

# Wigner RCP 2012

Annual Report

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Hungarian Academy of Sciences  
Budapest, Hungary  
2012



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Konkoly Thege Miklós út 29-33  
H-1121 Budapest  
Hungary

Mail: POB 49, H-1525 Budapest, Hungary  
Phone: +36 (1) 392-2512  
Fax: +36 (1) 392-2598  
E-mail: [titkarsag@wigner.mta.hu](mailto:titkarsag@wigner.mta.hu)  
<http://wigner.mta.hu>

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Wigner RCP 2012 – Annual Report  
Edited by V. Blázsik-Kozma, G. Konczos, G. Kriza, B. Selmeci, E. Szilágyi, and P. Ván  
*Closed on 8 December, 2012*

## ***Dear Reader,***

You are holding in your hand the first volume of a prospectively long series of Annual Reports published by the recently established Wigner Research Centre for Physics of the Hungarian Academy of Sciences (MTA Wigner RCP). Our research centre has been founded on 1<sup>st</sup> January 2012, as part of the reorganization of the academic research network. The MTA KFKI Research Institute for Particle and Nuclear Physics (RMKI) and the MTA Research Institute for Solid State Physics and Optics (SZFKI) were merged into this centre, following the decision of the MTA General Assembly on the 5<sup>th</sup> December 2011.

One of the “most problematic” issues was the name of our new research centre. Since so many disciplines were hosted in the above two institutes, listing all of them in a long name seemed pointless. The comforting solution was simple: Eugene P. Wigner, the widely known Hungarian-born genius, a modest and humble physicist of the 20<sup>th</sup> century could hallmark our institution. This idea received strong support from the family of Prof. Wigner. Being Wigner Research Centre for Physics means an honour and a service melded into a scientific mission fit for the 21<sup>st</sup> century. Many people remarked that such a weight might be too heavy for us – but real physicists are continuously looking for real challenges. During the past year our colleagues proved to be capable of fulfilling such a mission in several areas, maintaining scientific research in certain fields of physics and in related interdisciplinary fields at the level of the world’s leading research institutions. Although there is room for further alteration, but we want to move with caution, preserving our values and research-centred philosophy.

To summarize this first year: indeed it was difficult. We were running with a shrunk, reorganized, relocated Wigner Financial Department. Many thanks to the leaders and the members of this Department for serving the scientific community persistently. The renewal of the logistic groups is a time-consuming process. Finally we should not forget about the anxiety of people arising from any restructuring at times when world-wide financial turmoil is surrounding us.

Since two institutes with similar missions, similar structures, and similarly excellent people sharing similar scientific values united in the Wigner RCP, we expected a relatively fast and flawless merger concerning the scientific part, and, indeed, this is what we witnessed throughout the past year. If scientific activities are not compromised, it means that management work has been executed well. This volume displays the reassuring result. The Reader may get an impression on the potential of our research groups. The message is clear: these groups are willing to move along the lines of excellence, success, and sustainability. Furthermore, most of the groups have the ability to act on the European stage, to win tenders, and secure the financial background of their research. Next year will be crucial to reinforce these teams. The successful accomplishment depends on the people. The list on the following page with governmental and scientific awards demonstrates clearly that Wigner’s name is already in good hands, and we are looking forward to constructing a remarkable scientific centre here in Csillebérc – following the 60-year tradition of KFKI, including the last 20 years of RMKI and SZFKI, the two predecessor institutes.

I thank every Wigner researcher and staff member their last year’s efforts and their contribution to this Report. I wish them a more relaxed 2013 with plans fulfilled and successful work which will strengthen our research activities, and even open up new directions.

I ask the Reader to browse the Annual Report with an open mind, and if you are interested in physics and science, I am sure you will find novelties satisfying your taste.

Budapest, 8 December 2012

***Lévai Péter József***  
Director General

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## AWARDS AND PRIZES

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### Awards of the State of Hungary and Government of Hungary

T.S. Biró (RMI), Officer's Cross of the Order of Merit of Hungary (civil division), 2012  
Gy. Farkas (SZFI), Officer's Cross of the Order of Merit of Hungary (civil division), 2012  
D. Horváth (RMI), Széchenyi Prize, 2012  
L. Keszthelyi (RMI), Commander's Cross of the Order of Merit of Hungary (civil division), 2012  
N. Kroó (SZFI), Hungarian Heritage Award, 2012  
N. Kroó (SZFI), Lánchíd Award for Contribution to the International Relations of Hungary, 2012

### Awards of the Hungarian Academy of Sciences

I. Dézsi (RMI), Eötvös József Laurel Wreath, Hungarian Academy of Sciences, 2012  
L. Diósi (RMI), Academic Prize, Hungarian Academy of Sciences, 2012  
P. Hartmann (SZFI), Bolyai János Plaque of MTA, 2012  
P. Kostka (RMI), Mention of the Secretary General of MTA, 2012  
É. Kováts (SZFI), Award for Young Scientists of MTA, 2012  
T. Pusztai (SZFI), Physics Prize of MTA, 2012

### International Awards

T. Csörgő (RMI), State Alumni Member of the Month, USA State Department, February 2012  
S. Varró (SZFI), DAAD Professorship, Deutsche Akad. Ausstausch Dienst, Germany, 2012  
L. Vitos (SZFI), Lindbomska Award 2012 of the Royal Academy of Science, Stockholm, Sweden

### Professional Awards

J. Bakos (RMI), Medal of the Roland Eötvös Physical Society, 2012  
G.G. Barnaföldi (RMI), Jánossy Lajos Prize, Roland Eötvös Physical Society, 2012  
D. Dunai (RMI), In Memoriam Simonyi Károly Plaque, Hungarian Nuclear Society, 2012  
P. Hartmann (SZFI), Budó Ágoston Prize, Roland Eötvös Physical Society, 2012  
I. Korolov (SZFI), Applied Research Prize, Wigner RCP SZFI, 2012  
K. Kutasi (SZFI), Annual Publication Prize, Wigner SZFI, 2012  
G.Zs. Tóth (RMI), Györgyi Géza Prize, Wigner RCP RMI, 2012

### Awards of Foundations and Associations

Gy. Bencze (RMI), Wigner Jenő Prize 2012  
T. Csörgő (RMI), Charles Simonyi Research Fellowship, 2012  
J. Kadlecsik (RMI), Hungarnet Prize, 2012  
G. Tóth (SZFI), Junior Prima Prize 2012, Prima Primiissima Foundation, 2012

### “Lendület” (Momentum) Grant of MTA, 2012

Z. Bajnok (RMI)  
Ö. Legeza, (SZFI)  
G. Orbán (RMI)

### Bolyai János Research Scholarship of MTA

G.G. Barnaföldi (RMI), 2009-2012  
G. Bortel (SZFI), 2011-2014  
P. Dombi (SZFI), 2011-2014  
Á. Hegedüs (RMI), 2012-2015  
É. Kováts (SZFI), 2012-2014  
G. Szirmai (SZFI), 2010-2012  
G. Vankó (RMI), 2012-2014  
A. Vukics (SZFI), 2012-2014

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**CONTENTS**

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**KEY FIGURES AND ORGANIZATIONAL CHART**..... 1

**RESEARCH** .....3

**INSTITUTE FOR PARTICLE AND NUCLEAR PHYSICS**..... 3

        R-A. Field Theory .....4

        R-B. Heavy-ion physics ..... 7

        R-C. Gravitational physics ..... 11

        R-D. Femtoscopy ..... 14

        R-E. Theoretical neuroscience and complex systems ..... 17

        R-F. Hadron physics at CERN SPS and LHC ..... 19

        R-G. Particle detector research and development ..... 25

        R-H. New physics at CERN ..... 28

        R-I. Space physics ..... 34

        R-J. Space technology ..... 37

        R-K. X-ray spectroscopy ..... 40

        R-L. Magnetic thin films ..... 42

        R-M. Ion beam physics ..... 44

        R-N. Non-destructive study of cultural heritage objects (CHARISMA) ..... 46

        R-O. High temperature plasma physics ..... 48

        R-P. Low temperature plasma and atom physics in strong laser fields ..... 51

        R-Q. Laboratory of speech technology for rehabilitation (LSTR) ..... 53

**INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS** ..... 55

        S-A. Strongly correlated systems ..... 56

        S-B. Complex systems ..... 61

        S-C. Electronic states in solids ..... 63

        S-D. Semiconductor nanostructures ..... 66

        S-E. Non-equilibrium alloys ..... 69

        S-F. X-ray diffraction ..... 72

        S-G. Complex fluids ..... 76

        S-H. Radiofrequency spectroscopy ..... 80

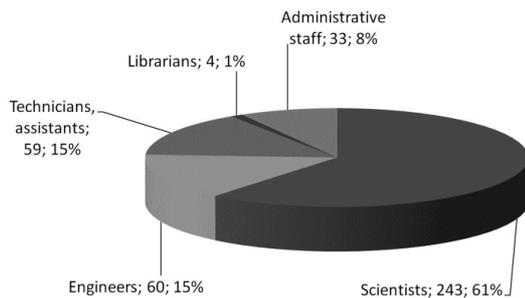
Annual Report 2012

S-I. Electrodeposited nanostructures .....	82
S-J. Metallurgy and magnetism .....	85
S-K. Neutron spectroscopy in condensed matter .....	89
S-L. Neutron scattering .....	93
S-M. Interactions of intense laser fields with matter .....	97
S-N. Gas Discharge Physics .....	101
S-O. Laser applications .....	105
S-P. Femtosecond lasers .....	108
S-Q. Optical thin films .....	111
S-R. Growth and characterization of optical crystals .....	112
S-S. Crystal physics and nonlinear optics .....	114
S-T. Quantum optics and quantum information .....	118
<b>SUPPLEMENTARY DATA</b> .....	123
EDUCATION .....	124
DISSERTATIONS .....	131
MEMBERSHIP .....	132
CONFERENCES .....	140
SEMINARS .....	142

# KEY FIGURES AND ORGANIZATIONAL CHART

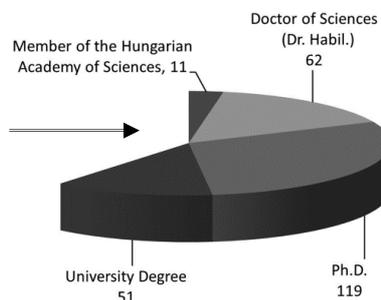
## Permanent staff by profession

Total: 399



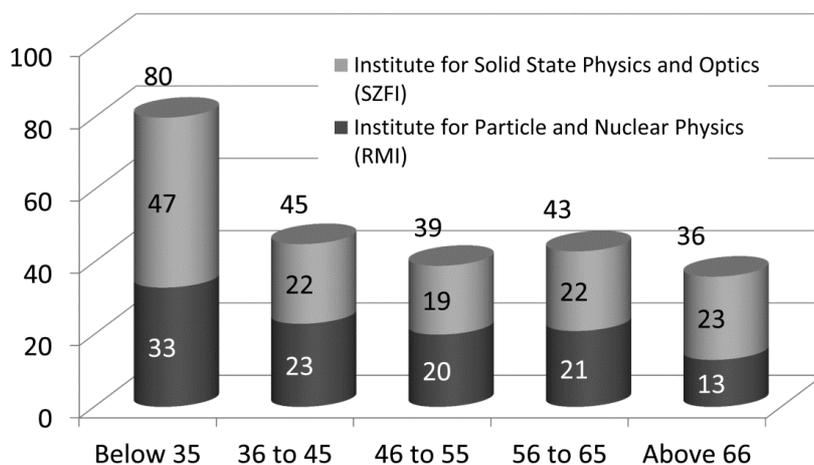
## Scientists by degree/title

Total: 243

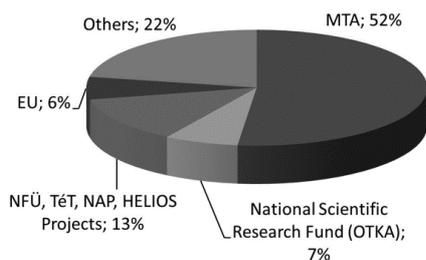


## Scientists by age group

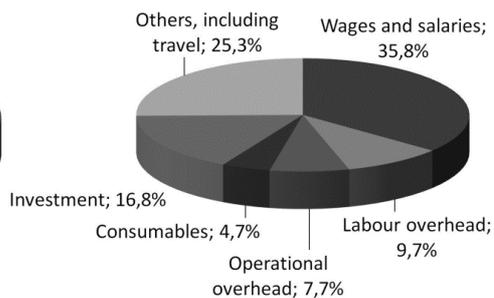
Total: 243



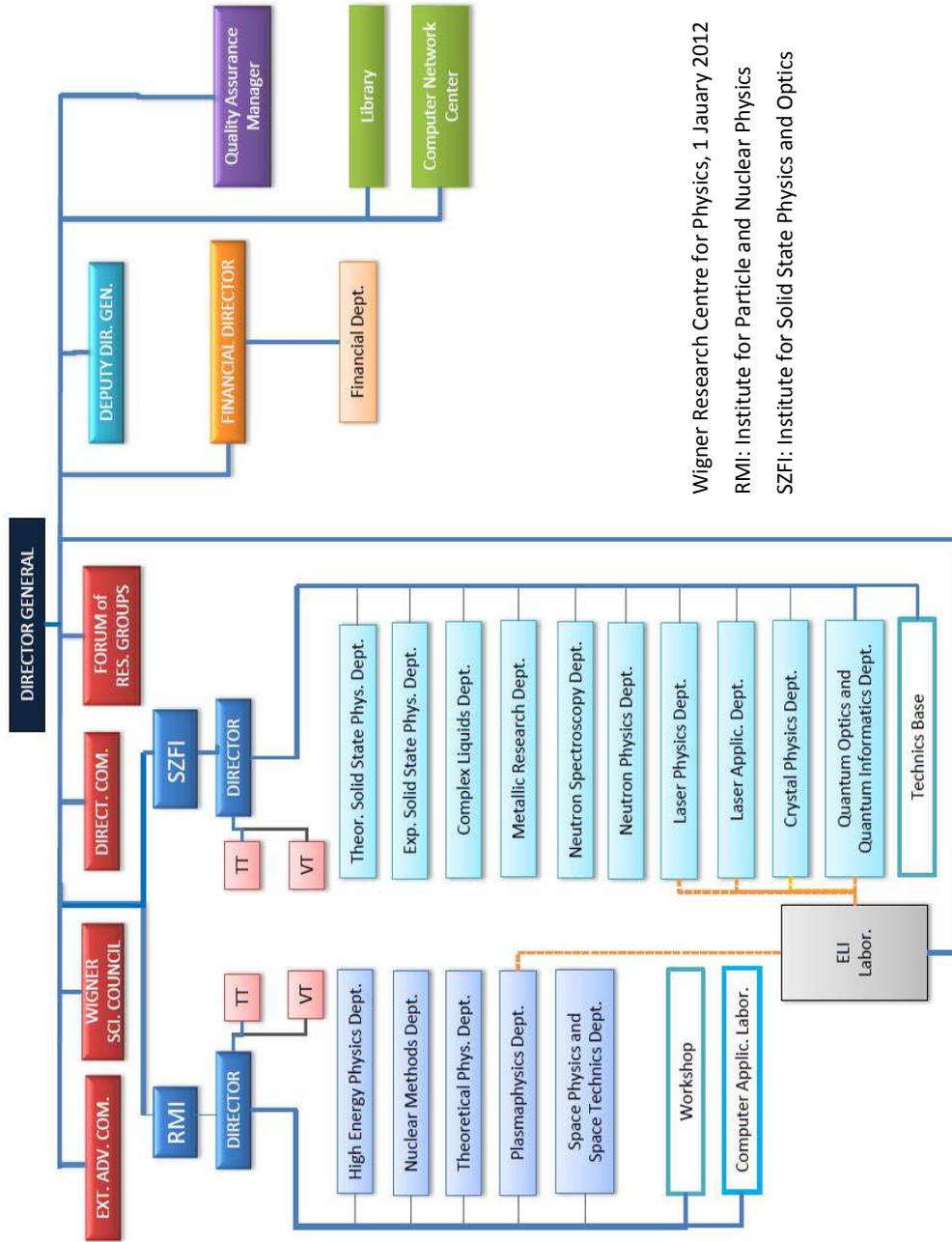
## Income



## Expenditure



Organizational Chart



Wigner Research Centre for Physics, 1 January 2012

RMI: Institute for Particle and Nuclear Physics

SZFI: Institute for Solid State Physics and Optics

**Research**

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**INSTITUTE FOR PARTICLE AND NUCLEAR PHYSICS**

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**R-A. FIELD THEORY**


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*János Balog, Gabriella Böhm, László Fehér, Gyula Fodor, Péter Forgács, Árpád Hegedűs, Tamás Herpay, Árpád Lukács, László Szabados, Kornél Szlachányi, Péter Vecsernyés*

Our field theory group has published results in the following areas: AdS/CFT correspondence and string theory; perturbative field theory; integrable particle interactions; algebraic field theory; general relativity; classical radiation theory.

**AdS/CFT correspondence.** — To verify the famous AdS/CFT conjecture, it is important to solve the so-called spectral problem, which means the exact determination of the energies of string theory, and anomalous dimensions in the dual super Yang-Mills theory. In the planar limit of the conjecture, using integrability techniques, a systematic method was worked out to derive and simplify the Thermodynamic Bethe Ansatz equations, which makes possible the exact determination of the spectrum.

**Nuclear forces from QCD.** — Employing perturbative methods which are applicable due to the property of QCD asymptotic freedom indicating that the interaction among quarks and gluons becomes weak at short distances, we show rigorously that short distance repulsion in three-nucleon forces do indeed emerge. Moreover, we derive functional forms of the repulsions in the limit that distances among three nuclei simultaneously go to zero.

Our results indicate that the Pauli exclusion principle of quarks and one-gluon exchange interactions between quarks induce short distance repulsions among nucleons. This interpretation leads to a general understanding of the short distance repulsions not only in three-nucleon forces, but also in the more fundamental two-nucleon forces. Our analysis can also be generalized to the case including hyperons made of strange quarks in addition to up and down quarks. This generalization is important since hyperons are expected to appear in the high-density state realized at the core of neutron stars.

**Ruijsenaars-Schneider models.** — We treat the trigonometric Ruijsenaars-Schneider model on the basis of quasi-hamiltonian reduction which connects this integrable particle system with the moduli space of  $SU(n)$  Yang-Mills fields on the punctured torus. The (compactified) phase space of this system is identified with the equivalence classes of flat  $SU(n)$  connections; the particle coordinates and action variables correspond to certain invariants of Wilson loops calculated along non-trivial cycles of the torus. This provides a natural interpretation of the Ruijsenaars self-duality transformations as the natural geometric action of the standard  $S$  element in the  $SL(2, \mathbb{Z})$  torus mapping group.

**Skew-monoidal categories.** — We introduced the notion of skew-monoidal categories. They are categories with a “skew-tensor product” and “skew-tensor unit” such that the associativity, left unit, and right unit constraints are not necessarily invertible. They are, however, required to obey the usual coherence axioms of a monoidal (i.e., tensor) category. The surprising result is that R-bialgebroids are in bijection with closed skew-monoidal structures on the category of one-sided R-modules (which does not possess any ordinary monoidal structure in general) with skew-monoidal unit being the regular R-module R. Extracting (co)representation theory of the bialgebroid H from the skew-monoidal category is very easy.

**Total mass in closed universes.** — A non-negative expression, built from the norm of the 3-surface twistor operator and the energy-momentum tensor of the matter fields on a spacelike

hypersurface, is found which, in the asymptotically flat/hyperboloidal case, provides a lower bound for the ADM/Bondi–Sachs mass, while on closed hypersurfaces it gives the first eigenvalue of the Sen–Witten operator. Also in the closed case, its vanishing is equivalent to the existence of non-trivial solutions of Witten’s gauge condition. Moreover, it is vanishing if and only if the closed data set is in a flat spacetime with toroidal spatial topology. Thus it provides a positive definite measure of the strength of the gravitational field (with physical dimension mass) on closed hypersurfaces, i.e. some sort of the total mass of closed universes.

**Radiation reaction force.** — We have computed the equations of motion of a spherically symmetric charged shell of radius  $R$ , taking into account the radiation reaction force exerted by the shell’s own electromagnetic field up to  $O(R^2)$ . In particular, we have shown that the authors of Phys. Rev. Lett. **105** (2010) 094802 are in error in their claim that the known result for the self force of the shell, as can be found, e.g. in Jackson’s textbook, be incorrect.

## GRANTS AND INTERNATIONAL COOPERATION

- OTKA K 83267 Relativistic particle systems (J. Balog, 2011-2015)  
 OTKA K 77400 Integrable many-body and field theoretic models (L. Fehér, 2009-2013)  
 OTKA K 101709 Nonlinear interactions of waves and particles in field theories with applications in astrophysics and cosmology (P. Forgács, 2012-2016)  
 OTKA K 68195 Algebraic methods in models of quantum field theory (K. Szlachányi, 2007-2012)

## PUBLICATIONS

### Articles

1. Balog J, Hegedűs Á; Hybrid-NLIE for the AdS/CFT spectral problem; *JHEP*; **1208**, 022/1-66, 2012
2. Balog J, Hegedűs Á; Quasi-local formulation of the mirror TBA; *JHEP*; **1205**, 039/1-13, 2012
3. Aoki\* S, Balog J, Weisz\* P; Short distance repulsion in 3 nucleon forces from perturbative QCD; *New Journal of Physics*; **14**, 043046/1-19, 2012
4. Fehér L, Klimcik\* C; Self-duality of the compactified Ruijsenaars-Schneider system from quasi-Hamiltonian reduction; *Nucl Physics*; **B860**, 464-515, 2012
5. Fehér L, Klimcik\* C; On the spectra of the quantized action variables of the compactified Ruijsenaars-Schneider system; *Theor Math Phys*; **171**, 704-714, 2012
6. Szlachányi K; Skew-monoidal categories and bialgebroids; *Advances in Mathematics*; **231**, 1694-1730, 2012
7. Szabados L; Mass, gauge conditions and spectral properties of the Sen-Witten and 3-surface twistor operators in closed universes; *Class Quant Grav*; **29**, 095001/1-34, 2012
8. Forgács P, Herpay T, Kovács P; Comment on “Finite Size Corrections to the Radiation Reaction Force in Classical Electrodynamics”, *Phys Rev Lett*; **106**, 029501/1-1, 2012
9. Balog J, Niedermayer\* F, Pepe\* M, Weisz\* P, Wiese\* U-J; Drastic Reduction of Cutoff Effects in 2-d Lattice O(N) Models; *JHEP*; **11**, 140-179, 2012

*Conference proceeding*

10. Forgács P, Herpay T, Kovács P; Massive scalar self-interaction in curved background space-time and its application to proton-pion interaction; In: *Proc. The Twelfth Marcel Grossmann Meeting (Paris, France, July 12-18, 2009)*; Eds.: T. Damour, RT Jantzen, R. Ruffini, World Scientific, Singapore; pp. 851-853, 2012

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## R-B. HEAVY-ION PHYSICS

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*Tamás Sándor Biró, Gergely Gábor Barnaföldi, Tamás Fülöp, Miklós Horváth, Péter Kovács, Péter Lévai, Etele Molnár, Péter Ván, György Wolf, Károly Ürmössi, Miklós Zétényi*

Our group conducts theoretical research both in fundamental questions and more practical ones related to phenomenology. In the past year we faced with the basic problems of chiral symmetry restoration in hadronic media and discussed questions of new entropy formulas by applying advanced statistical physics methods. In the followings we group our activities according to the research topics we are presently pursuing.

