
N. LASER PHYSICS	48
O. LASER APPLICATION	53
P. OPTICAL THIN FILMS	57
EDUCATION	60