**Relativistic hydrodynamics and kinetic theory.** — Relativistic hydrodynamics is applied to calculations of seeking for observable consequences of collective behavior in different properties of experimental particle spectra. It has both methodological and fundamental questions to settle. We have developed a first order and stable theoretical approach to relativistic dissipative fluids, circumventing the traditional Israel-Stewart second order approach. The relaxation dynamics of linear transport coefficients, like viscosity and heat conductivity, was shown to damp perturbations by our method. The Boltzmann-like kinetic theory and its non-extensive generalization also generate a dissipative hydrodynamical description. We studied the 14-moment Grad method and extended the usual derivation of hydrodynamical equations to a non-extensive Boltzmann equation. The latter uses an Ansatz defined by the  $q$ -exponential of the sum of  $q$ -logarithms instead of the original factorized form. Here  $q$ -exponential and  $q$ -logarithm are (Euler) power-law generalizations of the exponential and logarithm functions, widely used in the non-extensive context.

**Thermodynamics.** — Nonrelativistic continuum thermodynamics is a theoretical framework for classical continua, including heat conduction, continuum mechanics or electrodynamics. In our recent research we have derived unique measures of finite deformation and plasticity with a relativity motivated formulation of frame independence in nonrelativistic spacetime. We have also analysed the thermodynamic requirements of weakly nonlocal extensions of the Fourier type heat conduction, and obtained a common generalization of several known heat conduction equations like the Green-Naghdi or Gruyer-Krumhansl ones.

High-energy particle spectra were fitted by models based on thermal concepts, including different statistical models for jet-fragmentation in  $e+e-$  collisions and power-law tails observed in transverse momentum spectra in relativistic gold-gold and lead-lead nuclear collisions. Different possibilities of generalized non-additive thermostatistical theories were investigated.

**Unruh-like effects in semiclassical fields.** — The multiple successes of hydrodynamics in describing relativistic heavy-ion collisions and the interpretation of particle spectra in terms of an underlying temperature for a common fireball fascinate researchers since decades of research. We traced down the idea that a simple and long term acceleration may cause pseudo-thermal effects akin to the Unruh effect by calculating gamma photon spectra semiclassically, stemming from constantly accelerated point charges. Using the classical textbook formula, the radiation can be obtained with an exponential-dominated tail at high

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# PhD student

perpendicular momenta. This spectrum can be re-interpreted by a Fourier analysis as mimicking Unruh temperatures; a thermal-looking effect without the presence of any heat bath. In addition a hydrodynamic flow pattern is also simulated: for long term constant acceleration a Bjorken-flow, for short term acceleration the Landau hydrodynamics.

**Chiral symmetry restoration.** — The chiral symmetry is broken in the vacuum and restored both at high temperatures and high densities. We studied the signals of such a transition – most prominently a change in the basic properties of the particles. Based on a finite temperature generalization of the Witten-Veneziano formula, we concluded that the axial U(1) chiral symmetry breaking generated mass of  $\eta'$  is quenched in about the same proportion as the chiral quark condensate itself.

**Hadron phenomenology.** — The quark structure of mesons, especially the scalar ones, is not always straightforward. Our group, in collaboration with colleagues from the University of Frankfurt, developed an SU(3) symmetric linear sigma model including the scalar, pseudo scalar, vector, and axial vector mesons. In this model they could show that the quark-antiquark scalar states are the ones between 1 and 1.7 GeV, the scalars below 1 GeV are probably tetraquark states.

**Nuclear shadowing in heavy ions.** — We have predicted the size of the shadowing effect in p+Pb collisions applying DGLAP evolution in the nuclear shadowing function. Recent data from CERN LHC p+Pb experiments at 5.02 TeV energy validate our theoretical calculation and prove the existence of jet energy loss in hot dense deconfined matter in heavy ion collisions.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA NK77816 Theoretical and experimental investigation of high energy particle production in the CERN LHC ALICE experiment (P. Lévai, 2009-2013)

OTKA NK106119 Attometer physics phenomena: theoretical and experimental studies at the CERN LHC ALICE experiment (P. Lévai, 2012-2016)

OTKA PD73596 Jet fragmentation and end point effects in heavy ion collisions in RHIC and LHC energies (G.G. Barnaföldi, 2009-2012)

OTKA K71989 Nuclear matter in extreme condition at the FAIR (GSI Darmstadt) accelerator (Gy. Wolf, 2008-2013)

OTKA K81161 Experimental and theoretical investigation of heat conduction (Consortium leader: P. Ván, 2010-2014)

OTKA K104260 Particles and intense fields (Consortium leader: T.S. Biró, 2012-2016)

HIC for FAIR program participation with Frankfurt University, FIAS and GSI Darmstadt (T.S. Biró, Gy. Wolf)

HUNGARIAN–SOUTH-AFRICAN T&T Grant No. 10-1-2012-0061, MAG Zrt. Tender for Innovation, (Hungarian leader: T.S. Biró, South-African leader: A. Muronga, 2011-2013)

CERN ALICE, Barnaföldi G.G. (Wigner group leader) and Lévai P.

CERN ALICE VHMPID upgrade project, Barnaföldi G.G. (Wigner group leader)

**LONG TERM VISITORS**

- N. Mitsui, Research Center for Seismology, Volcanology and Disaster Mitigation, Graduate School of Environmental Studies, Nagoya University, Nagoya University, Japan, August 3-December 31, 2012 (host: P. Ván)
- M. Gyulassy, Columbia University, USA, August 1-31, 2012

**PUBLICATIONS***Articles*

1. Barnaföldi GG, Hamar G, Melegh<sup>\*</sup> HG, Oláh<sup>\*</sup> L, Surányi<sup>\*</sup> G, Varga<sup>\*</sup> D; Portable cosmic muon telescope for environmental applications; *Nuclear Instruments & Methods in Physics Research, Section A-Accelerators Spectrometers Detectors and Associated Equipment*; **689**, 60-69, 2012
2. Barnaföldi GG, Barrette<sup>\*</sup> J, Gyulassy M, Lévai P, Topor Pop<sup>\*</sup> V; Predictions for p + Pb at 4.4A TeV to test initial-state nuclear shadowing at energies available at the CERN Large Hadron Collider; *Phys Rev C*; **85**, 024903/1-7, 2012
3. Oláh L, Barnaföldi GG, Hamar G, Melegh HG, Surányi G, Varga D; CCC-based muon telescope for examination of natural caves; *Geosci Instrum Method Data Syst Discuss*; **2**, 781-800, 2012
4. Biró TS, Molnár E; Fluid dynamical equations and transport coefficients of relativistic gases with non-extensive statistics; *Phys Rev C*; **85**, 024905, 2012
5. Biró TS, Ürmössy K, Ván P, Barnaföldi GG, Schram<sup>\*</sup> Zs; Non-extensive statistical model for strange and non-strange hadron spectra at RHIC and LHC energies; *Acta Physica Polonica B*; **43**, 811-820, 2012
6. Biró TS, Gyulassy M, Schram<sup>\*</sup> Zs; Unruh gamma radiation at RHIC?; *Phys Lett B*; **708**, 276-279, 2012
7. Fülöp T, Ván P; Kinematic quantities of finite elastic and plastic deformations; *Mathematical Methods in the Applied Sciences*; **35**, 1825-1841, 2012
8. Denicol<sup>\*</sup> GS, Niemi<sup>\*</sup> H, Molnár E, Rischke<sup>\*</sup>; Derivation of transient relativistic fluid dynamics from the Boltzmann equation; *Phys Rev D*; **85**, 114047/1-22, 2012
9. Niemi<sup>\*</sup> H, Denicol<sup>\*</sup> GS, Huovinen<sup>\*</sup> P, Molnár E, Rischke<sup>\*</sup> DH, Influence of a temperature-dependent shear viscosity on the azimuthal asymmetries of transverse momentum spectra in ultrarelativistic heavy-ion collisions; *Phys Rev C*; **86**, 014909/1-13, 2012
10. Ürmössy K, Barnaföldi GG, Biró TS; Microcanonical Jet-fragmentation in proton-proton collisions at LHC Energy; *Phys Lett B*; 28942/1-7, 2012
11. Ürmössy K, Barnaföldi GG, Biró TS; Generalised microcanonical statistics and fragmentation in electron-positron collisions; *Acta Phys Polon B Supp*; **5/2**, 363-368, 2012
12. Ván P, Biró TS; First order and stable relativistic dissipative hydrodynamics; *Phys Lett B*; **709**, 106-110, 2012

13. Ván P, Fülöp T; Universality in heat conduction theory: weakly nonlocal thermodynamics, *Annalen der Physik*; **524**, 470-478, 2012
14. Deák\* F, Ván P, Vásárhelyi\* B; Hundred years after the first triaxial test; *Periodica Polytechnica- Civil Engineering*; **56**, 115-122, 2012
15. Ván P, Gróf\* Gy; What is thermodynamics and what is it for?; *INDECS - Interdisciplinary Description of Complex Systems*; **10**, 66-72, 2012
16. Wolf Gy, Kämpfer\* B, Zétényi M; Propagation of spectral functions and dilepton production at SIS energies, *Physics of Atomic Nuclei*; **75**, 718-720, 2012
17. Kwon\* Y, Lee\* SH, Morita\* K, Wolf Gy; Renewed look at eta' in medium; *Phys Rev D*; **86**, 034014/1-6, 2012

**Conference proceedings**

18. Berényi\* D, Lévai P, Skokov\* V; Simulation of pair production in extreme strong EM fields; In: *Proc. Light at Extreme Intensities 2011 (Szeged, Hungary, 14-18 November 2011)*; AIP Conference Proceedings, **1462**, 5-8, 2012

**Books, book chapters**

19. Fülöp, T., Egytengelyű eredő reológia, és relaxáció, mint deviatorikus kúszás (Uniaxial rheology as deviatoric creep, in Hungarian), In: *A képlékenység termodinamikájáról*, ed. Asszonyi Cs, Hungarian Printing House, Budapest, **13**, Mérnökgeológia-Kőzetmechanika Kiskönyvtár, 23-29, 2012
20. Asszonyi\* Cs, Szarka\* Z, Csatár\* A, Horváth\* R., Kocsis\* D., Ván P.; Tömör anyagok képlékeny deformációjáról (On the plastic deformation of dense solids, in Hungarian); In: *A képlékenység termodinamikájáról*, ed. Asszonyi Cs, Hungarian Printing House, Budapest, **13**, Mérnökgeológia-Kőzetmechanika Kiskönyvtár, 9-21, 2012
21. Asszonyi\* Cs, Doležalova\* M, Ván P, Vásárhelyi\* B; Gondolatok a porózus és töredezett anyagok mechanikai viselkedésének megértéséhez (Toward the understanding of mechanical properties of porose and cracked materials, in Hungarian); In: *A képlékenység termodinamikájáról*, ed. Asszonyi Cs, Hungarian Printing House, Budapest, **13**, Mérnökgeológia-Kőzetmechanika Kiskönyvtár, 9-21, 2012
22. Asszonyi\* Cs, Szarka\* Z, Doležalova\* M, Ván P; Porózus és töredezett anyagok reológiai viselkedése (Rheological properties of porose and cracked materials, in Hungarian) In: *A képlékenység termodinamikájáról*, ed. Asszonyi Cs, Hungarian Printing House, Budapest, **13**, Mérnökgeológia-Kőzetmechanika Kiskönyvtár, 9-21, 2012

*See also R-A.8, R-A.10, R-G.1- R-G.20, R-G.51, R-H.2, R-L.1*

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## R-C. GRAVITATIONAL PHYSICS

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*István Rácz, Péter Csizmadia, Gergely Debreczeni, Máté Ferenc Nagy<sup>#</sup>, Mátyás Vasúth*

The Gravitational Physics Group of RMI is involved in both experimental and theoretical studies of Einstein's theory of gravity. The principal part of our research interest is gravitational wave physics. Our group is involved in the Virgo Scientific Collaboration operating the European Virgo gravitational wave observatory. The most important contributions of our group members are as follows:

- Playing leading role in creating and maintaining a data transfer channel making possible the online data sharing between the LIGO and Virgo scientific collaborations.
- Developing the numerical packages *GridRipper* and *CBwaves* aimed at providing accurate waveforms for data analysis.
- Our engineers have been involved in modeling and realization of various parts of the vacuum system of the Advanced Virgo detector.
- Adaptation of graphical processing unit (GPU) technology to data analysis and development of new search algorithms to analyze the noisy data of the LIGO and Virgo detectors.
- Development of pilot packages for the Compact Binary Coalescence (CBC) group in the LIGO and Virgo collaborations aimed at creating various gravitational wave template banks and subsequent data analysis with computer clusters consisting of both CPUs and GPUs.

***CBwaves* software.** — The numerical package *CBwaves* models the gravitational radiation of binary systems with possibly spinning components on highly eccentric orbits. The code simultaneously determines the evolution of the binary system and the emitted gravitational waves within the post-Newtonian approach at the highest level of approximation available in the literature. With the development of this package we intended to provide an efficient tool for the CBC group which is capable of generating spinning and eccentric template banks for an effective detection of such sources. The capabilities of the code suit the needs of the collaboration and we have reported on the possible applications of *CBwaves* at teleconferences, collaboration seminars, and workshops. The software is publicly available, and we have received a request to integrate the software into the data analysis package of the Collaboration.

The software package *CBwaves* (the rpm and deb versions are also available) have been used in numerous applications with an increasing number of new tasks arising within the Collaboration. As an example, recently the decision was made to build *CBwaves* in the LAL/LALsimulation software package of the Collaboration which requires physically reliable gravitational wave templates for the search algorithms of inspiralling compact binary systems. *Cbwaves* will also be incorporated into the program package *GWTools* which is a GPU and OpenCL/C++ based general data analyzing tool under development.

***GridRipper* package.** — The program package *GridRipper* is developed to study the dynamical evolution of different astrophysical systems within the fully non-linear Einstein theory of gravity. The code is designed to be capable of describing in full details a large

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<sup>#</sup> PhD student

variety of gravitational wave production processes and the propagation of the emitted radiation. We are in the phase of implementing Einstein's equations in a gauge which suits the multipolar expansion applied in *GridRipper*.

## GRANTS AND INTERNATIONAL COOPERATION

- OTKA K67942 Study of gravitational wave production in general relativity  
(I. Rácz, 2007-2012)
- OTKA IN77395 Participation in the EGO-VIRGO scientific collaboration  
(I. Rácz, 2009-2012)
- NKTH TÉT\_10\_1\_2011\_0207 Research toward the realization of advanced gravitational wave detectors (M. Vasúth, 2012-2013)
- EGO-DIR-128 VESF Postdoctoral Fellowship (I. Rácz, 2009-2012)

## PUBLICATIONS

### Articles

1. Csizmadia P, Debreczeni G, Rácz I, Vasúth M; Gravitational waves from spinning eccentric binaries; *Class Quantum Grav*; **29**, 245002/1-32, 2012
2. Aasi\* J et al. [LIGO-Virgo Collaboration]; The characterization of Virgo data and its impact on gravitational-wave searches; *Class Quantum Grav*; **29**, 155002/1-41, 2012
3. Abadie\* J et al. [LIGO-Virgo Collaboration]; Upper limits on a stochastic gravitational-wave background using LIGO and Virgo interferometers at 600–1000 Hz; *Phys Rev D*; **85**, 122001/1-14, 2012
4. Abadie\* J et al. [LIGO-Virgo Collaboration]; Search for gravitational waves from low mass compact binary coalescence in LIGO's sixth science run and Virgo's science runs 2 and 3; *Phys Rev D*; **85**, 082002/1-12, 2012
5. Abadie\* J et al. [LIGO-Virgo Collaboration]; Implementation and testing of the first prompt search for gravitational wave transients with electromagnetic counterparts; *A&A*; **539**, A124/1-15, 2012
6. Abadie\* J et al. [LIGO-Virgo Collaboration]; Search for gravitational waves from intermediate mass binary black holes; *Phys Rev D*; **85**, 102004/1-13, 2012
7. Abadie\* J et al. [LIGO-Virgo Collaboration]; All-sky search for gravitational-wave bursts in the second joint LIGO-Virgo run; *Phys Rev D*; **85**, 122007/1-15, 2012
8. Abadie\* J et al. [LIGO-Virgo Collaboration]; First low-latency LIGO+Virgo search for binary inspirals and their electromagnetic counterparts; *A&A*; **541**, A155/1-12, 2012
9. Abadie\* J et al. [LIGO-Virgo Collaboration]; All-sky search for periodic gravitational waves in the full S5 LIGO data; *Phys Rev D*; **85**, 022001/1-19, 2012
10. Accadia\* T et al. [LIGO-Virgo Collaboration]; Characterization of the Virgo seismic environment; *Class Quantum Grav*; **29**, 025005/1-10, 2012
11. Accadia\* T et al. [LIGO-Virgo Collaboration]; A state observer for the Virgo inverted pendulum; *Rev Sci Instrum*; **82**, 094502/1-9, 2012
12. Accadia\* T et al. [LIGO-Virgo Collaboration]; Virgo: a laser interferometer to detect gravitational waves; *JINST*; **7**, P03012/1-124, 2012

**Conference proceedings**

13. Accadia\* T et al. [LIGO-Virgo Collaboration]; The NoEMi (Noise Frequency Event Miner) framework; *J Phys Conf Ser*; **363**, 012037, 1-10, 2012
14. Accadia\* T et al. [LIGO-Virgo Collaboration]; Noise monitor tools and their application to Virgo data; *J Phys Conf Ser*; **363**, 012024, 1-10, 2012
15. Accadia\* T et al. [LIGO-Virgo Collaboration]; Plans for the upgrade of the gravitational wave detector Virgo: advance Virgo, *Proc. The Twelfth Marcel Grossmann Meeting (Paris, France, July 12-18, 2009)*; Eds.: T. Damour, RT Jantzen, R. Ruffini, Singapore: World Scientific; p.1738, 2012
16. Accadia\* T et al. [LIGO-Virgo Collaboration]; Status of the commissioning of the Virgo interferometer; *AIP Conf Proc*; **1446**, 150-158, 2012

**Other**

17. Csizmadia P, Debreczeni G, Rácz I, Vasúth M; Gravitational waves from spinning eccentric binaries; technical note, 2012  
(<http://www.grid.kfki.hu/twiki/bin/view/RmkiVirgo/CBwaves>)
18. Csizmadia P, László A, Rácz I; GridRipper package; technical note, 2012.  
<http://www.rmki.kfki.hu/~gridripper/>

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**R-D. FEMTOSCOPY**


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*Tamás Csörgő, László P. Csernai, László Jenkovszky, Márton I. Nagy, Frigyes Nemes, Béla Lukács, András Ster, János Sziklai, Márton Vargyas, Róbert Vértesi*

**Solutions of (relativistic) hydrodynamics.** — The dynamical development of collective flow is studied in a (3+1)D fluid dynamical model with globally symmetric, peripheral initial conditions, which take into account the shear flow caused by the forward motion on the projectile side and the backward motion on the target side. While at  $\sqrt{s_{NN}} = 2.76$  TeV semi-peripheral Pb+Pb collisions the earlier predicted rotation effect is visible; at more peripheral collisions with high resolution and low numerical viscosity, the initial development of a Kelvin-Helmholtz instability is observed, which alters the flow pattern considerably. This effect provides a precision tool for studying the low viscosity of Quark-gluon Plasma.

**Partial  $U_A(1)$ /chiral symmetry restoration in relativistic heavy ion collisions.** — In  $\sqrt{s_{NN}} = 200$  GeV Au+Au collisions PHENIX reported a significant enhancement in the low-mass region ( $0.1 < m_{ee} < 0.7$  GeV) of the dielectron spectrum, which is still not fully understood. Several theoretical works and an indirect measurement suggest that, due to the possible restoration of the  $U_A(1)$  part of the chiral symmetry in a hot and dense medium, the mass of the  $\eta'$  meson may substantially decrease. We reported on a statistically acceptable description of the PHENIX low-mass dilepton enhancement using a radial flow dominated meson spectra, chain decays of long-lived resonances and an in-medium  $\eta'$  mass modification.

**Neutral pion production in Au+Au collisions at RHIC.** — New results from the 2010 RHIC low energy program show a substantial suppression of neutral pions in central Au+Au collisions at both  $\sqrt{s_{NN}} = 39$  and 62.4 GeV c.m.s. energies. At high  $p_T$  the 62.4 GeV and 200 GeV data follow the same suppression pattern. On the other hand, otherwise successful pQCD predictions do not describe the 39 GeV data. These observations indicate that initial state effects may play a dominant role at smaller c.m.s. energies and at lower  $p_T$ . The azimuthal dependence of the nuclear modification factor  $R_{AA}$  is strongly correlated with the (approximately elliptical) geometry of the overlap region. The dependence of  $R_{AA}$  on the reaction plane, determined up to  $p_T = 20$  GeV/c from 2007 high-luminosity  $\sqrt{s_{NN}} = 200$  GeV Au+Au data provides great selectivity among theories, and favours the ASW scenario with AdS/CFT correspondence over the pQCD-based models.

**Diffraction at LHC.** — Elastic p+p scattering data were analyzed at ISR and LHC energies, utilizing the quark-diquark model of protons in a form proposed by Bialas and Bzdak. The differential cross-section of elastic proton-proton collisions is analyzed in a detailed and systematic manner at small momentum transfers, starting from the energy range of CERN ISR at  $\sqrt{s_{NN}} \sqrt{s} = 23.5$  GeV, including also recent TOTEM data at the present LHC energies at  $\sqrt{s_{NN}} \sqrt{s} = 7$  TeV. These studies confirm the picture that the size of proton increases systematically with increasing energies, while the size of the constituent quarks and diquarks remains approximately independent of (or only increases only slightly with) the colliding energy. The detailed analysis indicates correlations between model parameters and also indicates an increasing role of shadowing at LHC energies. Within the investigated class of models, a simple and model-independent phenomenological relation was discovered that connects the total p+p scattering cross-section to the effective quark, diquark size and their average separation.

**GRANTS AND INTERNATIONAL COOPERATION**

OTKA NK 101438 Search for a critical point and a new domain of QCD using the PHENIX experiment at RHIC and the TOTEM experiment at LHC (T. Csörgő, 2012-2015)

Memorandum of Understanding on multilateral international collaboration signed with the PHENIX experiment at the Relativistic Heavy Ion Collider, Brookhaven National Laboratory, USA, (T. Csörgő, 2002-2016)

Memorandum of Understanding on multilateral international collaboration signed with the TOTEM experiment at the Large Hadron Collider at CERN, the European Research Center for Particle and Nuclear Physics, (T. Csörgő, from 2008)

Memorandum of Understanding on bilateral international collaboration signed with the State University of New York at Stony Brook, NY, USA, with the University of Nijmegen, Nijmegen, The Netherlands and University of Lund, Lund, Sweden, (T. Csörgő, from 2006)

**PUBLICATIONS***Articles*

1. Csernai LP, Skalvik\* AM, Wang\* DJ, Magas\* VK, Stocker\* H, Strottman\* DD, Cheng\* Y, Yan\* YL; Flow components and initial state CM fluctuations; *Acta Phys Polon*; **B43**, 803-810, 2012
2. Zhou\* DM, Limphirat\* A, Yan\* YL, Yun\* C, Yan\* YP, Cai\* X, Csernai LP, Sa\* BH; Higher moment singularities explored by the net proton non-statistical fluctuations; *Phys Rev C*; **85**, 064916/1-5, 2012
3. Csernai LP, Mocanu\* G, Neda\* Z; Fluctuations in hadronizing QGP; *Phys Rev C*; **85**, 068201/1-4, 2012
4. Csernai LP, Eyyubova\* G, Magas\* VK; New method for measuring longitudinal fluctuations and directed flow in ultrarelativistic heavy ion reactions; *Phys Rev C*; **86**, 024912/1-7, 2012
5. Csernai LP, Strottman\* DD, Anderlik\* Cs; Kelvin-Helmholz instability in high energy heavy ion collisions; *Phys Rev C*; **85**, 054901, 2012
6. Jenkovszky LL, Magas\* VK, Londergan\* JT, Szczepaniak\* AP; Explicit model realizing parton-hadron duality; *Int J Mod Phys A*; **27**, 1250157/1-19, 2012
7. Afanasiev\* S. et al. [PHENIX Collaboration]; Measurement of direct photons in Au+Au collisions at  $\sqrt{s_{NN}}=200$  GeV; *Phys Rev Lett*; **109**, 152302, 2012
8. Adare\* A. et al. [PHENIX Collaboration]; Direct-photon production in p+p collisions at  $\sqrt{s}=200$  GeV at midrapidity; *Phys Rev D*; **86**, 072008, 2012
9. Adare\* A et al. [PHENIX Collaboration]; Evolution of  $\pi^0$  suppression in Au+Au collisions from  $\sqrt{s_{NN}}=39$  to 200 GeV; *Phys Rev Lett*; **109**, 152301, 2012

10. Adare\* A et al. [PHENIX Collaboration]; Nuclear-modification factor for open-heavy-flavor production at forward rapidity in Cu+Cu collisions at  $\sqrt{s_{NN}}=200$  GeV; *Phys Rev C*; **86**, 024909, 2012
11. Adare\* A et al. [PHENIX Collaboration]; Deviation from quark-number scaling of the anisotropy parameter  $v_2$  of pions, kaons, and protons in Au+Au collisions at  $\sqrt{s_{NN}}=200$  GeV; *PhysRev C*; **85**, 064914, 2012
12. Adare\* A et al. [PHENIX Collaboration]; Observation of direct-photon collective flow in  $\sqrt{s_{NN}}=200$  GeV Au+Au collisions; *Phys Rev Lett*; **109**, 122302, 2012
13. Adare\* A et al. [PHENIX Collaboration]; Ground and excited charmonium state production in p+p collisions at  $\sqrt{s}=200$  GeV; *PhysRev D*; **85**, 092004, 2012
14. Antchev\* G et al. [TOTEM Collaboration]; Measurement of the forward charged particle pseudorapidity density in pp collisions at  $\sqrt{s}=7$  TeV with the TOTEM experiment; *Europhys Lett*; **98**, 31002, 2012
15. Csörgő T et al. [TOTEM Collaboration]; Elastic scattering and total cross-section in p+p reactions measured by the LHC Experiment TOTEM at  $\sqrt{s}=7$  TeV; *Prog Theor Phys; Suppl.* **193**, 180-183, 2012
16. G. Abbiendi et al. [OPAL Collaboration]; Search for charged Higgs bosons in  $e^+e^-$  collisions at  $\sqrt{s}=189$ -209 GeV; *Eur Phys J C*; **72**, 2076, 2012
17. Nemes F, Csörgő T; Detailed analysis of p+p elastic scattering data in the quark-diquark model of Bialas and Bzdak from  $\sqrt{s}=23.5$  GeV to 7 TeV; *Int J Mod Phys A*; **27**, 1250175/1-26, 2012

**Conference proceedings**

17. De Kock\* MB, Eggers\* HC, Csörgő T; From chi2-squared to Bayesian model comparison and Levy expansions of Bose-Einstein correlations in  $e^+e^-$  reactions; In: *Proc. The Seventh Workshop on Particle Correlations and Femtoscopy (WPCF2011, Tokyo, Japan, Sept. 20-24, 2011, ed. T.Hirano)*; Published by Proceedings of Science (a service of SISSA) **154**, 33, 2012 (e-Print: arXiv:1206.1680 [nucl-th])

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**R-E. THEORETICAL NEUROSCIENCE AND COMPLEX SYSTEMS**


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*Fülöp Bazsó, Mihály Bányai,<sup>#</sup> Dorottya Cserpán,<sup>#</sup> Péter Érdi, László Négyessy, Zoltán Somogyvári, Balázs Ujfalussy, László Zalányi*

**Microelectric imaging techniques.** — One of the main obstacles to decipher the information processing and the neural communication in the brain is the lack of any experimental technique which is able to measure the spatio-temporal distribution of synaptic currents on individual neurons in freely behaving animals. Thus, we developed a new micro electric imaging technique which is able to determine the currents flowing on single neurons during action potentials. Our results show that by using new mathematical source localization methods and high density, chronically implanted micro electrode arrays, fine details of initiation and spatio-temporal dynamics of neural action potentials can be revealed, which was not directly observable before. The new method will provide better description of cortical microcircuits and their dynamics, which is essential for the understanding of their computation and helps to bridge the gap between the microscopic and the macroscopic neuro-electric phenomena.

**Tactile functions of the cerebral cortex.** — Tactile information acquired by the fingers via e.g. haptic exploration, is transmitted to the somatosensory cortex where this information is processed and integrated for perception and other behavioral purposes. In the primate somatosensory cortex the hand and particularly the fingers, the primary sensory organ of touch, has well-defined representations as part of the so called “homunculus”. Accordingly, topographically organized cortical territories are dedicated to the processing of information originating from the individual fingers with the finger tips having disproportionately large representations. The aim of our studies is to understand how information is integrated, i.e., how coherent perceptual representations are formed, in such a distributed system. Our results indicate that global tactile percepts which are assumed to emerge at high stage of somatosensory cortical processing, are

- beginning to form in the primary somatosensory cortex via connections,
- formed between neighboring fingertip representations, and that this
- information is transmitted to higher cortical stages in a
- digit-specific manner.

**Statistical characterisation of neural behaviour.** — Interspike interval (ISI) series exhibit multimodal distribution and can be described by different types of probability distributions. These observations point to the rich dynamical properties underlying the behavior of the cortical neurons and partly objectify them in probabilistic terms. Using autocorrelation functions we found that stationary processes can be used to model the generation of ISI time series. In order to remove the effects of trend in ISI data we used two methods: multifractal detrended fluctuation analysis and the analysis of ISI differences. The analysis of the detrended signal revealed the presence of memory effects which could be partly interpreted as network level phenomena. The analysis indicated existence of at least two different network-level dynamical processes. The correlation of local field potential (LFP) with the ISI series required the removing of the effect of action potentials from the LFP.

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<sup>#</sup> PhD student

**Complex networks.** — The network of patents connected by citations is an evolving graph which provides a representation of the innovation process. A patent citing another implies that the cited patent reflects a piece of previously existing knowledge that the citing patent builds upon. The methodology presented identified actual clusters of patents, i.e., technological branches, and gave predictions about the temporal changes of the structure of the clusters. We identified evolving patent groups and were able to predict the emerging technological fields. The clustering technique adopted was able to detect the new emerging recombinations, and successfully predicted emerging new technology clusters. New tools of predictive analytics could support policy decision making processes in science and technology, and help formulate recommendations for action.

## GRANTS

TÉT 10-1-2011-0001: Statistical characterisation of neural behaviour in the cerebral cortex of behaving animals (L. Négyessy, 2010-2012)

## PUBLICATIONS

### *Articles*

1. Négyessy L, Bányai M, Bazsó F; What makes the prefrontal cortex so appealing in the era of brain imaging? A network analytical perspective; *Acta Biologica Hungarica*; **63**(S1), 38-53, 2012
2. Hanics\* J, Barna\* J, Xiao\* J, Millán\* JL, Fonta\* C, Négyessy L; Ablation of TNAP function compromises myelination and synaptogenesis in the mouse brain; *Cell and Tissue Research*; **349**, 459-471, 2012
4. Somogyvári Z, Cserpán D, Ulbert\* I, Érdi P; Localization of single cell current sources based on extracellular potentials patterns: the spike CSD method; *European Journal of Neuroscience*; **36**, 3299-3313, 2012.

## R-F. HADRON PHYSICS AT CERN SPS AND LHC

*Ferenc Siklér, András Agócs<sup>#</sup>, László Boldizsár, Zoltán Fodor, Endre Futó, Sándor Hegyi, Gábor Jancsó, József Kecskeméti, Krisztián Krajczár, András László, Krisztina Márton<sup>#</sup>, Levente Molnár, Gabriella Pállya, Sona Pochybová<sup>#</sup>, Zoltán Seres, János Sziklai, Anna Julianna Zsigmond<sup>#</sup>*

**CERN-ALICE experiment.** — We took part in the data analysis of the HMPID subdetector, as well as in the research and development of the DAQ system for the planned VHMPID detector. Beside these activities, we also participated in the operation of the ALICE GRID Tier-2 site, and performed detector control tasks. Our most important result was the theoretical and experimental analysis of the pseudorapidity density and nuclear modification factors in  $\sqrt{s} = 5$  TeV center-of-mass energy p-Pb collisions. Our model predictions, published at the beginning of the year, are in good agreement with the results of these first measurements.

**CERN-CMS experiment, hadron physics.** — We have determined the inelastic p-p cross section with a simple event counting method at  $\sqrt{s} = 7$  TeV, and have contributed to a combined cross section paper, together with a pile-up counting analysis. We have measured the spectra of identified charged hadrons in p-p collisions at  $\sqrt{s} = 0.9, 2.76,$  and 7 TeV. Charged pions, kaons, and protons in the transverse-momentum ( $p_T$ ) range 0.1-1.7 GeV/c were identified via their energy loss in the silicon tracker. The average  $p_T$  increases rapidly with the mass of the hadron and the event charged-particle multiplicity, independently of the center-of-mass energy. We have presented both results at the DIS2012 conference.

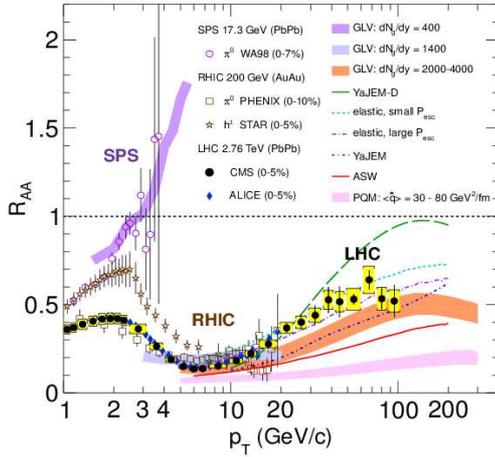


Fig 1. CMS: The nuclear modification factor  $R_{AA}$  in central heavy-ion collisions for neutral and charged hadrons, at several center-of-mass energies.

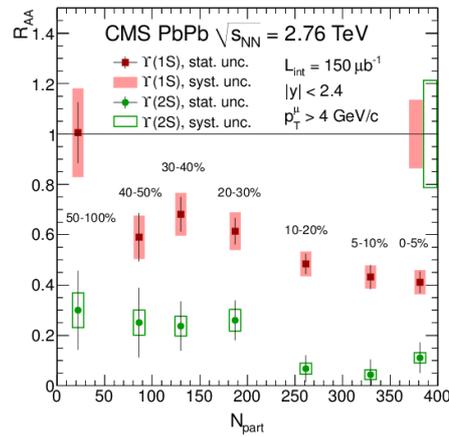


Fig 2. CMS: The nuclear modification factor  $R_{AA}$  for upsilon states as a function of the centrality of the heavy-ion collision.

We have participated in the measurement of the relative and absolute suppression of Y states in Pb-Pb collisions. We see the expected sequential melting of quarkonium states. We have

<sup>#</sup> PhD student

performed a study of Z boson production in Pb-Pb collisions with a high statistics data set, obtained in 2011. The measurements compared to NLO calculations show that the production of Z bosons is not modified by the strongly interacting matter produced in heavy-ion collisions. We also have participated in the measurement of the nuclear modification factor of charged particles in Pb-Pb collisions, using the data set mentioned above. The results were presented at the HP2012 conference. We took part in the analysis of jet-track correlations by evaluating the performance of tracking and the related uncertainties of the final results. We have developed the trigger menu used to record the first p-Pb collisions, and also contributed to the measurement of two-particle correlations by developing the event selection and performing various cross-checks.

**CERN-NA61 experiment.** — We have measured the spectra of charged pions and kaons in minimum bias p-C collisions at 31 GeV/c beam momentum. These data have been used as reference data to for a precise calculation of neutrino fluxes produced at the T2K neutrino beam experiment. We have also recorded a large statistics minimum bias p-Pb data set at 158 GeV/c beam momentum, a unique reference for comparisons with heavy-ion collisions. For event centrality determination in these collisions a new detector, the Low Momentum Particle Detector, was developed in the framework of the REGARD group, in close collaboration with us. We have significantly upgraded the DAQ system of the experiment, making it possible to record data with sufficient speed and quality. Furthermore, we also started to develop a new offline software system, for fast data reconstruction and analysis.

**Independent works.** — We have studied the estimation of energy loss rate ( $dE/dx$ ) for charged particles in tracking detectors. The truncated mean method was generalized to the weighted mean of the measurements. The optimized weights are rather independent of particle momentum and track segment length, and their values are given by a simple universal description as a function of the number of measured track segments. We have approximated the energy loss distribution of charged particles in silicon by a simple analytical parametrization. With the help of energy deposits in sensing elements of the detector, the position of track segments and the corresponding deposited energies were estimated with improved accuracy and less bias. The parametrization was successfully used to estimate the energy loss rate of charged particles, and applied to detector gain calibration tasks.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA K 81614	New analysis methods and tests of quantum chromodynamics at the LHC (F. Siklér, 2010-2014)
OTKA NK 81447	Hungary in the CMS experiment of the Large Hadron Collider (D. Horváth, 2010-2013)
OTKA K 68506	Experimental and model study of high momentum transfer phenomena at pp, pA and AA reactions (Z. Fodor; 2007-2012)
CERN-NA49	D. Barna, Z. Fodor, A. László, G. Pála, F. Siklér, Gy. Vesztergombi
CERN-NA61	L. Boldizsár, Z. Fodor, A. László, G. Pála, Gy. Vesztergombi
CERN-ALICE	A. Agócs, GG. Barnaföldi, D. Berényi, L. Boldizsár, E. Dénes, G. Hamar, P. Lévai, S. Pochybova, L. Molnár
CERN-CMS	Cs. Hajdu, P. Hidas, D. Horváth, F. Siklér, V. Veszprémi, Gy. Vesztergombi, AJ. Zsigmond, K. Krajczár

**PUBLICATIONS***Articles*

1. Yoshikawa\* A et al [ALICE ITS Collaboration]; Development of resistive electrode gas electron multiplier (RE-GEM); *JINST*; **7**, C06006/1-9, 2012
2. Abelev\* B et al [ALICE Collaboration];  $K_s^0$ - $K_s^0$  correlations in pp collisions at  $\sqrt{s} = 7$  TeV from the LHC ALICE experiment; *Phys Lett B*; **717**, 151-161, 2012
3. Abelev\* B et al [ALICE Collaboration]; Neutral pion and  $\eta$  meson production in proton-proton collisions at  $\sqrt{s} = 0.9$  TeV and  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **717**, 162, 2012
4. Zichichi\* A [LVD, EEE, TOF (ALICE) Collaboration]; Proposal for an MRPC system with high-precision timing in the LVD structure; *Eur Phys J Plus*; **127**, 42, 2012
5. Abelev\* B et al [ALICE Collaboration]; Measurement of charm production at central rapidity in proton-proton collisions at  $\sqrt{s} = 2.76$  TeV; *JHEP*; **07**, 191, 2012
6. Ahn\* S et al [ALICE Collaboration]; Commissioning of the ALICE muon spectrometer trigger at LHC; *Nucl Instrum Meth A*; **661**, S41, 2012
7. Gagliardi\* M [ALICE Collaboration]; Commissioning and first performance of the resistive plate chambers for the ALICE muon arm; *Nucl Instrum Meth A*; **661**, S45, 2012
8. De Gruttola\* D [ALICE Collaboration]; Study of the cosmic data taken with the ALICE TOF detector at the LHC; *Nucl Instrum Meth A*; **661**, S102, 2012
9. Abelev\* B et al [ALICE Collaboration]; Suppression of high transverse momentum D mesons in central Pb-Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *JHEP*; **09**, 112, 2012
10. Abelev\* B et al [ALICE Collaboration];  $J/\Psi$  Production as a Function of Charged Particle Multiplicity in pp Collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **712**, 165, 2012
11. Abelev\* B et al [ALICE Collaboration];  $J/\Psi$  suppression at forward rapidity in Pb-Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *Phys Rev Lett*; **109**, 072301, 2012
12. Abelev\* B et al [ALICE Collaboration]; Heavy flavour decay muon production at forward rapidity in proton-proton collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **708**, 265, 2012
13. Abelev\* B et al [ALICE Collaboration]; Measurement of event background fluctuations for charged particle jet reconstruction in Pb-Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *JHEP*; **03**, 053, 2012
14. Abelev\* B et al [ALICE Collaboration]; Light vector meson production in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **710**, 557, 2012
15. Abelev\* B et al [ALICE Collaboration]; Underlying Event measurements in pp collisions at  $\sqrt{s} = 0.9$  and 7 TeV with the ALICE experiment at the LHC; *JHEP*; **07**, 116, 2012
16. Abelev\* B et al [ALICE Collaboration]; Measurement of charm production at central rapidity in proton-proton collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **01**, 128, 2012

17. Abelev<sup>\*</sup> B et al [ALICE Collaboration];  $J/\Psi$  polarization in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Rev Lett*; **108**, 082001, 2012
18. Aamodt<sup>\*</sup> K et al [ALICE Collaboration]; Particle-yield modification in jet-like azimuthal di-hadron correlations in Pb-Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *Phys Rev Lett*; **108**, 092301, 2012
19. [ALICE Collaboration]; Multi-strange baryon production in pp collisions at root  $s = 7$  TeV with ALICE; *Phys Lett B*; **712**, 309-318, 2012. Schukraft<sup>\*</sup> J [ALICE Collaboration]; Heavy Ion physics with the ALICE experiment at the CERN LHC; *Phil Trans Roy Soc Lond A*; **370**, 917, 2012
20. Aamodt<sup>\*</sup> K et al [ALICE Collaboration]; Harmonic decomposition of two-particle angular correlations in Pb-Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *Phys Lett B*; **708**, 249, 2012
21. [CMS Collaboration]<sup>♦</sup>; Measurement of the inelastic proton-proton cross section at  $\sqrt{s} = 7$  TeV; *CMS-PAS-QCD-11-002*, <http://cdsweb.cern.ch/record/1433413>, 2012
22. [CMS Collaboration]<sup>♦</sup>; Study of the inclusive production of charged pions, kaons, and protons in pp collisions at  $\sqrt{s} = 0.9, 2.76$ , and 7 TeV; *Eur Phys J C*; **72**, 2164, 2012
23. [CMS Collaboration]<sup>♦</sup>; Observation of sequential Y suppression in PbPb collisions; *CMS-HIN-11-011*, <http://cdsweb.cern.ch/record/1472750>, 2012
24. <sup>♦</sup>[CMS Collaboration]<sup>♦</sup>; Z boson production with the 2011 data in PbPb collisions; *CMS-PAS-HIN-12-008*, <http://cdsweb.cern.ch/record/1472723>, 2012
25. [CMS Collaboration]<sup>♦</sup>; Study of high- $p_T$  charged particle suppression in PbPb compared to pp collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *Eur Phys J C*; **72**, 1945, 2012
26. [CMS Collaboration]<sup>♦</sup>; Detailed characterization of jets in heavy ion collisions using jet shapes and jet fragmentation functions; *CMS-PAS-HIN-12-013*, <http://cdsweb.cern.ch/record/1472734>, 2012
27. [CMS Collaboration]<sup>♦</sup>; Observation of long-range near-side angular correlations in proton-lead collisions at the LHC; *CMS-HIN-12-015*, <http://cdsweb.cern.ch/record/1486180>, 2012
28. Chatrchyan<sup>\*</sup> S et al [CMS Collaboration]; Measurement of the underlying event activity in pp collisions at  $\sqrt{s} = 0.9$  and 7 TeV with the novel jet-area/median approach; *JHEP*; **08**, 130, 2012
29. Chatrchyan<sup>\*</sup> S et al [CMS Collaboration]; Measurement of the pseudorapidity and centrality dependence of the transverse energy density in PbPb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *Phys Rev Lett*; **109**, 152303, 2012
30. Chatrchyan<sup>\*</sup> S et al [CMS Collaboration]; Shape, transverse size, and charged hadron multiplicity of jets in pp collisions at 7 TeV; *JHEP*; **06**, 160, 2012
31. Chatrchyan<sup>\*</sup> S et al [CMS Collaboration]; Azimuthal anisotropy of charged particles at high transverse momenta in PbPb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV; *Phys Rev Lett*; **109**, 022301, 2012

---

<sup>♦</sup> Highlighted publication, where the contribution of our group was decisive.

32. Chatrchyan\* S et al [CMS Collaboration]; Jet momentum dependence of jet quenching in PbPb collisions at  $\sqrt{s_{NN}}=2.76$  TeV; *Phys Lett B*; **712**, 176, 2012
33. Chatrchyan\* S et al [CMS Collaboration]; Inclusive b-jet production in pp collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **04**, 084, 2012
34. Chatrchyan\* S et al [CMS Collaboration]; Measurement of the inclusive production cross sections for forward jets and for dijet events with one forward and one central jet in pp collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **06**, 036, 2012
35. Chatrchyan\* S et al [CMS Collaboration]; Suppression of non-prompt  $J/\Psi$ , prompt  $J/\Psi$ , and  $Y(1S)$  in PbPb collisions at  $\sqrt{s_{NN}}=2.76$  TeV; *JHEP*; **05**, 063, 2012
36. Chatrchyan\* S et al [CMS Collaboration]; Centrality dependence of dihadron correlations and azimuthal anisotropy harmonics in PbPb collisions at  $\sqrt{s_{NN}}=2.76$  TeV; *Eur Phys J C*; **72**, 2012, 2012
37. Chatrchyan\* S et al [CMS Collaboration]; Measurement of isolated photon production in pp and PbPb collisions at  $\sqrt{s_{NN}}=2.76$  TeV; *Phys Lett B*; **710**, 256, 2012
38. Chatrchyan\* S et al [CMS Collaboration]; Measurement of the production cross section for pairs of isolated photons in pp collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **01**, 133, 2012
39. Chatrchyan\* S et al [CMS Collaboration]; Jet Production Rates in Association with W and Z Bosons in pp Collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **01**, 010, 2012
40. Chatrchyan\* S et al [CMS Collaboration]; Measurement of energy flow at large pseudorapidities in pp collisions at  $\sqrt{s}=0.9$  and 7 TeV; *JHEP*; **02**, 055, 2012
41. Chatrchyan\* S et al [CMS Collaboration]; Forward Energy Flow, Central Charged-Particle Multiplicities, and Pseudorapidity Gaps in W and Z Boson Events from pp Collisions at 7 TeV; *Eur Phys J C*; **72**, 1839, 2012
42. [NA61 Collaboration]\*; Measurement of production properties of positively charged kaons in proton-carbon interactions at 31 GeV/c; *Phys Rev C*; **85**, 035210, 2012
43. Cetner\* T et al. [NA61 Collaboration]; Methods to study event-by-event fluctuations in the NA61/SHINE experiment at the CERN SPS; *Phys Atom Nucl*; **75**, 567, 2012
44. Davis\* N et al [NA49 Collaboration]; Searching for the QCD critical point in A A collisions at CERN SPS; *Phys Atom Nucl*; **75**, 661, 2012
45. Anticic\* T et al [NA49 Collaboration]; Antideuteron and deuteron production in mid-central Pb+Pb collisions at 158A GeV; *Phys Rev C*; **85**, 044913, 2012
46. Reisdorf\* W et al [FOPI Collaboration]; Systematics of azimuthal asymmetries in heavy ion collisions in the 1 A GeV regime; *Nucl Phys A*; **876**, 1-60, 2012
47. Siklér F, Szeles\* S; Optimized estimation of energy loss rate for charged particles from energy deposit measurements in tracking detectors; *Nucl Instrum Meth A*; **687**, 30-39, 2012
48. Siklér F, A parametrisation of the energy loss distributions of charged particles and its applications for silicon detectors, *Nucl Instrum Meth A*; 691, 16-29, 2012
49. Salgado\* C et al, incl Siklér F; Proton-nucleus collisions at the LHC: Scientific opportunities and requirements; *J Phys G*; 39, 015010, 2012

*Conference proceedings*

50. László A; A linear iterative unfolding method; In:*Proc. of the 14th International Workshop on Advanced Computing and Analysis Techniques in Physics Research ACAT 2011, (Uxbridge, London, UK, Sept 5-9, 2011)*; J Phys: Conf Ser; **368**, 012043, 2012;
51. Mackowiak\* M et al. [NA49 Collaboration]; Identity method - a new tool for studying chemical fluctuations; In: *Proc. CPOD 2010 (August 23-29, Dubna, Russia)*; Phys Atom Nucl; **75**, 651, 2012
52. Agócs AG, Barnaföldi GG, Lévai P; Underlying event in pp collisions at LHC Energies; In: *Proc. 6th International Workshop on High-pT physics at LHC (Utrecht, Netherlands, April 4-7, 2011)*; CERN-Proceedings-2012-001, 33-37, 2012

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**R-G. PARTICLE DETECTOR RESEARCH AND DEVELOPMENT**

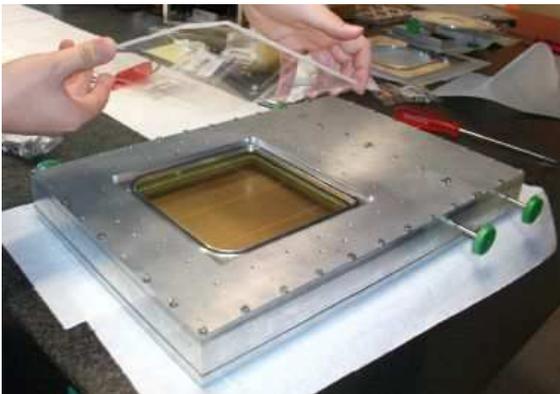

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*György Bencze, Gyula Bencédi, Ervin Dénes, Gergő Hamar, Tivadar Kiss, Levente Kovács, Tamás Tölyhi*

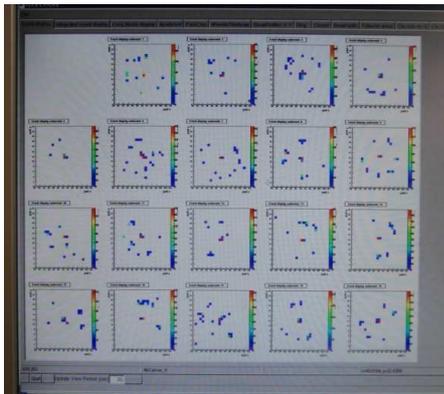
Our task is to study and develop advanced micropattern gas-avalanche detector technologies for applications in and outside high energy physics in close collaboration with the Lorand Eötvös University, including frontend and data acquisition electronics and software.

In 2012 the work was concentrated on further improvement of the detectors and technologies, which has been started during the past three years:

**VUV-photon detector for the ALICE-VHMPID upgrade project.** —A 200x200 mm<sup>2</sup> prototype detector based on CsI-covered ThickGEM (Fig. 1) has been tested at CERN with 6 GeV pions, and a full Cherenkov ring could be seen for the first time with GEM-type detector (Fig. 2).



*Fig. 1: ThickGEM-based photon detector during assembly*



*Fig. 2: Some detected Cherenkov ring events*

A new and very perspective method has been developed for characterization of the TGEM-based detectors by scanning and extracting photo-electrons from the surface with focused UVlight (Fig. 3).

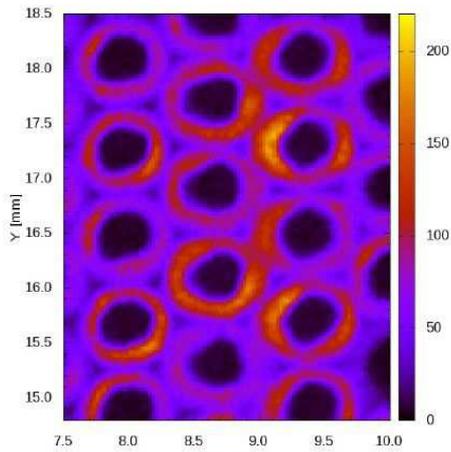


Fig.3: Efficiency-map of the ThickGEM detector surface



Fig. 4: Large-size CCC-chamber

**Further development of the CCC (Close Cathode Chamber) technology and its application for muon tomography.** — We have proposed and developed a light-weight low-cost chamber which can be built in large size (Fig.4). The design has been accepted as the candidate for the particle-track detector of the VHMPID. A small prototype (Fig. 5) was already used during the VHMPID beam tests at CERN.



Fig. 5: CCC-chamber used during the VHMPID-beamtests at CERN



Fig. 6: The portable Muon Tomograph in the Ajándék-cave

The improved version of the Muon Tomograph based on CCC-chambers has been applied in different caves in Hungary and measured the relief and possible cavities by detecting cosmic muons. The particularity of this device is its portability and autonomy during data taking (Fig.6).

**GRANTS AND INTERNATIONAL COOPERATION:**

OTKA-NKTH CK77815 (György Bencze, 2009-2013)

CERN CMS collaboration (Gy. Bencze)

CERN RD51 collaboration, (Gy. Bencze Wigner group leader, G. Hamar, L. Kovács, E. Dénes)

CERN NA61 collaboration (T. Tölyhi)

CERN ALICE collaboration (Gy. Bencédi, G. Hamar, E. Dénes, T. Kiss)

CERN ALICE VHMPID upgrade project (Gy. Bencze, Gy. Bencédi, G. Hamar, E. Dénes)

**PUBLICATIONS**

*Articles*

1. Hamar G, Varga\* D; High resolution surface scanning of thick-GEM for single photoelectron detection; *Nucl Inst and Meth A*; **694**, 16-23, 2012
2. Hamar G, Lévai P; Strange and nonstrange hadron resonance production by quark coalescence, investigating quark number scaling; *Acta Phys Polon*; Suppl 5; 451-456, 2012
3. Varga\* D, Kiss\* G, Hamar, G, Bencédi Gy; Close cathode chamber: low material budget MWPC; *Nucl Inst and Meth*; **698**, 11-18, 2012
4. Arce\* P, et al.; CMS structural equilibrium at constant magnetic field as observed by the link alignment system; *Nucl Instrum Meth*; **A675**, 84-96, 2012

*See also: R-B.I., R-F (Alice, NA61)*

## R-H. NEW PHYSICS AT CERN

*György Vesztegombi, Ádám Agócs,<sup>#</sup> Dániel Barna, Lajos Diósi, Csaba Hajdú, Pál Hidas, Dezső Horváth, Gabriella Pásztor, Viktor Veszprémi*

**Higgs-boson discovery.** — All members of the CMS collaboration got the following message in July 5 from Joseph Robert Incandela, the spokesperson of the experiment, who was returning from the Melbourne conference presentation of Higgs discovery on July 4th:

*Dear CMS colleagues - dear friends!*

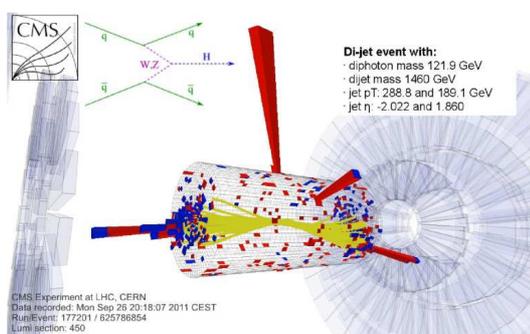
*I want to congratulate the whole collaboration on an amazingly beautiful result under incredible time pressure. It is the consequence of decades of work and it is something we all made possible and we now all share together.*

*I had to rush off to Melbourne so I could not send this message sooner than this moment while waiting for a connecting flight in Singapore, reading Wall Street Journal Asia which has a CMS event display on the front page and another one covering a full half page on the inside!!*

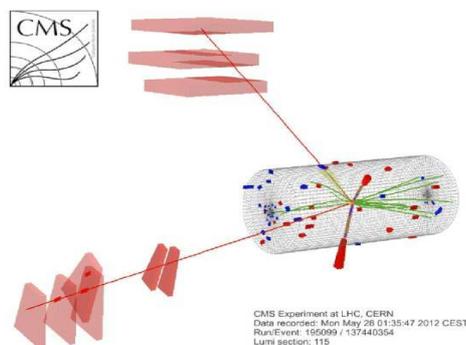
*We have really made an impression worldwide.*

*Enjoy the moment everyone. It is a truly historic one.*

*Joe*



*Fig. 1. The figure shows a CMS event similar to a Higgs particle. The boson is born when two quarks are scattered on each other and decays to two high energy photons denoted by red rectangles. The two quarks are flying away and initiate a hadron shower (yellow). The two hadron showers show the possible starting point of the Higgs boson, where the photons are initiated, and this is helpful in the determination of the mass of the boson.*



*Fig. 2 A CMS event where the hypothetical Higgs boson decays onto a pair of electrons and muons, respectively. The electrons are absorbed by the electromagnetic calorimeter, but the muons leave the system, triggering the muon detectors farther away.*

<sup>#</sup> PhD student

The Hungarian physicists as senior funding fathers of RD5=proto-CMS and junior members of the Wigner CMS team had the feeling that the 2 events mentioned by WSJ and shown below really represent the reward of their 20-year work.

Of course, the Wigner team's contribution was marginal in size, but essential in the final outcome, like in a very long chain the breaking of one single element would destroy the whole system. Though the expert teams consisted of much more members than the Hungarian collaborators, the Wigner participants had a considerable share in the pixel and the alignment.

The heart of the CMS detector is the Silicon TRACKER which contains almost 100 million active channels. The heart of the heart is the pixel detector which, practically, consists of hundreds of CCD cameras producing pictures with nanosecond time resolution. It was the responsibility of the Hungarian team to ensure that these cameras make the exposition in the right time. The method was worked out and the continuous monitoring was accomplished.

Another task of the Wigner team was the radiation damage control. The pixel detector is standing in the very front-line only few centimeters away from the collision point (which is one of the hottest points of the Universe). Due to the wonderfully intensive collision rate these detector elements are rapidly collecting huge radiation dose, which causes the performance of the system to deteriorate. This effect was foreseen during design, and one can correct for it by adjusting the voltage on the detector chips. The work-out of this correction method and its regular updating application was also done by the Wigner team.

The in-situ determination of alignment constants for the CMS Silicon Tracker is also an important task. Though it is not known for the public, the accurate determination of the alignment constants is crucial for the physics performance of the experiment. Position and angular orientation, as well as shape parameters are determined at the level of individual sensors, resulting in up to 200000 alignment parameters. An algorithm based on the global minimization of track-to-hit residuals is used, which determines all alignment and track parameters simultaneously. Systematic biases in the geometry are controlled by adding further information into the alignment workflow in form of the known mass of resonances decaying into muons. The time evolution of the position of large structures in the tracker is also a central issue. The Hungarian contribution in these activities mainly was concentrated on the monitoring task. Recently a new method was proposed for the treatment of the so-called weak modes by the Wigner team.

**SUSY search.** — The discovery of Higgs-boson has double meaning: it is the END and the BEGINNING at the same time. It is the coronation of the Standard Model, the last missing element in the jig-saw puzzle. But if there exists one Higgs then any number of additional Higgs bosons may exist, too. One of the most popular candidates with 5 bosons is the SUSY model which would solve many fundamental problems of particle physics.

Unfortunately the observed  $125 \text{ GeV}/c^2$  mass for Higgs is strongly disfavours the most popular SUSY versions (CMSSM, mSUGRA)

, therefore working out a new search strategy is on the agenda, where the Wigner team is actively participating in the Single Lepton group.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA NK 81447 Hungary in the CMS experiment of the Large Hadron Collider (D. Horváth, 2010-2013)

- OTKA K 72172 Study of fundamental symmetries using antiprotons (D. Horváth, 2008-2012)
- OTKA K 75129 Theory of quantum effects in nano-systems (L. Diósi, 2009-2013)
- SCOPES 128079 (Swiss National Science Foundation) First years of data taking with the CMS experiment at the LHC (Dissertori\* G; 2009-2012)
- EU COST M1016 Fundamental problems in quantum physics (L. Diósi, 2011-2014)

## PUBLICATIONS

### Articles

1. Chatrchyan\* S et al. [CMS Collaboration]; Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC; *Phys Lett B*; **716**, 30, 2012
2. Hoff\* J et al. [CMS Collaboration]; Readout chip for an L1 tracking trigger using asynchronous logic; *JINST*; **7**, C08004, 2012
3. Chatrchyan\* S et al. [CMS Collaboration]; Search for heavy Majorana neutrinos in  $\mu^\pm\mu^\pm$  and  $e^\pm e^\pm$  events in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **717**, 109, 2012
4. Chatrchyan\* S et al. [CMS Collaboration]; Search for pair production of first- and second-generation scalar leptoquarks in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Rev D*; **86**, 052013, 2012
5. Chatrchyan\* S et al. [CMS Collaboration]; Search for supersymmetry in hadronic final states using MT2 in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1210**, 018, 2012
6. Chatrchyan\* S et al. [CMS Collaboration]; Search for a fermiophobic Higgs boson in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1209**, 111 (2012)
7. Chatrchyan\* S et al. [CMS Collaboration]; Search for stopped long-lived particles produced in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1208**, 026, 2012
8. Chatrchyan\* S et al. [CMS Collaboration]; Inclusive and differential measurements of the  $t$   $\bar{t}$  charge asymmetry in proton-proton collisions at 7 TeV; *Phys Lett B*; **717**, 129, 2012
9. Chatrchyan\* S et al. [CMS Collaboration]; Search for a light pseudoscalar Higgs boson in the dimuon decay channel in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Rev Lett*; **109**, 121801, 2012
10. Chatrchyan\* S et al. [CMS Collaboration]; Search for dark matter and large extra dimensions in monojet events in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1209**, 094, 2012
11. Chatrchyan\* S et al. [CMS Collaboration]; Performance of CMS muon reconstruction in pp collision events at  $\sqrt{s} = 7$  TeV; *JINST*; **7**, P10002, 2012
12. Chatrchyan\* S et al. [CMS Collaboration]; Measurement of the electron charge asymmetry in inclusive W production in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Rev Lett*; **109**, 111806, 2012
13. Chatrchyan\* S et al. [CMS Collaboration]; Search for narrow resonances in dilepton mass spectra in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **714**, 158, 2012

14. Chatrchyan\* S et al. [CMS Collaboration]; Search for high mass resonances decaying into tau-lepton pairs in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **716**, 82, 2012
15. Chatrchyan\* S et al. [CMS Collaboration]; Search for a  $W'$  or Techni-rho decaying into WZ in pp collisions at  $\sqrt{s}=7$  TeV; *Phys Rev Lett*; **109**, 141801, 2012
16. Chatrchyan S et al. [CMS Collaboration]; Search for new physics with same-sign isolated dilepton events with jets and missing transverse energy; *Phys Rev Lett*; **109**, 071803, 2012
17. Chatrchyan S et al. [CMS Collaboration]; Study of W boson production in PbPb and pp collisions at  $\sqrt{s[NN]} = 2.76$  TeV; *Phys Lett B*; **715**, 66, 2012
18. Chatrchyan S et al. [CMS Collaboration]; Search for a light charged Higgs boson in top quark decays in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1207**, 143, 2012
19. Chatrchyan S et al. [CMS Collaboration]; Search for new physics in events with same-sign dileptons and b-tagged jets in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1208**, 110, 2012
20. Chatrchyan\* S et al. [CMS Collaboration]; Measurement of the  $\lambda(b)$  cross section and the anti- $\Lambda(b)$  to  $\Lambda(b)$  ratio with  $\Lambda(b)$  to  $J/\Psi$   $\Lambda(b)$  decays in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **714**, 136, 2012
21. Chatrchyan\* S et al. [CMS Collaboration]; Search for heavy long-lived charged particles in pp collisions at  $\sqrt{s}=7$  TeV; *Phys Lett B*; **713**, 408, 2012
22. Chatrchyan\* S et al. [CMS Collaboration]; Observation of a new  $\Xi(b)$  baryon; *Phys Rev Lett*; **108**, 252002, 2012
23. Chatrchyan\* S et al. [CMS Collaboration]; Search for anomalous production of multilepton events in pp collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **1206**, 169, 2012
24. Chatrchyan\* S et al. [CMS Collaboration]; Search for leptonic decays of  $W'$  bosons in pp collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **1208**, 023, 2012
25. Chatrchyan\* S et al. [CMS Collaboration]; Search for physics beyond the standard model in events with a Z boson, jets, and missing transverse energy in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **716**, 260, 2012
26. Chatrchyan\* S et al. [CMS Collaboration]; Measurement of the mass difference between top and antitop quarks; *JHEP*; **1206**, 109, 2012
27. Chatrchyan\* S et al. [CMS Collaboration]; Search for anomalous t t-bar production in the highly-boosted all-hadronic final state; *JHEP*; **1209**, 029, 2012
28. Chatrchyan\* S et al. [CMS Collaboration]; Measurement of the  $Z/\gamma^* + b$ -jet cross section in pp collisions at 7 TeV; *JHEP*; **1206**, 126 (2012)
29. Chatrchyan\* S et al. [CMS Collaboration]; Search for heavy bottom-like quarks in 4.9 inverse femtobarns of pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1205**, 123 (2012)
30. Chatrchyan\* S et al. [CMS Collaboration]; Search for dark matter and large extra dimensions in pp collisions yielding a photon and missing transverse energy; *Phys Rev Lett*; **108**, 261803, 2012
31. Chatrchyan\* S et al. [CMS Collaboration]; Measurement of the top quark pair production cross section in pp collisions at  $\sqrt{s} = 7$  TeV in dilepton final states containing a  $\tau$ ; *Phys Rev D*; **85**, 112007, 2012

32. Chatrchyan\* S et al. [CMS Collaboration]; Search for heavy, top-like quark pair production in the dilepton final state in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **716**, 103, 2012
33. Carrillo\* C [CMS Collaboration]; The CMS RPC project, results from 2009 cosmic-ray data, *Nucl Instrum Meth A*; **661**, S19, 2012
34. Iorio\* AOM [CMS Collaboration]; Study of the RPC level-1 trigger efficiency in the compact muon solenoid at LHC with cosmic ray data; *Nucl Instrum Meth A*; **661**, S27, 2012
35. Sharma\* A et al. [CMS RPC Collaboration]; A data-driven performance evaluation method for CMS RPC trigger through CMS muon trigger; *Nucl Instrum Meth A*; **661**, S30, 2012
36. Pant\* LM [CMS Collaboration]; Characterization of CMS end-cap RPCs assembled in India; *Nucl Instrum Meth A*; **661**, S34, 2012
37. Jindal\* M [CMS Collaboration]; Estimation of level-1 trigger efficiency of RPC detectors in CMS experiment using cosmic muon data; *Nucl Instrum Meth A*; **661**, S37, 2012
38. Lee\* KS [CMS Collaboration]; Six-gap resistive plate chambers for high-rate muon triggers; *Nucl Instrum Meth A*; **661**, S90, 2012
39. Chatrchyan\* S et al. [CMS Collaboration]; Search for  $B_s^0 \rightarrow \mu^+ \mu^-$  and  $B^0 \rightarrow \mu^+ \mu^-$  decays; *JHEP*; **1204**, 033, 2012
40. Chatrchyan\* S et al. [CMS Collaboration]; Measurement of the cross section for production of  $b \bar{b} X$ , decaying to muons in pp collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **1206**, 110, 2012
41. Chatrchyan\* S et al. [CMS Collaboration]; Search for microscopic black holes in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1204**, 061, 2012
42. Chatrchyan\* S et al. [CMS Collaboration]; Search for quark compositeness in dijet angular distributions from pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1205**, 055, 2012
43. Chatrchyan\* S et al. [CMS Collaboration]; Search for the standard model Higgs boson decaying to bottom quarks in pp collisions at  $\sqrt{s}=7$  TeV; *Phys Lett B*; **710**, 284, 2012
44. Chatrchyan\* S et al. [CMS Collaboration]; Search for neutral Higgs bosons decaying to tau pairs in pp collisions at  $\sqrt{s}=7$  TeV; *Phys Lett B*; **713**, 68, 2012
45. Chatrchyan\* S et al. [CMS Collaboration]; Search for large extra dimensions in dimuon and dielectron events in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **711**, 15, 2012
46. Chatrchyan\* S et al. [CMS Collaboration]; Search for the standard model Higgs boson in the  $H \rightarrow ZZ \rightarrow 2l 2\gamma$  channel in pp collisions at  $\sqrt{s} = 7$  TeV, *JHEP*; **1203**, 040 (2012)
47. Chatrchyan\* S et al. [CMS Collaboration]; Search for the standard model Higgs boson in the  $H \rightarrow ZZ \rightarrow l^+ l^- \tau \tau$  decay channel in pp collisions at  $\sqrt{s}=7$  TeV; *JHEP*; **1203**, 081, 2012
48. Chatrchyan\* S et al. [CMS Collaboration]; Search for the standard model Higgs boson in the decay channel  $H \rightarrow ZZ \rightarrow 4$  leptons in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Rev Lett*; **108**, 111804, 2012

49. Chatrchyan\* S et al. [CMS Collaboration]; Search for the standard model Higgs boson decaying to a W pair in the fully leptonic final state in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **710**, 91, 2012
50. Chatrchyan\* S et al. [CMS Collaboration]; Combined results of searches for the standard model Higgs boson in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **710**, 26, 2012
51. Chatrchyan\* S et al. [CMS Collaboration], Search for the standard model Higgs boson decaying into two photons in pp collisions at  $\sqrt{s}=7$  TeV; *Phys Lett B*; **710**, 403, 2012
52. Chatrchyan\* S et al. [CMS Collaboration], Search for a Higgs boson in the decay channel  $H$  to  $ZZ^{(*)}$  to  $q\bar{q}l^+l^+$  in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1204**, 036, 2012
53. Chatrchyan\* S et al. [CMS Collaboration], Measurement of the charge asymmetry in top-quark pair production in proton-proton collisions at  $\sqrt{s} = 7$  TeV; *Phys Lett B*; **709**, 28, 2012
54. Chatrchyan\* S et al. [CMS Collaboration], Exclusive photon-photon production of muon pairs in proton-proton collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1201**, 052, 2012
55. Chatrchyan\* S et al. [CMS Collaboration],  $J/\psi$  and  $\psi(2S)$  production in pp collisions at  $\sqrt{s} = 7$  TeV; *JHEP*; **1202**, 011, 2012
56. Chatrchyan\* S et al. [CMS Collaboration], Measurement of the rapidity and transverse momentum distributions of Z bosons in pp collisions at  $\sqrt{s}=7$  TeV; *Phys Rev D*; **85**, 032002, 2012
57. C. Collaboration et al. [CMS Collaboration], Performance of tau-lepton reconstruction and identification in CMS; *JINST*; **7**, P01001, 2012
58. Chatrchyan\* S et al. [CMS Collaboration], Inclusive search for squarks and gluinos in pp collisions at  $\sqrt{s} = 7$  TeV; *Phys Rev D*; **85**, 012004, 2012
59. Diósi L; Non-Markovian open quantum systems: Input-output fields, memory, monitoring; *Phys Rev A*; **85**, 03410/1-5, 2012

#### *Conference proceedings*

60. Diósi L; Classical-quantum coexistence: a 'free will' test; In: Emergent Quantum Mechanics 2011; *Journal of Physics Conference Series*; **361**, 012028-7, 2012
61. Diósi L; Thermodynamic and quantum entropy gain of frame averaging; In: Quantum Africa 2010: Theoretical and Experimental Foundations of Recent Quantum Technologies; *AIP Conference Proceedings*; **1469**, 16-22, 2012

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**R-I. SPACE PHYSICS**


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*Géza Erdős, Zsófia Bebesi, Lajos Földy, Antal Juhász, Károly Kecskeméty, Péter Király, Katalin Lukács, Zoltán Németh, Károly Szegő, Mariella Tátrallyay*

**Magnetic field in the Heliosphere.** — Some portion of the solar magnetic field is frozen into the solar wind and carried out to the interplanetary space. The magnetic flux in the heliosphere is best characterized by the radial component of the magnetic field vector measured by spacecraft, which is a complex function of the location and time of observation. We have shown that the complexity is mainly due to magnetohydrodynamical waves and we have introduced a new data analysis method which largely reduces the effect of fluctuations. This widened the possibility to study the sunspot cycle variations of the solar magnetic field.

**Energetic particles in the Heliosphere.** — In contrast to energetic ions arriving predominantly from the Sun, the main source of electrons with energies above about 1 MeV is planet Jupiter. The penetration of Jovian electrons into the inner heliosphere during periods of optimum magnetic connection between Jupiter and Earth is a well-known phenomenon, however, a special magnetic configuration is necessary for periods when such a connection is absent. Based on near-Earth electron measurements we have shown that long-living magnetic traps corotating with the Sun filled by energetic electrons can account for the periodic variations observed in 2007-2008. By analyzing spacecraft observations of 0.03-1 MeV/n ions during quiet solar activity we pointed out that the elementary composition of such ions split into three well-defined groups. These correspond to those of solar energetic particle events, the solar corona, and the solar wind, respectively, and suggest that various acceleration mechanisms are at work in the different groups.

**The plasma environment of non-magnetic solar system bodies.** — Venus, Mars and Titan, the largest moon of Saturn, are the only non-magnetic solar system bodies having a relatively dense atmosphere. As a consequence, their ionospheres interact directly with the high speed plasma flow surrounding them. Accordingly, these objects provide a wide parameter range for the investigations of the interaction of non-magnetic bodies with their plasma environment. It is remarkable that the global structures formed by these interactions are very similar, although the two planets are immersed in the supersonic solar wind flow. Titan, however, is located inside Saturn's hot, rapidly rotating but subsonic magnetospheric flow.

We studied the plasma environment of these solar system objects and also participated in the comparative studies concerning the similarities and differences of these environments. We investigated the induced magnetospheres formed by the magnetized plasma enfolding the highly conducting ionosphere; provided a classification of the possible plasma types of Titan's plasma environment, and reviewed results about the ionosphere of Titan.

**The magnetodisk of Saturn** – In situ measurements around Jupiter and Saturn revealed that both giant planets possess a complex magnetic/plasma structure, called magnetodisk. It is established that the magnetodisk is the result of the interaction of the planetary magnetic field with the relatively dense co-rotating plasma surrounding these planets. This structure plays a very important role in the magnetospheres of the giant planets. The density and composition of the magnetospheric plasma, as well as the properties of the magnetic fields show a strong dependence

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# PhD student

pendence on the position of the measurements site relative to the central sheet of the magnetodisk. On the other hand, these properties strongly influence the interaction of the magnetosphere with the various bodies orbiting around the planet, including its moons. Thus the location of the magnetodisk is a very important property of Saturn's plasma environment. Using ion densities derived from measurements by the Cassini Plasma Spectrometer, we determined the location of the magnetodisk in the nightside outer magnetosphere of Saturn near equinox conditions.

### GRANTS AND INTERNATIONAL COOPERATION

EU-FP7-CPS CSA Number 228319      Europlanet RI (K. Szegő, 2008-2012)

PECS Experimental Arrangement No. 98077 "Cluster Data Exploitation" (M. Tátrallyay, 2008-2012)

PECS Experimental Arrangement No. 98080 "Participation in the development of the Rosetta Consortium Experiment on board Orbiter RPC" (S. Szalai, 2008-2013)

### Publications

#### Articles

1. Bebesi Z, Krupp\* N, Szegő K, Fränz\* M, Németh Z, Krimigis\* SM, Mitchell\* DG, Erdős G, Young\* DT, Dougherty\* MK; Analysis of energetic electron drop-outs in the upper atmosphere of Titan during flybys in the dayside magnetosphere of Saturn; *Icarus*; **218**, 1020-1027, 2012
2. Coates\* AJ, Wellbrock\* A, Lewis\* GR, Arridge\* CS, Crary\* FJ, Young\* DT, Thomsen\* MF, Reisenfeld\* DB, Sittler\* EC Jr, Johnson\* RE, Szegő K, Bebesi Z, Jones\* GH; Cassini in Titan's tail: CAPS observations of plasma escape; *J Geophys Res*; **117**, A05324/1-11, 2012
3. Erdős G, Balogh\* A; Magnetic flux density measured in fast and slow solar wind streams; *Astrophys J*; **753**, 130, 2012
4. Ishkov\* VN, Zeldovich\* MA, Kecskeméty K, Logachev\* YuI; Relative ion Fe, C and O abundances in quiet time particle fluxes in the 23 SC; *Adv Space Res*; **50**, 757-761, 2012
5. McKenna-Lawlor\* SMP, Fry\* CD, Dryer\* M, Heynderickx\* D, Kecskeméty K, Kudela\* K, Balaz\* J; A statistical study of the performance of the Hakamada-Akasofu-Fry version 2 numerical model in predicting solar shock arrival times at Earth during different phases of solar cycle 23; *Ann Geophys*; **30**, 405-419, 2012
6. Szegő K, Németh Z, Erdős G, Földy L, Bebesi Z, Thomsen\* M, Delapp\* D; Location of the magnetodisk in the nightside outer magnetosphere of Saturn near equinox based on ion densities; *J Geophys Res*; **117**, A09225/1-11, 2012

#### Articles in Hungarian

7. Király P; Kettős centenárium. A kozmikus sugárzás és Jánossy Lajos (Double centenary. The cosmic radiation and Lajos Jánossy, in Hungarian); *Természet Világa*; **143**, 10-12, 2012

***Conference proceedings***

8. Kecskeméty K, Daibog\* EI, Logachev\* YuI; Homogeneity of interplanetary space according to charged particle observations; In: *Proc. of 32th Int. Cosmic Ray Conference of IUPAP, (Beijing 2011)*; vol. 11, pp. 186-189, 2012
9. Kecskeméty K, Zeldovich\* MA, Logachev\* YuI; Relative abundances of quiet-time suprathermal ions at 1 AU; In: *Proc. of 32th Int. Cosmic Ray Conference of IUPAP, (Beijing 2011)*; vol. 11, pp. 117-120, 2012

***Books and book chapters***

10. Szegő K (ed.); *The Plasma Environment of Venus, Mars, and Titan*; Space Sciences Series of ISSI, Vol. **37**, Springer, 2012.

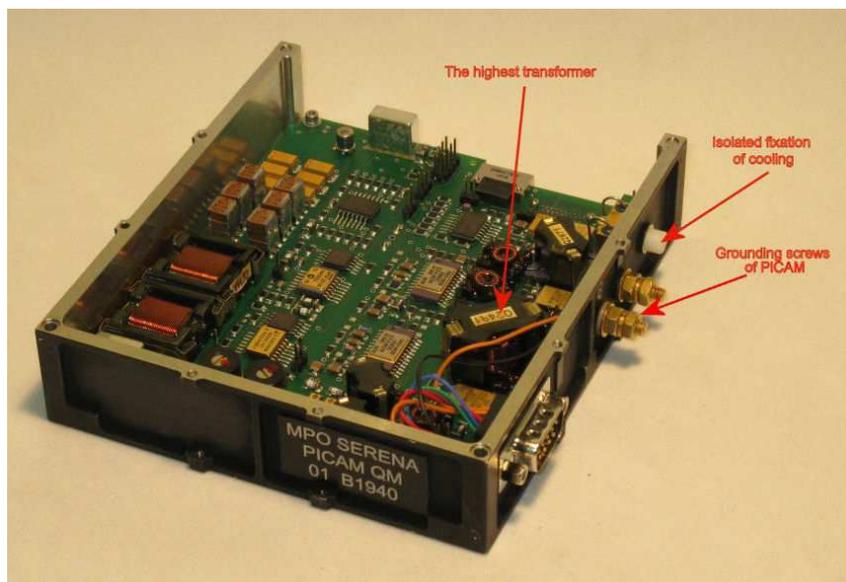
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**R-J. SPACE TECHNOLOGY**

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*Sándor Szalai, Attila Baksa, Kálmán Balajthy, András Balázs, László Heyesi, István Horváth, János Nagy, Zoltán Pálos, Bálint Sódor, Lajos Szalai, András Szekeres, Gábor Tróznai, Pál G. Vizi*

**Development of the SERENA/PICAM instrument on MPO BepiColombo mission.** — BepiColombo is Europe's first mission to Mercury. It will set off in 2015 on a journey to the smallest and least explored terrestrial planet in our Solar System. It will arrive to Mercury in January 2022. The mission comprises two spacecrafts: the Mercury Planetary Orbiter (MPO) and the Mercury Magnetospheric Orbiter (MMO). The task of the Wigner RCP RMI is to develop the Direct Current Converter (DCC) for the PICAM instrument. PICAM is a spectrometer dedicated to the measurement of the ions in Mercury's exosphere; it is part of a set of instruments named SERENA (neutral and ionised particle analyser). The DCCs supply the instrument's electronic circuits with several appropriate voltages, all galvanically isolated from the on-board power supply. The instrument's Control Electronics requires 6 different fixed voltages, while the Gate Electronics requires two symmetric, bipolar and variable voltages. The PICAM DCC has 3 functional units: Input Filter and Inrush Limiter; Fixed output voltage DC/DC converter units; Controllable output voltage DC/DC converter for Gate Electronics. In 2012 the Qualification Model (QM) has been manufactured which integrated all the functional parts into a single PCB. The PICAM-DCC-QM unit was transferred to Graz where it was integrated to PICAM-QM. Parallel with these tests the Flight Model (FM) topology was designed.



*Fig 1. The Qualification Model of the DCC for the PICAM instrument*

**Development of the Command Data Management Subsystem (CDMS) for the Rosetta Lander.** — Rosetta is the ESA's first mission designed to orbit and land on a comet. It comprises a large orbiter and a small lander. The spacecraft was launched in March 2004 and it will meet its target, 67P/Churyumov-Gerasimenko, in 2014. The task of the Wigner RCP RMI is to develop the software for the central data acquisition and control computer (CDMS) for the lander. The actual software version is functionally complete and equipped with mechanisms for fault tolerance in the relevant respects and is flight tested prior to entering the Deep Space Hibernation phase of the spacecraft. The autonomous overlaying technique is considered to be an applicable mechanism to cope with accepted requirements.

Since a substantial part of the SW – that for controlling the on-comet Long Term Science operations – could be tested only in an environment simulated configuration, the SW had to be adapted also to the Ground Reference Model (GRM) of the lander. In contrast to the Lander SW Simulator, the GRM is equipped with real hardware components. The adaptation and the test phase required more than a year. In this year we have solved the double-storage of the executable SW, so that it does not get corrupted during the on-comet Long Term Science phase.

In order to facilitate the prediction of the Sun orbit the SunTracker tool has also been upgraded this year. The aim was to reconstruct the on-comet in-situ Sun orbit with respect to the lander, and to predict the Sun orbit on long term under cometary conditions. This will allow for solar power and thermal conditions prediction over longer term of comet operations. A general mathematical model has been set up and various methods have been worked out to in-situ calibrate this model for Sun orbit reconstruction.

**Development of on-board computers of “Obstanovka” project of ISS.** — The goal of the Obstanovka project of International Space Station (ISS) is to investigate the space weather. Our task was to develop a distributed intelligence system containing three computers, which realized data acquisition and control of eleven sensors measuring different space weather parameters on the ISS. During the project we completed two flight models of on-board computers which were tested in Moscow this year. We supported the test job by personal participation and we were in continuous contact with the Russian colleagues. In order to facilitate tests we wrote software which converted data coming from IUS (IUS is a special on-board system bus in the Russian Segment on ISS using User Datagram Protocol ) and BITS telemetry channel into our Electrical Ground Support Equipment (EGSE) display format to visualize them. We have verified the command cycle algorithm of the measuring scenario software developed by Russian side.

The Obstanovka unit tests were carried out successfully and according to our current knowledge, the Russian side plans to deliver the Obstanovka system to the International Space Station in February 2013 on board of a Progress.



Fig. 2. The distributed computer system of the Obstanovka

## GRANTS

ESA PECS No. 98091; Participation in development of the SERENA/PICAM instrument on MPO BepiColombo mission (K Szegő; 2008–2013, Participants: S. Szalai, K. Balajthy, L. Hevesi, I. Horváth, L. Szalai)

ESA PECS No. 98098; Participation in the development of the Command Data Management Subsystem (CDMS) for the Rosetta Lander (K Szegő, 2008–2013, Participants: S. Szalai, A. Baksa, A. Balázs, Z. Pálos, B. Sódor, G. Tróznai, A. Szekeres\*)

ISS URKUT\_09-1-2009-0014; Development of on-board computers of “Obstanovka” project of ISS, National Development Agency (J. Nagy, 2010-2012, Participants: J. Nagy, K. Balajthy, I. Horváth, B. Sódor, S. Szalai)

## PUBLICATIONS

### Article in Hungarian

1. Nagy J, Szalai S; Az űridőjárás megfigyelése, magyar műszerek a Nemzetközi Űrállomáson, (Monitoring space weather, Hungarian instruments on the International Space Station, in Hungarian); *Élet és Tudomány*; **LXVII**, 329-331, 2012

### Others

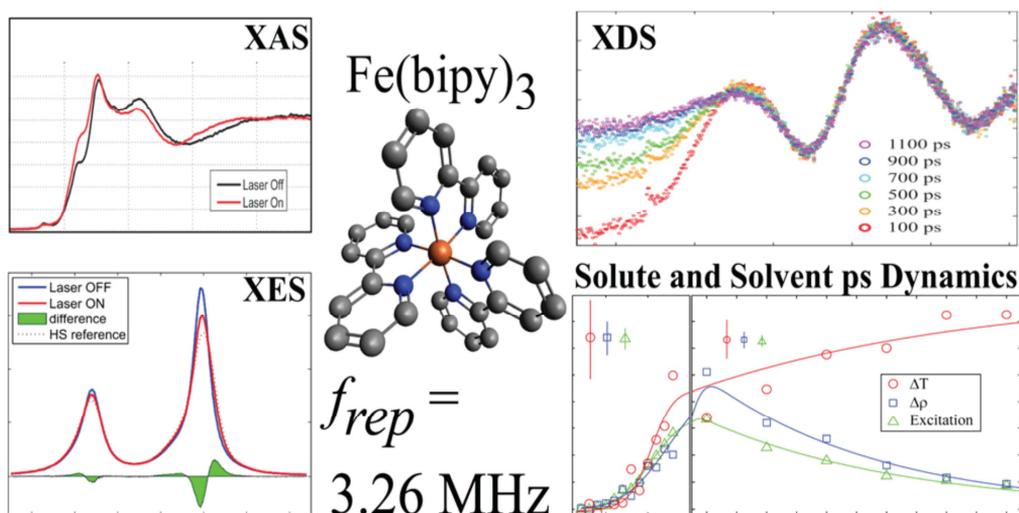
2. Szalai S, Nagy J; Instruments for Mars & Solar System research; Mars workshop, Budapest, 2012. Jul. 06-07 (<http://www.rmki.kfki.hu/tfo/UK-T-website/>)
3. Balázs A; SunTracker; LSWT workshop, Graz, 2012. October 29-31 (<http://www.rmki.kfki.hu/tfo/UK-T-website/>)
4. Nagy J, Sódor B, Szalai S; Improvement of EGSE Architecture and Software in Last Decade; poster in: SESP 2012, Simulation and EGSE facilities; ESTEC, Noordwijk, 25-27 September 2012 (<http://www.rmki.kfki.hu/tfo/UK-T-website/>)

## R-K. X-RAY SPECTROSCOPY

György Vankó, Csilla Bogdán, Amélie Bordage, Zoltán Németh, Mátyás Pápai<sup>#</sup>

Switchable transition-metal-based molecular systems have great potential in future IT applications in very high density devices including data storage systems, molecular switches, and display devices. We employ powerful static and time-resolved X-ray spectroscopy techniques to explore the fine details of the switching mechanisms.

**Ultrafast molecular transitions.** — Unveiling the elementary steps of light-induced molecular switching requires ultrafast pump-probe experiments. We have been making efforts to introduce element-sensitive high-resolution X-ray spectroscopy as probes in ultrafast experiments. We report a relevant advance from the first proof-of-principle X-ray emission experiment to collecting picosecond-resolved data employing a MHz laser system with count rates similar to those in static experiments. Moreover, we have realized a setup to combine elastic scattering and spectroscopy, to obtain information on the electronic and structural dynamics at the same time. Combining information from X-ray emission spectroscopy and scattering on a photo-induced spin-state transition of  $[\text{Fe}(\text{bipy})_3]^{2+}$  in aqueous solution, the excitation fraction as well as the temperature and density changes of the solvent can be closely followed on the subnanosecond time scale of the lifetime of the transient excited state. An analysis approach directly utilizing the spectroscopic data in the XDS analysis effectively reduces the number of free parameters, and both combined permit extraction of information about the ultrafast structural dynamics of the caging solvent, in particular, a decrease in the number of water molecules in the first solvation shell is inferred, as predicted by recent theoretical work.



**Fig. 1.** Combined X-ray absorption and X-ray emission spectra, and X-ray diffuse scattering results that resolve a subnanosecond-lived excited Fe(II) state.

<sup>#</sup> PhD student

**X-ray induced effects.** — Exploring alternative modes for molecular switching can provide us with insights into the interplay of the strongly coupled degrees of freedoms that shape the electronic structure and magnetic properties of such materials. Following our recent finding of hard X rays trigger spin-state switching in Fe(II) complexes, we have now observed they can also induce a thermal hysteresis at the switching of molecular magnets; the observation can provide us with a new tool to monitor cooperativity among the switching units.

#### GRANTS AND COOPERATION

- ERC-StG 259709 ERC Starting Grant: Electronic transitions and bistability: states, switches, transitions and dynamics studied with high-resolution X-ray spectroscopy, (G. Vankó, 2010-2015)
- OTKA K 72597 Novel approaches to lasting problems: spectroscopic studies of the electronic structure of transition metal-based strongly correlated systems (G. Vankó, 2012-2013)
- NFÜ T&T French-Hungarian Bilateral Intergovernmental S&T Cooperation: Investigation of switching mechanisms in Fe molecular complexes by hard X-ray spectroscopies: contribution from experiments and theory, (G. Vankó, 2012-2013)

#### PUBLICATIONS

##### Articles

1. Haldrup\* K, Vankó G, Gawelda\* W, Galler\* A, Doumy\* G, March\* AM, Kanter\* EP, Bordage A, Dohn\* A, van Driel\* TB, Kjør\* KS, Lemke\* HT, Canton\* SE, Uhlig\* J, Sundström\* V, Young\* L, Southworth\* SH, Nielsen\* MM, Bressler\* C; Guest–host interactions investigated by time-resolved X-ray spectroscopies and scattering at MHz rates: solvation dynamics and photoinduced spin transition in aqueous Fe(bipy)<sub>3</sub><sup>2+</sup>; *J Phys Chem A*; **116**, 9878-9887, 2012
2. Renz\* F, Vankó G, Homenya\* P, Saadat\* R, Németh Z, Huotari\* S; Hard-X-ray-induced thermal hysteresis (HAXITH) in a molecular switchable solid; *Eur J Inorg Chem*; **2012**, 2653-2655, 2012
3. Bordage A, Rossano\* S, Horn\* AH, Fuchs\* Y; Site partitioning of Cr<sup>3+</sup> in the trichroic alexandrite BeAl<sub>2</sub>O<sub>4</sub>:Cr<sup>3+</sup> crystal: contribution from x-ray absorption spectroscopy; *J Phys: Condens Matter*; **24**, 225401/1-8, 2012
4. Manuel\* D, Cabaret\* D, Brouder\* Ch, Sainctavit\* Ph, Bordage A, Trcera\* N; Experimental evidence of thermal fluctuations on the x-ray absorption near-edge structure at the aluminum K edge; *Phys Rev B*; **85**, 224108/1-13, 2012

*See also R-L.3*

## R-L. MAGNETIC THIN FILMS

László Bottyán, László Deák, Miklós Dolgos<sup>#</sup>, János Major, Dániel Géza Merkel, Béla Nagy<sup>#</sup>, Dénes Lajos Nagy, Szilárd Sajti

**Introduction.** — Reduced dimensions and the presence of interfaces alter the properties of magnetic materials which are being made extensive use of world-wide applying up-to-date controlled deposition techniques. Film-perpendicular anisotropy, sign-changing interlayer coupling, giant and tunnelling magnetoresistance are already commercialized phenomena in this field. The group's activity covers research and development of magnetic thin films and heterostructures including their characterization by nuclear methods. Besides, the group offers services in ultrahigh vacuum preparation and polarized neutron reflectometry.

**Reciprocity in the scattering theory.** — Reciprocity requires the scattering amplitude be symmetric upon transposition of detector and source. Reciprocity violation in magneto-optical gyrotropy, a well known property of the Mössbauer nuclear medium was studied. Following the theoretical elucidation ([MR.1], Fig. 1) we experimentally found large non-reciprocity in nuclear resonance scattering at special orientations of the magnetic hyperfine fields.

**Development of neutron optical elements.** — As a result of simulations, in collaboration with our industrial partner, we developed new types of polarizing neutron monochromators and band filter layer systems, and optimized sputtering parameters of neutron supermirrors for optimum reflectivity and tolerable internal stress.

**Controlling exchange coupling in thin bilayers.** — As part of our continued research in superconductor/weak ferromagnet proximity effects, we succeeded in controlling magnetic exchange coupling strength in  $\text{Ni}_x\text{Cu}_{100-x}$  ( $x = 55, 65$ ) alloy films of a few nanometer thickness and found an induced magnetic proximity contribution in  $\text{V}(d_S)/\text{Ni}_x\text{Cu}_{100-x}(d_F)$  bilayers beyond the finite size effect upon  $d_F$ .

**Neutron instrumentation.** — We designed and constructed a new high-precision slit system, a new multielement graphite monochromator, and a high performance supermirror neutron polarizer. We also installed a 12 K to 300 K cryostat for the GINA neutron reflectometer.

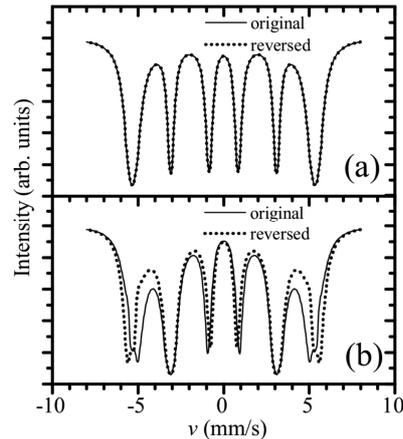


Fig.1. Simulation of reciprocity-obeying (a) and violating (b) arrangements in Mössbauer scattering [MR.1].

<sup>#</sup> PhD student

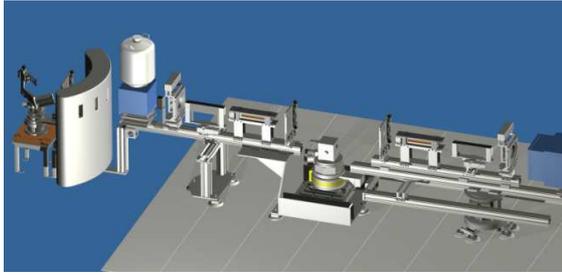


Figure 2. Layout of the GINA neutron reflectometer with the upgraded monochromator and slits



Figure 3. The installed low temperature sample environment of the GINA reflectometer

## GRANTS AND INTERNATIONAL COOPERATION

NAP-VEENEUS'08 Visegrad Cooperation for Development and Application of Neutron Spectroscopy Techniques in Multidisciplinary Research (L. Bottyán, 2009-2012)

TÉT-10-1-2011-0671 Hungarian-Vietnamese Bilateral Intergovernmental S&T Cooperation: Porous materials and residual stress in metals studied by nuclear microscopies (L. Bottyán, 2012-2014)

## LONG TERM VISITOR

— Luu Anh Tuyen, Center for Nuclear Techniques in Hochiminh City, Vietnam, from 23 July to 3 September, 2012, (host: L. Bottyán)

## PUBLICATIONS

### Articles

1. Deák L, Fülöp T; Reciprocity in quantum, electromagnetic and other wave scattering; *Ann Phys - New York*; **327**, 1050-1077, 2012
2. Bottyán L, Merkel DG, Nagy B, Major J; Neutron reflectometer with polarization option at the Budapest Neutron Centre; *Neutron News*; **23**, 21-24, 2012
3. Deák L, Bottyán L, Fülöp T, Kertész G, Nagy DL, Ruffer\* R, Spiering\* H, Tanczikó F, Vankó G; Switching reciprocity on and off in a magneto-optical x-ray scattering experiment using nuclear resonance of  $\alpha$ - $^{57}\text{Fe}$  foils; *Phys Rev Lett*; **109**, 237402/1-4, 2012

*See also R-L.3*

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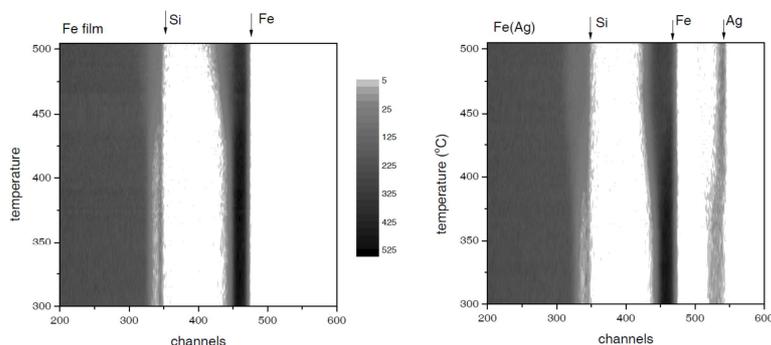
**R-M. ION BEAM PHYSICS**


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*Endre Kótai, Pál Kostka, Attila Németh, Edit Szilágyi*

**Real-time backscattering.** — Applying in situ backscattering spectrometry (BS) during annealing opens a new possibility to characterise both composition and thickness of the formed layers. Since only a few minutes are needed to collect a BS spectrum, this may be done continuously to provide a real-time analysis of the reactions. Detailed depth sensitive information on the film composition is crucial to comprehend the full formation of the growth process. Annealing can be carried out either isothermally or with a linearly ramped temperature, depending on the type of kinetic analysis to be performed. From isothermal annealing the constants of linear-parabolic growth law of solid-state reactions can be determined. When the sample temperature ramped linearly with time and evaluated at each temperature, the thickness of the formed layers allows the determination of the interdiffusion coefficient (both the pre-exponential factor and activation energy) from a single sample.

Due to the high sensitivity of BS to heavy elements, real-time BS is an ideal technique to study the redistribution of heavier elements during various silicide formations that play important role in semiconductor technology as well.



*Fig. 1. Real-time BS measurements using 2000 keV  $^4\text{He}^+$ -beam on a 50 nm Fe film (left) and Fe film containing 1 at. % Ag (right) on Si(100) using ramped annealing (1.9 °C/min). Every horizontal line in such a contour plot corresponds to an RBS spectrum, with a tone scale representing the backscattering yield.*

This year we set up the instrumental requirements of the real-time BS experiments. Computer controlled annealing experiments can be performed both with linearly ramped voltage or current, which allow us to change the temperature as a function of the annealing time. In order to check the temperature calibration at first NiSi formations were studied, and we observed similar processes as can be found in the literature.

To study the impurity effect of Ag on the iron silicide formation, 50 nm of Fe layer was grown on Si(100) substrate with and without of 1 at% Ag. The samples were covered by a 5 nm Si layer to avoid oxidation. Fig. 1 shows the results of real-time BS of both samples using ramped annealing (1.9°C/min) up to 500°C. In case of pure Fe film, no change on the Fe layer can be observed up to 425°C. Then suddenly, the whole iron layer transformed into Fe<sub>2</sub>Si, above at 450°C the left side of the iron peak gradually smeared out, which can be interpreted

as formation of various iron silicide ( $\text{FeSi}$ ,  $\text{FeSi}_2$ ,  $\text{FeSi}_3$ ) interface layers. In the Ag containing film the reaction started about  $400^\circ\text{C}$  ( $\text{Fe}_4\text{Si}$  and  $\text{Fe}_3\text{Si}$ ), and suddenly (around  $425^\circ\text{C}$ ) the composition of the whole layer changed to  $\text{Fe}_1\text{Si}_1$ , moreover Ag segregation can be observed at the surface. No sign of starting other solid state reaction up to  $500^\circ\text{C}$ .

## **PUBLICATIONS**

### *Articles*

1. Baji\* Zs, Szanyo\* A, Molnár\* Gy, Tóth\* AL, Petó\* G, Frey\* K, Kótai E, Kaptay\* G; Formation of nanoparticles by ion beam irradiation of thin films; *J Nanosci Nanotechnol*; **12**, 5009-5015, 2012
2. Jeynes\* C, Barradas\* NP, Szilágyi E; Accurate determination of quantity of material in thin films by Rutherford backscattering spectrometry; *Anal Chem*; **84**, 6061-6069, 2012

## R-N. NON-DESTRUCTIVE STUDY OF CULTURAL HERITAGE OBJECTS (CHARISMA)

Zoltán Szőkefalvi-Nagy, Imre Kovács

Preservation and conservation of our cultural heritage has become one of the main concerns today all over the world. In particular there is an increasing need for non-destructive investigations, as sampling from the unique and precious objects of art and archaeology is inadmissible in most cases. The external beam version of particle induced X-ray emission spectroscopy (PIXE), where the bombarding particles (few MeV protons in most cases) are extracted from the vacuum chamber of the particle accelerator through a thin foil “window” into the atmosphere is specially suited for elemental analysis of even extended objects, too. Our work in this field is carried out in the frame the EU-funded integrating activity project CHARISMA (Cultural Heritage Advanced Research Infrastructures: Synergy for a Multidisciplinary Approach to Conservation/Restoration, carried out in the FP7 Capacities Specific Programme "Research Infrastructures"). Successful applicants from eligible EU countries visit the Van de Graaff accelerator laboratory for missions of few days bringing along their valuable object to investigate. Measurements, data evaluation and interpretation of the results are made in common.

**Technical developments.** — The former ponderous external beam PIXE setup was radically modified. The simplified mounting of the accelerator beam tube and the enforced sample holding stage allow much easier rough positioning of larger and heavier objects. The new mechanical sighting arrangement together with a monitoring video camera makes more accurate final beam spot adjustment. In addition the computer controlled compact Peltier-cooled Amptek X-123 x-ray spectrometer with SDD detector simplifies data acquisition and reduces running cost.

**An illustrative example.** — The PIXE spectrum clearly shows that an ancient metal night-light holder from Italy was manufactured from almost pure Zn in contrast to former supposition of bronze (CHARISMA project of M. Rogante).

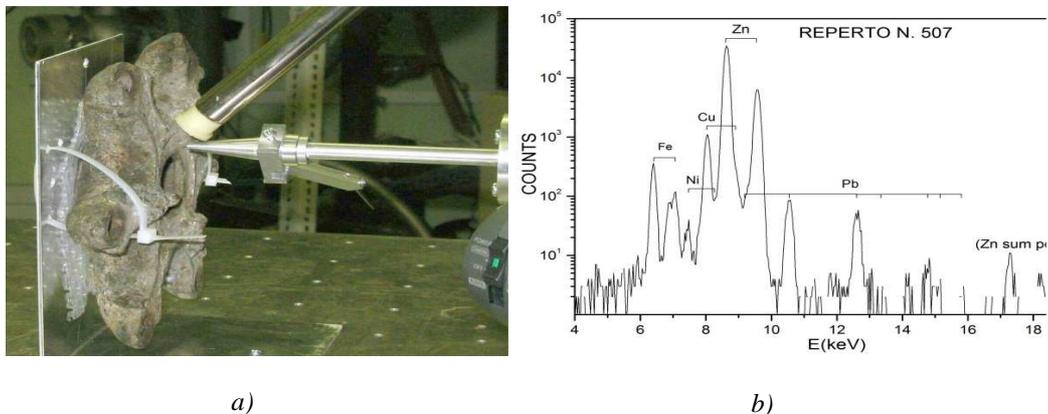


Fig 1.a) The sample-beam pipe- detector arrangement of the external beam PIXE set-up; b) The PIXE spectrum obtained with dominating Zn K x-ray lines.

R-N. Non-destructive study of cultural heritage objects (CHARISMA)

**GRANTS AND COOPERATIONS**

CHARISMA Grant Agreement No. 228330 (2009-2014)

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**R-O. HIGH TEMPERATURE PLASMA PHYSICS**

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*Gábor Kocsis, Márk Aladi,<sup>#</sup> Gábor Cseh, Angéla Barňa,<sup>#</sup> Attila Bencze, Gábor Cseh,<sup>#</sup> Dániel Dunai, István Földes, Sándor Kálvin, Máté Lampert,<sup>#</sup> Gábor Petravich, Dániel Réfy, Tamás Szepesi, Balázs Tál,<sup>#</sup> Gábor Veres, Sándor Zoletnik*

The largest portion of our activities is connected to ITER, the fusion test reactor being built in Cadarache, France. Our group is responsible for several diagnostic developments and technical services financed by the ITER's European Domestic Agency, the Fusion for Energy. Our group is heading a consortium of three Hungarian institutions to deliver the electrical services of in-vessel, in-cryostat and in-divertor diagnostic components in ITER.

A second important field is the development of intelligent fast framing camera. Event Detection Intelligent CAMera (EDICAM) was designed for the video survey diagnostics system of the Wendelstein 7-X stellarator (W7-X). Taking into account the harsh environment and the difficult availability of the W7-X tangential port, a special camera has to be designed: small (camera body diameter is limited to 6 cm, the length to 20 cm) and resistant against strong (2.5 T) and fast changing magnetic field. The camera is divided into a small sensor module (SM) and an Image Processing and Control Unit (IPCU) residing in a commercial personal computer. Owing to the steady state operation the images cannot be stored in memory located in SM but rather they are directly transferred via a 10-Gbit optical link into IPCU. The maximum bandwidth of the sensor selected is high (6.5 Gbit/s) therefore this diagnostics produces tremendous amount of data. It is clear that to manage this problem special hardware is needed to make real time processing to be able to react on events dangerous for the environments or interesting for the scientific investigations and – if it is reasonable – to reduce the amount of the stored data. This is done by the FPGA based IPCU.

The IPCU controls the SM operation, receives and processes data from SM, and sends data to PC via PCIe DMA channel. IPCU translates the periodic image read operations into individual sensor readout operations. It can support the image processing functions as well, which means it makes IPCU a real time pre-processor. Trigger signal inputs and outputs are located at the IPCU. These hardware level inputs can force readouts or change the exposure control during operation.

Presently camera hardware and firmware tests are ongoing and the W7-X video survey diagnostics will be fully operational in 2013.

The Korea Research Council of Fundamental Science and Technology (KRCF) awarded a grant in 2011 for the establishment of a joint Hungarian-Korean laboratory. Since then several Korean researchers visited Wigner RCP for evaluating data obtained with the trial system and participating in the design of the final BES system. The joint work revealed signatures of turbulence at the edge of the KSTAR plasma and showed that turbulence eddies extend to at least 2 m along magnetic field lines. In 2012 a final BES observation system has been designed in collaboration with the Budapest University of Technology and Economics. The setup transmits light along the 2 m long port tube out from the tokamak where it is filtered using a carefully designed interference filter and detected by a 4×8 pixel avalanche photodiode camera built by Adimtech Kft, a spin-off company of Wigner RCP. A CCD

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<sup>#</sup> PhD student

camera is used for spatial calibration. This optical system is looking onto the heating Deuterium beam of the KSTAR tokamak. To improve diagnostic performance at the plasma edge, design work for a neutral Lithium beam injector has also started in 2012. This beam will go through in 2013 the same observation volume as the BES optics has. By selecting between two interference filters the diagnostic will be capable of measuring both the Li-beam and the heating beam light.

The BES observation system was built in summer 2012 and installed on the KSTAR tokamak in September 2012. First measurements showed that a signal-to-noise ratio up to 100 can be reached.

## GRANTS AND INTERNATIONAL COOPERATION

Hungarian National Development Agency No. NAP-1-2005- 0013 (S. Zoletnik, 2005-2012)

European Communities under the contract of Association between EURATOM and the Hungarian Academy of Sciences. (S. Zoletnik, 1999-)

Hungarian-Korean Joint Laboratory Program in Science and Technology: Joint fusion laboratory. (S. Zoletnik, 2011-2013)

Fusion for Energy, F4E-FPA-328, (G. Veres 2012-2016)

## LONG-TERM VISITORS

- Minjun Choi, POSTECH Pohang, South Korea, January 2012 (host: S. Zoletnik)
- Kyu Dong Lee, NFRI, Daejeon, South Korea, May-July 2012 (host: S. Zoletnik)

## PUBLICATIONS

### Articles

1. Nam<sup>\*</sup> YU, Zoletnik S, Lampert M, Kovácsik<sup>\*</sup> Á; Analysis of edge density fluctuation measured by trial KSTAR beam emission spectroscopy system; *Rev Sci Instrum*; **83**, 10D531/1-3, 2012
2. Guszejnov<sup>\*</sup> D, Pokol<sup>\*</sup> GI, Pusztai<sup>\*</sup> I, Refy D, Zoletnik S, Lampert M, Nam<sup>\*</sup> YU; Three-dimensional modeling of beam emission spectroscopy measurements in fusion plasmas; *Rev Sci Instrum*; **83**, 113501/1-7, 2012

### Conference proceedings

3. Nam<sup>\*</sup> YU, Zoletnik S, Lee<sup>\*</sup> KD, Lampert M; Edge density fluctuation patterns at the KSTAR tokamak measured by two-dimensional beam emission spectroscopy; In: *Proc. 39<sup>th</sup> EPS Conference & 16<sup>th</sup> Int. Congress on Plasma Physics EPS/ICPP (Stockholm, Sweden, 2-6 July 2012)*; Eds: S. Ratynskaya, L. Blomberg, A. Fasoli, EPS; P.4.069, 2012
4. Lampert M, Choi<sup>\*</sup> M, Guszejnov<sup>\*</sup> D, Jeon<sup>\*</sup> YM, Kiss I, Kovácsik<sup>\*</sup> Á, Nam<sup>\*</sup> YU, Park<sup>\*</sup> H, Pokol<sup>\*</sup> G, Veres G, Zoletnik S; Beam emission spectroscopy measurements on KSTAR, In: *Proc. 39<sup>th</sup> EPS Conference & 16<sup>th</sup> Int. Congress on Plasma Physics EPS/ICPP (Stockholm, Sweden, 2-6 July 2012)*; Eds: S. Ratynskaya, L. Blomberg, A. Fasoli, EPS; P1.075, 2012

5. Zoletnik S, Buday Cs, Dunai D, Kálvin S, Krämer-Flecken\* A, Liang\* Y, Petravich G, Soldatov\* S, Pearson\* J, Réfy D, TEXTOR Team\*; Dynamics of the Electron Density Profile and Plasma Turbulence during the L-H transition and ELMs in TEXTOR; In: *Proc. 39<sup>th</sup> EPS Conference & 16<sup>th</sup> Int. Congress on Plasma Physics EPS/ICPP (Stockholm, Sweden, 2-6 July 2012)*; Eds: S. Ratynskaya, L. Blomberg, A. Fasoli, EPS;O3.107, 2012
6. Dodt\* D, Brix\* M, Beurskens\* MNA, Flanagan\* J, Kempenaars\* M, Maslov\* M, Fischer\* R, Schweinzer\* J, Zoletnik S, Dunai D, Nedzelskiy\* IS, Refy D, Petravich G., Leyland\* MJ and JET-EFDA contributors\*; Pedestal Density Profiles from the Upgraded Lithium Beam Diagnostic at JET and Comparison to Expectations from Neutral Penetration; In: *Proc. 39<sup>th</sup> EPS Conference & 16<sup>th</sup> Int. Congress on Plasma Physics EPS/ICPP (Stockholm, Sweden, 2-6 July 2012)*; Eds: S. Ratynskaya, L. Blomberg, A. Fasoli, EPS;P1.020, 2012

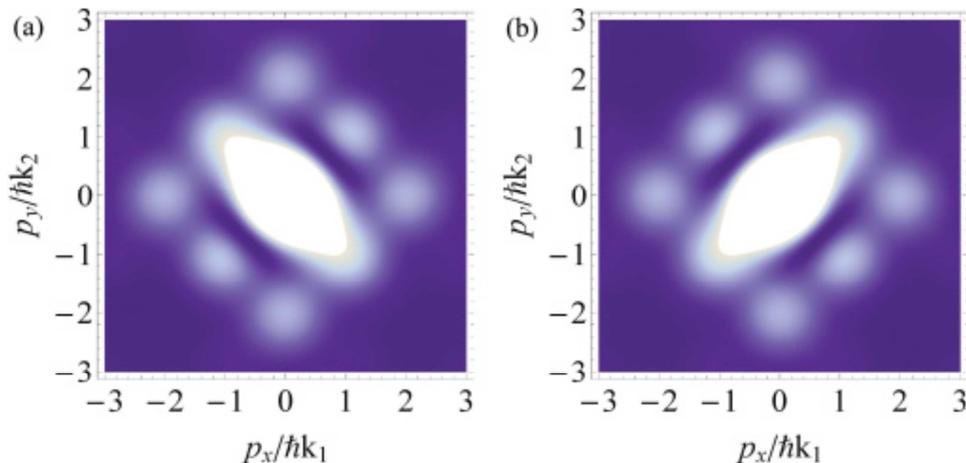
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**R-P. LOW TEMPERATURE PLASMA AND ATOM PHYSICS IN STRONG LASER FIELDS**


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*Gagik Dzsotjan, József Bakos, Gábor Demeter, Dávid Dzsotjan, Miklós Kedves, Béla Ráczkevi, Nóra Sándor, Zsuzsanna Sörlei*

One of the basic processes of atom optics is the manipulation of atomic ensembles by external laser fields. It turns out that the results depend strongly on the initial preparation of the atomic systems. We have proposed and analyzed novel schemes for creation of coherent superposition of meta-stable states in multi-level atoms using frequency-chirped laser pulses with negligible excitation of the atoms. We have shown that the proposed schemes may be equally efficient in homogeneously and Doppler-broadened media. By numerically solving the master equation for the density matrix operator, we have analyzed the influence of relaxation processes on the efficiency of the creation of superposition states and have shown that the proposed schemes are robust against small-to-medium variations of the laser field's parameters.



*Fig.1. 2D momentum distribution of two-level model atoms for two cases of the initial preparation: a)- initial populations of the states are equal with the zero phase of the coherence (a) and with the phase of the coherence equal to pi radian (b).*

We have shown in our investigation how the atomic inner dynamics may be visualized in coherent acceleration of an atomic cloud cooled and trapped in magneto-optical trap (MOT) by short laser pulses, as well as in deflection of the atoms by standing light waves in an optical cavity.

In the case of MOT, we have demonstrated experimentally how the dynamics of the population transfer in atoms induced by laser pulses is reflected in the transfer of mechanical moment from pulsed laser fields to atomic ensemble. In particular, we have analyzed acceleration of a cloud of trapped and cooled Rb atoms in the field of counter-propagating short laser pulses with special form of the frequency chirp. Namely, the direction of the chirp was changing during the laser pulse providing multiple population transfer between the working levels and, respectively, transfer of multiple mechanical momentum to the atoms

compared with the case of the monotonic chirp. The results of the experiment are compared with the theoretical analysis and reasonable agreement is revealed.

In the case of optical cavity, we have demonstrated that initial preparation of atoms in coherent superposition states is qualitatively displayed in two-dimensional patterns of atoms deflected on two crossed standing waves (Fig.1). The analysis is done in quantum treatment for three-level atoms in a lambda configuration, interacting with two crossed standing light waves.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA NN 78112 Light slowing down by frequency-chirped laser pulses (G. Dzsotjan, 2010-2013)

OTKA K68240 Nonlinear effects in the interaction of frequency modulated laser pulses with rubidium atoms in magneto-optical trap (G. Dzsotjan, 2007-2012)

Hungarian National Development Agency: ELI-09-1-2010-0010, "HELIOS" grant (G. Dzsotjan, 2012-2013)

Bilateral collaboration project with the Institute of Physics of the Jagellonian university, Krakow, Poland in the frame of cooperation between the Hungarian and Polish Academies of Sciences (G. Dzsotjan, 2010-2013)

Bilateral collaboration project with the Institute for Physical Research, Ashtarak, Armenia in the frame of cooperation between the Hungarian and Armenian Academies of Sciences (G. Dzsotjan, 2010-2012)

## PUBLICATIONS

### Articles

1. Abovyan\* GA, Djotyan GP, Kryuchkian\* GYu; Visualization of superposition states and Raman processes with two-dimensional atomic deflection; *Phys Rev A*; **85**, 013846/1-7, 2012
2. Demeter G, Kis Z, Hohenester\* U; Nonlinear pulse propagation phenomena in ion-doped dielectric crystals; *Phys Rev A*; **85**, 033819/1-8, 2012

### Conference proceedings

3. Sándor N, Bakos JS, Sörlei Zs and Djotyan GP; Creation of coherent superpositions between metastable atomic states in Doppler-broadened media; *J Phys Conf Ser*, **350**, 012002/1-6, 2012
4. Djotyan GP, Sandor N, Bakos JS, Sörlei Zs; Optical storage in quantized media; *Proc. SPIE* **8414**, 84140X/1-5, 2012; <http://dx.doi.org/10.1117/12.923473>
5. Dzsotjan D, Fleischhauer\* M; Long-range coupling of single atoms mediated by metallic nano-wires and metamaterials: collective decay rate modifications and level shifts, *Proc. SPIE: Plasmonics: Metallic Nanostructures and Their Optical Properties X*, **8457**, 84573R/1-15, 2012

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## R-Q. LABORATORY OF SPEECH TECHNOLOGY FOR REHABILITATION (LSTR)

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*András Arató, Norbert Márkus, Szabolcs Malik*

The two main activities of LSTR are talking aids for the blind and talking aids for people living with autism.

**The Mobile SlateTalker (MOST)** system was ported to different versions of the Android operating system (2.2, 2.3, 3.0 and 4.0) and different models of smartphones including Motorola Milestone2 and Defy, Sony Ericsson Xperia Mini Pro 2. Different text-to-speech programs were included into MOST and the user can easily switch from one to other. Our Brailab text-to-speech program was modified for use with the Hungarian free NVDA (Non Visual Desktop Access) screen reader program. This task continues into next year.

A stuttering autistic boy was taught the *Morse language* which he can reproduce fluently. The Morse language is used today only by radio amateurs, so we built a radio station with the call sign HA5RST (R)ehabilitation with (S)peech (T)echnology or (R)eadability (S)ignal strength (T)one which is the report abbreviation in Morse transmission. Our speaking TalkPad program was ported to the Android operating system to facilitate communication. Three autistic children use TalkPad which helps us to understand more the nature of autism. Morse language and spoken speech can be compared and investigated to understand the nature of communication disorders.



*TalkPad for facilitated communication*

*MOST smartphones with Braille mask*

## PUBLICATIONS

### *Conference proceedings*

1. Arató A, Márkus N, Juhász Z; Speaking and understanding Morse language, speech technology and autism; In: *Proc. ICCHP 2012 13th International Conference on Computers Helping People with Special Needs (University of Linz, Austria, June 10-14, 2012)*; Ed: K. Miesenberger et al., Springer-Verlag, Linz, Austria; Part II. pp. 311-314, 2012.

2. Márkus N, Malik Sz, Juhász Z, Arató A; Accessibility for the Blind on an Open-Source Mobile Platform, MObile Slate Talker (MOST) for Android; In: *Proc. ICCHP 2012, 13<sup>th</sup> International Conference on Computers Helping People with Special Needs (University of Linz, Austria, June 10-14)*; Ed: K. Miesenberger et al., Springer-Verlag, Linz, Austria; Part II. pp. 599-606, 2012.

**Research**

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**INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS**

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**S-A. STRONGLY CORRELATED SYSTEMS**


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*Örs Legeza, Gergely Barcza,<sup>#</sup> Imre Hagymási,<sup>#</sup> Annamária Kiss, Miklós Lajkó,<sup>#</sup> Karlo Penc, Judit Romhányi,<sup>#</sup> Jenő Sólyom, Ferenc Woytnarovich*

**Anderson and Kondo problems.** — Available analytical methods to study strongly correlated systems – which form the basis of present-day development of electronic devices – are very limited, thus application of numerical procedures is mandatory. We have investigated an extended version of the periodic Anderson model (the so-called periodic Anderson-Hubbard model) with the aim of understanding the role of interaction between conduction electrons in the formation of the heavy-fermion and mixed-valence states. Two methods were used: (i) variational calculation with the Gutzwiller wave function optimizing numerically the ground-state energy and (ii) exact diagonalization of the Hamiltonian for short chains. The  $f$ -level occupancy and the renormalization factor of the quasiparticles were calculated as a function of the energy of the  $f$  orbital for a wide range of the interaction parameters. The results obtained by the two methods are in reasonably good agreement for the periodic Anderson model. The agreement is maintained even when the interaction between band electrons,  $U_d$ , is taken into account, except for the half-filled case. This discrepancy can be explained by the difference between the physics of the one and higher dimensional models. We have found that this interaction shifts and widens the energy range of the bare  $f$  level, where heavy-fermion behaviour can be observed. For large enough  $U_d$  this range may lie even above the bare conduction band. The Gutzwiller method indicates a robust transition from Kondo insulator to Mott insulator in the half-filled model, while  $U_d$  enhances the quasi-particle mass when the filling is close to half filling.

**Exotic magnetic orders of high-spin ultracold atoms.** — Recently ultracold atomic and molecular systems have been in the focus of theoretical and experimental studies as they can also be used as simulators of condensed matter physics. For a long time magnetic ordering and superconductivity were thought to be incompatible. In fact, homogeneous ferromagnetic order excludes a homogeneous superconducting order of singlet Cooper pairs. We have shown that the system of ultracold atoms with hyperfine spin  $F = 3/2$  might be unstable against the formation of quintet pairs if the interaction is attractive in the quintet channel. We have investigated the behaviour of correlation functions in a model including only s-wave interactions at quarter filling by large-scale density-matrix renormalization-group simulations. We have shown that the correlations of quintet pairs become quasi-long-ranged, when the system is partially polarized, leading to the emergence of various mixed superfluid phases in which BCS-like pairs carrying different magnetic moments coexist.

**Multiferroics.** — The research of the technologically important multiferroics – materials simultaneously exhibiting ordering of different degrees of freedom, such as charge, spin, and orbitals – requires a multidisciplinary approach. In the magnetoelectric multiferroics, ferroelectricity is induced by different kinds of magnetic orders via the relativistic spin-orbit interaction. As a direct consequence of the cross-coupling between spins and electric polarization, the control of the ferroelectric polarization by external magnetic field and the manipulation of the magnetic order via electric field can be realized in these systems. Though the basic symmetry requirements for the existence of this cross-coupling are known, the possible microscopic mechanisms behind need to be clarified in order to optimize the

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<sup>#</sup> PhD student

synthesis of multiferroics. To address this question, we have studied the static and dynamic properties of one such compound,  $\text{Ba}_2\text{CoGe}_2\text{O}_7$ , in close collaboration with experimentalists. Due to the magnetoelectric coupling, the material acquires new optical properties. The spins are excited not only by the magnetic, but also by the electric component of the light. We have identified spin modes where the spins change their length periodically, in contrast to usual spin waves where the spins precess. Using a simple model, we were able to describe the absorption of infrared light in magnetic fields up to 30 T. (Fig. 1)

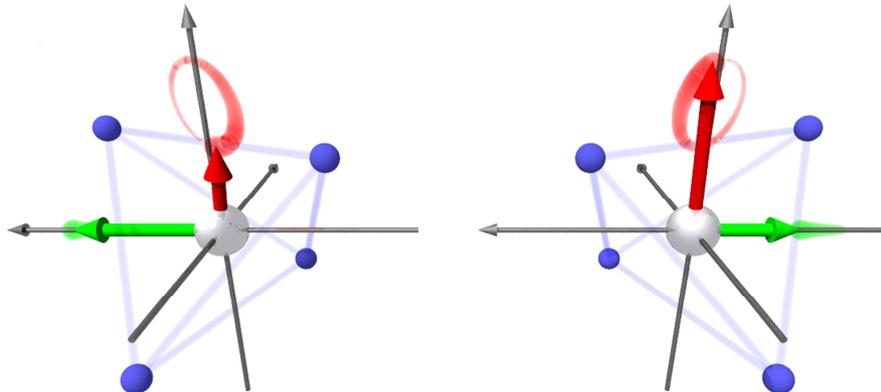


Fig. 1. Motion of the magnetizations (green, light arrows) and the local electric polarizations (red, dark arrows) in the two sublattices for the spin stretching mode. The blue (darker) spheres are the oxygen atoms forming tetrahedral cages around the central Co ions in  $\text{Ba}_2\text{CoGe}_2\text{O}_7$ .

**Spin-relaxation in metals and semiconductors.** — Spin transport electronics, or spintronics, is an emerging field of modern physics due to possible novel devices that carry out efficient transport and storage of information. The central issues in spintronics are the control and manipulation of spin degree of freedom, which requires precise knowledge of the interaction between the spin and its environment in solids. By taking selected semiconductors with zinc-blende crystal structure we have studied the Elliott-Yafet (EY) and Dyakonov-Perel (DP) spin-relaxation mechanisms under inversion symmetry breaking. The band structures in the presence of spin-orbit interaction are obtained within the pseudopotential approximation, and the spin relaxation is treated phenomenologically. Phase diagrams with crossover between the EY and DP processes are obtained as a function of inversion asymmetry, chemical potential, and momentum relaxation rate. According to the widely accepted picture it is expected that the EY mechanism dominates when the inversion symmetry is just slightly broken, while DP mechanism is the most important process in semiconductors with large inversion asymmetry. However, we have found a non-monotonic dependence on the inversion asymmetry for spin-relaxation, which leads to unusual characteristics for semiconductors with large inversion asymmetry such as ZnSe from group II-VI.

**Frustrated magnetic systems.** — We have revisited the phase diagram of the frustrated  $S = 1/2$  spin ladder with antiferromagnetic rungs and diagonal couplings. In particular, we have reexamined the evidence for the columnar dimer phase predicted from an analytic treatment of the model and claimed to be found in numerical calculations. We have found no positive numerical evidence for a finite dimer order parameter in the thermodynamic limit anywhere in the parameter regime in which the columnar dimer phase is expected to appear. Conservative error estimates in the scaling of our data placed stringent limits on the

maximum possible value of the dimer order parameter and the maximum possible extent of the parameter regime in which a sufficiently weak dimer phase could still exist.

**Tensor factorization in high-dimensional spaces.** — The treatment of high-dimensional problems such as the Schrödinger equation can be approached by concepts of tensor product approximation. We have presented general techniques that can be used for the treatment of high-dimensional optimization tasks and time-dependent equations, and connect them to concepts already used in many-body quantum physics.

**Quantum-chemical applications of the DMRG algorithm.** — We have presented a novel approach based on the density-matrix renormalization group (DMRG) algorithm for the calculation of spin density distributions for molecules that require very large active spaces for a qualitatively correct description of their electronic structure. Our approach is based on calculating the spin-density matrix elements as basic quantity for the spatially resolved spin-density distribution.

Electron correlation effects are essential for an accurate *ab initio* description of molecules. A quantitative *a priori* knowledge of the single- or multireference nature of electronic structures as well as of the dominant contributions to the correlation energy can facilitate the decision regarding the optimum quantum chemical method of choice. We have proposed concepts from quantum information theory, such as orbital entanglement measures, that allow one to evaluate the single- and multireference character of any molecular structure in a given orbital basis set. By studying these measures we can detect possible artifacts of small active spaces.

We have continued our study of the elementary excitations of a model Hamiltonian for the  $\pi$ -electrons in poly-diacetylene chains including electron-phonon interactions as well. We have shown that inclusion of lattice relaxation, local potentials, different spring constants for the double and triple bonds as well as an accurate description of the long-ranged screened Coulomb potential are mandatory to reproduce experimental values. Optimization tasks and DMRG calculations have been carried out in a seven-dimensional parameter space.

## GRANTS AND INTERNATIONAL COOPERATION

- OTKA K68340      Quantum phase transitions in low-dimensional magnetic and fermionic systems (J. Sólyom, 2007–2012)
- OTKA K73455      Quantum phases and phase transitions in tunable correlated systems (K. Penc, 2008-2012)
- OTKA K100908    Simulating strongly correlated systems with fermionic alkaline earth atom isotopes in optical lattices and related quantum chemistry of transition metal complexes (Ö. Legeza, 2012–2016)
- Marie Curie Grant: Numerical study of dynamics and magnetic properties of PIRG-GA-strongly correlated electron systems (A. Kiss, 2011-2015)
- 2010-276834: MTA-EAS NMR and ESR studies of low dimensional strongly correlated electron systems (K. Penc, 2010-2012).
- Momentum Award of MTA: Tensor factorization in high-dimensional spaces and applications to ultracold atomic systems and transition metal complexes (Ö. Legeza 2012-2017).

## PUBLICATIONS

## Articles

1. Romhányi J, Lajkó M, Penc K; Zero- and finite-temperature mean field study of magnetic field induced electric polarization in  $\text{Ba}_2\text{CoGe}_2\text{O}_7$ : The effect of the antiferroelectric coupling; *Phys Rev B*; **84**, 224419/1-8, 2011
2. Hagymási I, Itai\* K, Sólyom J; Periodic Anderson model with d-f interaction, Proceedings of the European Conference Physics of Magnetism 2011, Poznan; *Acta Physica Polonica A*; **121**, 1070/1-3, 2012
3. Hagymási I, Itai\* K, Sólyom J; Periodic Anderson model with correlated conduction electrons: Variational and exact diagonalization study; *Phys Rev B*; **85**, 235116/1-13, 2012
4. Barcza G, Legeza Ö, Noack\* RM, Sólyom J; Dimerized phase in the cross-coupled antiferromagnetic spin ladder; *Phys Rev B*; **86**, 075133/1-6, 2012
5. Boguslawski\* K, Marti\* KH, Legeza Ö, Reiher\* M; Accurate ab initio spin densities; *J Chem Theory Comput*; **8**, 1970-1982, 2012
6. Corboz\* P, Penc K, Mila\* F, Läuchli\* AM; Simplex solids in  $\text{SU}(N)$  Heisenberg models on the kagome and checkerboard lattices; *Phys Rev B*; **86**, 041106(R)/1-5, 2012
7. Penc K, Romhányi J, Rössler\* T, Nagel\* U, Antal\* Á, Fehér\* T, Jánossy\* A, Engelkamp\* H, Murakawa\* H, Tokura\* Y, Szaller\* D, Bordács\* S, Kézsmárki\* I; Spin-stretching modes in non-centrosymmetric magnets: spin-wave excitations in the multiferroic  $\text{Ba}_2\text{CoGe}_2\text{O}_7$ ; *Phys Rev Lett*; **108**, 257203/1-5, 2012
8. Korshunov\* SE, Mila\* F, Penc K; Degeneracy and ordering of the non-coplanar phase of the classical bilinear-biquadratic Heisenberg model on the triangular lattice; *Phys Rev B*; **85**, 174420/1-9, 2012
9. Pereira\* R, Penc K, White\* SR, Sacramento\* PD, Carmelo\* JMP; Charge dynamics in half-filled Hubbard chains; *Phys Rev B*; **85**, 165132/1-19, 2012
10. Tóth\* TA, Läuchli\* AM, Mila\* F, Penc K; Competition between two- and three-sublattice ordering for  $S=1$  spins on the square lattice; *Phys Rev B*; **85**, 140403(R)/1-5, 2012
11. Bauer\* B, Corboz\* P, Läuchli\* AM, Messio\* L, Penc K, Troyer\* M, Mila\* F; Three-sublattice order in the  $\text{SU}(3)$  Heisenberg model on the square and triangular lattice; *Phys Rev B*; **85**, 125116/1-11, 2012
12. Shannon\* N, Sikora\* O, Pollmann\* F, Penc K, Fulde\* P; Quantum ice: a quantum Monte Carlo study; *Phys Rev Lett*; **108**, 067204/1-5, 2012
13. Lajkó M, Sindzingre\* P, Penc K; Exact ground states with deconfined gapless excitations for the 3 leg spin-1/2 tube; *Phys Rev Lett*; **108**, 017205/1-5, 2012
14. Boguslawski\* K, Tecmer\* P, Legeza Ö, Reiher\* M; Entanglement measures for single- and multireference correlation effects; *J Phys Chem Lett*; **3**, 3129-3135; 2012
15. Corboz\* P, Lajkó M, Läuchli\* AM, Penc K, Mila\* F; Spin-orbital quantum liquid on the honeycomb lattice; *Phys Rev X*; **2**, 041013/1-11, 2012

16. Romhányi J, Penc K; Multiboson spin-wave theory for Ba<sub>2</sub>CoGe<sub>2</sub>O<sub>7</sub>, a spin-3/2 easy-plane Néel antiferromagnet with strong single-ion anisotropy; *Phys. Rev. B*; **86**, 174428/1-10, 2012

***Other***

17. Woynarovich F; Milyen tantárgy a fizika? (What kind of school subject is Physics? in Hungarian); *Fizikai Szemle*; **62/6**,205-207, 2012

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**S-B. COMPLEX SYSTEMS**


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*Ferenc Iglói, Róbert Juhász, István Kovács,<sup>#</sup> Gergely Roósz,<sup>#</sup> András Süttő, Péter Szépfalussy*

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

**Phase transitions and critical behaviour.** — We have calculated the entanglement entropy of the random transverse-field Ising model by a numerical implementation of the asymptotically exact strong disorder renormalization group method in  $2d$ ,  $3d$  and  $4d$  hypercubic lattices for different shapes of the subregion. We have found that the area law is always satisfied, but there are analytic corrections due to  $E$ -dimensional edges ( $1 \leq E \leq d - 2$ ). We have observed that the contribution arising from corners is logarithmically divergent at the critical point and its prefactor in a given dimension is universal, i.e. independent of the form of disorder.

We have studied the time evolution of the entanglement entropy  $S(t)$  of a block of spins in the random transverse-field Ising chain after a sudden change of the parameters of the Hamiltonian by means of free fermionic techniques. We have considered global quenches, when the parameters are modified uniformly in space, as well as local quenches, when two disconnected blocks are suddenly joined together. For a non-critical final state, the dynamical entanglement entropy is found to approach a finite limiting value for both types of quenches. If the quench is performed to the critical state, the entropy grows for an infinite block as  $S(t) \sim \ln \ln t$ . This type of ultraslow increase is explained through the strong disorder renormalization group method.

We have analysed the contact process, the simplest model for propagation phenomena, with node-dependent infection rates (i.e. intrinsic quenched disorder) on complex networks. We have found Griffiths phases and other rare region effects leading rather generically to anomalously slow (algebraic, logarithmic, etc.) relaxation on Erdős-Rényi networks. Similar effects are predicted to exist for other topologies as long as a non-vanishing percolation threshold exists. More strikingly, we have found that Griffiths phases can also emerge, even with constant epidemic rates, as a consequence of mere topological heterogeneity. In particular, we have observed Griffiths effects in finite dimensional networks as, for instance, a family of generalized small-world networks.

Considering diffusion in the presence of asymmetric disorder, an exact relationship between the strength of weak disorder and the electric resistance of the corresponding resistor network has been revealed, which is valid in arbitrary networks. This implies that the dynamics are stable against weak asymmetric disorder if the resistance exponent  $\zeta$  of the network is negative. In the case of  $\zeta > 0$ , numerical analyses of the mean first-passage time  $\tau$  on various fractal lattices have shown that the logarithmic scaling of  $\tau$  with the distance  $l$ ,  $\ln \tau \sim l^\psi$ , is a general rule, characterized by a new dynamical exponent  $\psi$  of the underlying lattice.

**Quantum systems.** — We have considered global quenches in the quantum XY chain in a transverse field and studied the nonequilibrium relaxation of the magnetization and the correlation function as well as the entanglement entropy in finite systems. For quenches in the ordered phase the exact results are explained and well described by a semiclassical theory in terms of ballistically moving quasiparticle pairs. For finite systems quasiperiodic behaviour of the dynamical evolution of the local order parameter and the correlation functions is predicted correctly including the period length, an exponential relaxation, a quasistationary

regime and an exponential recurrence in one period. In the thermodynamic limit the semiclassical theory is exact for the entanglement entropy and its modified version is exact for the magnetization and the correlation function, too. The stationary correlation function is shown to be described by a generalized Gibbs ensemble.

The three fluid hydrodynamics of the spin-1 spin or Bose gas has been shown to be valid even when the Bose condensation occurs in all the three Zeeman levels. We discussed the damping of the quadrupolar spin waves in the critical region, where three fluid hydrodynamics goes over to the usual two fluid ones.

We have continued the application of the pseudopotential theory generalized to trapped superfluid Fermi gases. We determined the excess energy when one atom is added to a system with even number of particles in cases in anisotropic traps as well.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA T075324 Effects of disorder in many body systems (F. Iglói, 2009-2013)

OTKA K77629 Investigation of fundamental problems of phase transitions and symmetry breaking phases (P. Szépfalusy, 2009-2013)

## PUBLICATIONS

### Articles

1. Kovács IA, Iglói F; Universal logarithmic terms in the entanglement entropy of 2d, 3d and 4d random transverse-field Ising models; *EPL*; **97**, 67009/1-6, 2012
2. Iglói F, Szatmári\* Zs, Lin\* Y-C; Entanglement entropy dynamics of disordered quantum spin chains; *Phys Rev B*; **85**, 094417/1-8, 2012
3. Blaß\* B, Rieger\* H and Iglói F; Quantum relaxation and finite size effects in the XY chain in a transverse field after global quenches; *EPL*; **99**, 30004/1-6, 2012
4. Juhász R; Competition between quenched disorder and long-range connections. A numerical study of diffusion; *Phys Rev E*; **85**, 011118/1-8, 2012
5. Juhász R, Ódor\* G, Castellano\* C, Munoz\* MA; Rare region effects in the contact process on networks; *Phys Rev E*; **85**, 066125/1-14, 2012
6. Juhász R; The effect of asymmetric disorder on the diffusion in arbitrary networks; *EPL*; **98**, 30001/1-5, 2012
7. Juhász R and Ódor\* G; Anomalous coarsening in disordered exclusion processes; *J Stat Mech*; P08004/1-17, 2012
8. Csordás\* A, Homa\* G and Szépfalusy P; Calculation of the even-odd energy difference in superfluid Fermi systems using the pseudopotential theory; *EPL*; **97**, 37005/1-6, 2012

*See also: S-T.13*

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**S-C. ELECTRONIC STATES IN SOLIDS**


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*IstvánTüttő, Krisztina Kádas, Balázs Újfalussy, Attila Virosztek,<sup>+</sup> Levente Vitos*

**Magnetic structure and impurities.** — We investigated the interactions of magnetic impurities on surfaces of random substitutional alloys. We found that the interaction acquires an exponential decay due to the smearing of the states at the Fermi level. We also obtained a new type of interaction in platinum and palladium rich alloys.

We performed a detailed study of the ground-state magnetic structure of *ultrathin Fe films* on the surface of fcc Ir(001). We used the spin-cluster expansion technique in combination with the relativistic disordered local moment scheme to obtain the parameters of spin models and, subsequently, determined the favored magnetic structure of the system by means of a mean-field approach as well as by atomistic spin dynamics simulations. For the case of a single monolayer of Fe, we find that layer relaxations very strongly influence the ground-state spin configurations, whereas Dzyaloshinskii-Moriya (DM) interactions and biquadratic couplings also have remarkable effects. To characterize the latter effect, we introduced and analysed the spin collinearity maps of the system. While for two monolayers of Fe we obtained a single- $q$  spin spiral as ground state due to DM interactions, for the case of four monolayers, the system shows a noncollinear spin structure with nonzero net magnetization. These findings are consistent with experimental measurements indicating ferromagnetic order in films of four monolayers and thicker.

Landau phenomenological theory in combination with first-principles calculations was used to reveal the origin of the meta-magnetic nature and the unusually strong dependence of the ordering temperature with doping of the  $Fe_2P$  compound. We show that the magnetism of the two sublattices occupied by Fe atoms has an entwined codependency, which is strongly influenced by alloying.

**Mechanical properties of alloys.** — The *elastic properties* of paramagnetic (PM) Fe- $M$  ( $M = Al, Si, V, Cr, Mn, Co, Ni,$  and  $Rh$ ) solid solutions in the body-centered-cubic (bcc) and face-centered-cubic (fcc) structures were investigated using the exact muffin-tin orbital density functional method in combination with the coherent-potential approximation and disordered local-magnetic-moment model. All impurities considered enlarge or leave nearly constant the equilibrium volume of PM Fe. At the same time, however, they produce both positive and negative changes in the elastic parameters. Some of the alloying elements induce opposite effects on cubic shear elastic parameters of PM bcc and fcc Fe. With a few exceptions, we find that the alloying effects on PM bcc Fe are smaller than on PM fcc Fe. Trends in the tetragonal elastic constant show a general correlation with the trends obtained for the bcc-fcc lattice energy difference.

The *effect of Cr and Ti on the fundamental mechanical properties of V-Cr-Ti alloys* has been investigated using the all-electron exact muffin-tin orbitals method in combination with the coherent-potential approximation. The static lattice constant and elastic parameters have been calculated for the body-centered-cubic V-Cr-Ti random solid solution as a function of composition. Our theoretical predictions are in good agreement with the available experimental data. Alloys along the equicomposition region are found to exhibit the largest shear and Young's modulus as a result of the opposite alloying effects obtained for the two

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<sup>+</sup> Permanent position: Budapest University of Technology and Economics

cubic shear elastic constants. The classical solid-solution hardening (SSH) model predicts larger strengthening effect in V-Ti than in V-Cr. By considering a phenomenological expression for the ductile-brittle transition temperature (DBTT) in terms of Peierls stress and SSH, it is shown that the present theoretical results can account for the variations of DBTT with composition.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA K84078      Magnetic, mechanical and thermal properties of alloys and their surfaces (B. Újfalussy, 2011-2015)

STINT Swedish-Hungarian joint project, Atomic-scale investigation of steel materials by first principles method (L. Vitos, 2009-2014)

Oak Ridge National Laboratory, Research on magnetic properties, (B. Újfalussy, 2012-2013)

## LONG TERM VISITOR

— Hugo Aramberri, University of Madrid, Spain

## PUBLICATIONS

### Articles

1. Kádas K, Ahuja\* R, Johansson\* B, Eriksson\* O, Vitos L; Theoretical prediction of the elastic properties of body-centered cubic Fe-Ni-Mg alloys under extreme conditions; *Philosophical Magazine*; **92**, 888-898, 2012
2. Zhang\* H, Johansson\* B, Ahuja\* R, Vitos L; First-principles study of solid-solution hardening in steel alloys; *Computational Materials Science*; **55**, 269-272, 2012
3. Hu\* Q-M, Luo\* H-B, Li\* C-M, Vitos L, Yang\* R; Composition dependent elastic modulus and phase stability of Ni<sub>2</sub>MnGa based ferromagnetic shape memory alloys; *Science China*; **55**, 295-305, 2012
4. Zhang\* H, Marko\* P, Punkkinen\* J, Johansson\* B, Vitos L; Elastic parameters of paramagnetic iron-based alloys from first-principles calculations; *Phys Rev B*; **85**, 054107, 2012
5. Al-Zoubi\* N, Skorodumova\* N V, Medvedeva\* A, Andersson\* J, Nilson\* G, Johansson\* B, Vitos L; Tetragonality of carbon-doped ferromagnetic iron alloys: A first-principles study; *Phys Rev B*; **85**, 014112, 2012
6. Lu\* S, Hu\* Q-M, Krisztina\* E, Delczeg-Czirjak\* K, Johansson\* B, Vitos L; Determining the minimum grain size in severe plastic deformation process via first-principles calculations; *Acta Materialia*; **60**, 4506-4513, 2012
7. Tian\* F-Y, Chen\* N-X, Shen\* J, Vitos L; A novel potential: the interlayer potential for the fcc (111) plane family; *J Phys: Cond Matter*; **24**, 045001, 2012
8. Delczeg\* L, Johansson\* B, Vitos L; Ab initio description of mono-vacancies in austenitic stainless steels; *Phys Rev B*; **85**, 174101, 2012
9. Kádas K, Teles da Costa\* M, Vitos L, Andersson\* Y, Bergman\* A, and Eriksson\* O; On the icosahedral metal-phosphorus coordination in melliniite; a gift from the sky for materials chemistry; *J Mater Chem*; **22**, 14741, 2012

### S-C. Electronic states in solids

10. Li<sup>\*</sup> X, Zhang<sup>\*</sup> H, Lu<sup>\*</sup> S, Li<sup>\*</sup> W, Zhao<sup>\*</sup> J, Johansson<sup>\*</sup> B and Vitos L; Elastic properties of vanadium-based alloys from first-principles theory; *Phys Rev B*; **86**, 014105, 2012
11. Hoffmann<sup>\*</sup> M, Marmodoro<sup>\*</sup> A, Nurmi<sup>\*</sup> E, Kokko<sup>\*</sup> K, Vitos L, Ernst<sup>\*</sup> A, Hergert<sup>\*</sup> W; Elastic anomalies and long/short range ordering effects: a first-principles investigations of the Ag<sub>c</sub>Pd<sub>1-c</sub> solid solution; *Phys Rev B*; **86**, 094106, 2012
12. Delczeg-Czirjak<sup>\*</sup> K, Bergqvist<sup>\*</sup> L, Eriksson<sup>\*</sup> O, Gercsi<sup>\*</sup> Z, Nordblad<sup>\*</sup> P, Szunyogh<sup>\*</sup> L, Johansson<sup>\*</sup> B, and Vitos L; Microscopic theory of magnetism in the magnetocaloric material Fe<sub>2</sub>P<sub>1-x</sub>T<sub>x</sub> (T = B and Si); *Phys Rev B*; **86**, 045126, 2012
13. Tian<sup>\*</sup> F-Y, Chen<sup>\*</sup> N-X, Delczeg<sup>\*</sup> L and Vitos L; Interlayer potentials for fcc (111) planes of Pd-Ag random alloys; *Computational Materials Science*; **63**, 20-27, 2012
14. Delczeg-Czirjak<sup>\*</sup> E K, Gercsi<sup>\*</sup> Z, Bergqvist<sup>\*</sup> L, Eriksson<sup>\*</sup> O, Szunyogh<sup>\*</sup> L, Nordblad<sup>\*</sup> P, Johansson<sup>\*</sup> B and Vitos L; Magnetic exchange interactions in B-, Si- and As-doped Fe<sub>2</sub>P from first principles theory; *Physical Review B*; **85**, 224435, 2012
15. Vitos L, Zhang<sup>\*</sup> H, Al-Zoubi<sup>\*</sup> N, Lu<sup>\*</sup> S, Nilsson<sup>\*</sup> J-O, Hertzman<sup>\*</sup> S, Nilson<sup>\*</sup> G, and Johansson<sup>\*</sup> B; Stainless Steel Alloys from First-principles Theory; *Metallurgia Italiana*; **5**, 19-27, 2012
16. Luo<sup>\*</sup> H-B, Hu<sup>\*</sup> Q-M, Li<sup>\*</sup> C-M, Yang<sup>\*</sup> R, Johansson<sup>\*</sup> B, Vitos L; Phase stability of Ni<sub>2</sub>(Mn<sub>1-x</sub>Fe<sub>x</sub>)Ga: A first-principles study; *Phys Rev B*; **86**, 024427, 2012
17. Vajna<sup>\*</sup> Sz, Simon<sup>\*</sup> E, Szilva<sup>\*</sup> A, Palotas<sup>\*</sup> K, Ujfalussy B, and Szunyogh<sup>\*</sup> L; Higher-order contributions to the Rashba-Bychkov effect with application to the Bi/Ag(111) surface alloy; *Phys Rev B*; **85**, 075404-075411, 2012
18. Deák<sup>\*</sup> A, Szunyogh<sup>\*</sup> L, Ujfalussy B; Thickness-dependent magnetic structure of ultrathin Fe/Ir(001) films: From spin-spiral states toward ferromagnetic order ; *Phys Rev B*; **84**, 224413- 224422, 2011
19. Virosztek A and Bácsi<sup>\*</sup> A; Friedel oscillations around a short range scatterer: the case of graphene; *J Supercond Nov Magn*; **25**, 691-697, 2012

#### **Conference proceeding**

20. Landa<sup>\*</sup> A, Söderlind<sup>\*</sup> P, Grabowski<sup>\*</sup> B, Turchi<sup>\*</sup> P E A, Ruban<sup>\*</sup> AV, and Vitos L; Ab Initio Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors; in: *Actinides – Basic Science, Applications, and Technology*; *Mater Res Soc Symp Proc*; **v1444**, 67-78, 2012

#### **Book chapter**

21. Vitos L, Zhang<sup>\*</sup> H L, Lu<sup>\*</sup> S, Al-Zoubi<sup>\*</sup> N, Johansson<sup>\*</sup> B, Nurmi<sup>\*</sup> E, Ropo<sup>\*</sup> M, Punkkinen<sup>\*</sup> M P J and Kokko<sup>\*</sup> K, First-principles Quantum Mechanical Approach to Stainless Steel Alloys; In: *Alloy Steel: Properties and Use*, Ed: Eduardo Valencia Morales, InTech, ISBN 978-953-307-888-5, pp. 3-28, 2011

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## S-D. SEMICONDUCTOR NANOSTRUCTURES

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Ádám Gali, Dávid Beke,<sup>#</sup> Thomas Chanier, Tamás Demjén,<sup>#</sup> Tamás Hornos, Viktor Ivády,<sup>#</sup> Hugo Pinto, Bálint Somogyi,<sup>#</sup> Krisztián Szász,<sup>#</sup> Márton Vörös,<sup>#</sup> Viktor Zólyomi

The research team is active in three main fields: develop new type of (i) biomarkers, (ii) spintronics, and (iii) 3rd generation solar cells. Tibor Szilvási (who is an MSc student in physics and PhD student in chemistry), Gergő Thiering (MSc student in physics) and Tamás Simon (MSc student in physics) are also active members of the group.

Particularly, silicon carbide (SiC) nanocrystals were studied by theory and experiments in the research field of biomarkers. The experimental group developed a new method to fabricate fluorescent SiC nanoparticles that were tested in different biological systems. We found that our SiC nanoparticles show no toxicity even at high concentration, which makes them indeed promising for *in vivo* bioimaging. In addition, we demonstrated the two-photon response from a neuron cell injected with our SiC nanoparticles. These results were published in focused issues of *Journal of Materials Research*. We continued to characterize the color centers in SiC by theoretical calculations that might be useful in bioimaging. For example, we identified near-infrared emitters in small SiC nanoparticles. Our results were published in prestigious journals such as *Nanoscale* and *Applied Physics Letters*. The theory group applies beyond state-of-the-art methods where the group leader was invited to write a feature article about the application of the methods. Besides, a 35-page printed review article has been published about the recent results of SiC nanostructures achieved by the group. We also suggested a new solution for *in vivo* bioimaging by preparing sulfurized nanodiamonds. This result was published in *Physical Review Letters*.

Nitrogen-vacancy defect in diamond is a very promising candidate to realize solid state quantum bits. The manipulation of single nitrogen-vacancy center by external electric field was demonstrated where our theoretical calculations helped to understand and interpret the electro-luminescence signals. This breakthrough was published in *Nature Photonics*. We calculated and analysed the photo-excitation and ionization of a nitrogen-vacancy defect by explaining this complex process (our study is under consideration at *Physical Review Letters*). Carbon nanostructures were also investigated. In addition, we proposed to use ultrathin silicon nanowires to host *P*-donors acting as quantum bits that may operate at elevated temperatures as we show in our *Nano Letters* paper.

We could achieve a breakthrough in first-principles calculation of impact ionization rates in semiconductor nanocrystals where the enhanced probability of impact ionization could lead to a big boost in the efficiency of solar cells. The results were presented at conferences and are under review at *Physical Review Letters*.

### GRANTS AND INTERNATIONAL COOPERATION

- |              |   |
|--------------|---|
| OTKA K101819 | Design, fabrication and analysis of luminescent silicon carbide nanocrystals for <i>in vivo</i> biomarker applications (Á. Gali, 2012-2016) |
| OTKA K106114 | Development of novel silicon carbide nanomarkers and more effective glutamate and GABA uncaging materials for measurement of neuronal       |

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<sup>#</sup> PhD student

## S-D. Semiconductor nanostructures

network activity and dendritic integration with three-dimensional real-time two-photon microscopy (Á. Gali, 2012-2017)

EU FP7 No. 270197: DIAMANT-Diamond based atomic nanotechnologies (Á. Gali, 2011-2014)

PRACE Distributed European Computing Initiative (DECI-7) project DIAVIB (Á. Gali, 2011-2012)

## PUBLICATIONS

### Articles

1. Vörös M, Gali Á; Electronic and optical properties of silicon carbide nanotubes and nanoparticles studied by density functional theory calculations: effect of doping and environment; *J Computational and Theoretical Nanoscience*; **9**, 1906-1940, 2012
2. Son\* NG, Trinh\* XT, Gällström\* A, Leone\* S, Kordina\* O, Janzén\* E, Szász K, Ivády V, Gali Á; Electron paramagnetic resonance and theoretical studies of Nb in 4H- and 6H-SiC; *J Appl Phys*; **112**, 083711, 2012
3. Yan\* B, Ruráli\* R, Gali Á; Ab initio study of phosphorus donors acting as quantum bits in silicon nanowires; *Nano Letters*; **12**, 3460-3465, 2012
4. Vörös M, Demjén T, Szilvási T, Gali Á; Tuning the optical gap of nanometer-size diamond cages by sulfurization: a time-dependent density functional study; *Physical Review Letters*; **108**, 267401, 2012
5. Gällström\* A, Magnusson\* B, Beyer\* FC, Gali Á, Son\* NT, Leone\* S, Ivanov\* IG, Hemmingsson\* CG, Henry\* A, Janzén\* E; Optical identification and electronic configuration of tungsten in 4H- and 6H-SiC; *Physica B: Condensed Matter*; **407**, 1462-1466, 2012
6. Yan\* F, Devaty\* R P, Choyke\* W J, Gali Á, Kimoto\* T, Ohshima\* T, and Pensl\* G; Anharmonic vibrations of the dicarbon antisite defect in 4H-SiC; *Applied Physics Letters*; **100**, 132107, 2012
7. Mizuochi\* N, Makino\* T, Kato\* H, Takeuchi\* D, Ogura\* M, Okushi\* H, Nothhaft\* M, Neumann\* P, Gali Á, Jelezko\* F, Wrachtrup\* J, Yamasaki\* S; Electrically driven single photon source at room temperature in diamond; *Nature Photonics*; **6**, 299-303, 2012
8. Vörös M, Gali Á, Kaxiras\* E, Frauenheim\* T, Knaup\* JM; Identification of defects at the interface between 3C-SiC quantum dots and a SiO<sub>2</sub> embedding matrix; *physica status solidi b*; **249**, 360-367, 2012
9. Gali Á; Excitation spectrum of point defects in semiconductors studied by time-dependent density functional theory; *J Materials Research*; **27**, 897-909, 2012
10. Somogyi B, Zólyomi V, Gali A; Near-infrared luminescent cubic silicon carbide nanocrystals for in vivo biomarker applications: an ab initio study; *Nanoscale*; **4**, 7720-7726, 2012

### Conference proceedings

11. Gali Á; Excitation properties of silicon vacancy in silicon carbide; In: *Proc. 14th Int. Conf. on Silicon Carbide and Related Materials (Cleveland, USA, September 11-16, 2011)*; *Mater Sci Forum*; **717-720**, 255-258, 2012

12. Ivády\* V, Somogyi B, Zólyomi V, Gällström\* A, Son\* N T, Janzén\* E and Gali Á; Transition Metal Defects in Cubic and Hexagonal Polytypes of SiC: Site Selection, Magnetic and Optical Properties from ab initio Calculations; In: *Proc. 14th Int. Conf. on Silicon Carbide and Related Materials (Cleveland, USA, September 11-16, 2011)*; *Mater Sci Forum*; **717-720**, 205-210, 2012
13. Gällström\* A, Magnusson\* B, Beyer\* FC, Gali Á, Son\* N T, Leone\* S, Ivanov\* IG, Henry\* A, Hemmingsson\* CG, Janzén\* E; Electronic Configuration of Tungsten in 4H-, 6H-, and 15R-SiC; In: *Proc. 14th Int. Conf. on Silicon Carbide and Related Materials (Cleveland, USA, September 11-16, 2011)*; *Mater Sci Forum*; **717-720**, 211-216, 2012
14. Son\* N T, Ivády\* V, Gali Á, Gällström\* A, Leone\* S, Kordina\* O and Janzén\* E; Identification of Niobium in 4H-SiC by EPR and ab initio Studies; In: *Proc. 14th Int. Conf. on Silicon Carbide and Related Materials (Cleveland, USA, September 11-16, 2011)*; *Mater Sci Forum*; **717-720**, 217-220, 2012
15. Devaty\* R P, Yan\* F, Choyke\* W J, Gali Á, Kimoto\* T and Ohshima\* T; Local Thermal Expansion and the C-C Stretch Vibration of the Dicarbon Antisite in 4H-SiC; In: *Proc. 14th Int. Conf. on Silicon Carbide and Related Materials (Cleveland, USA, September 11-16, 2011)*; *Mater Sci Forum*; **717-720**, 263-266, 2012

*See also: S-I.7.*

## S-E. NON-EQUILIBRIUM ALLOYS

*Imre Vincze, Judit Balogh, László Bujdosó, Dénes Kaptás, Tamás Kemény, László Ferenc Kiss*

**Investigation of half-metallic ferromagnetic alloys.** – The density of states of half metallic ferromagnets exhibits a gap for minority electrons around the Fermi energy. As a result, these materials display a 100% spin polarized transport at low temperatures showing huge potential for device applications in the field of “spintronics.”

A promising class of such materials is that of the Co-based Heusler alloys,  $\text{Co}_2\text{FeZ}$ , where Z is a main group element (like Al, Ga, Si, and Ge). In general, these compounds crystallize in the  $L2_1$  structure shown in Fig. 1a, which is decisive for the expected half-metallic behaviour. The symmetry of the  $L2_1$  structure decreases and the material transforms to B2 structure because of the disorder between the Fe and metalloid sites. This structural change has strong influence on the half-metallic property. The position of the Fermi energy within the gap is important for the temperature dependence of spin-polarized transport; the optimum behaviour is expected when it is in the middle of the gap. Shift of the Fermi level is achieved by changing the valence contribution of the metalloid. Theoretical calculations assuming  $L2_1$  structure predict  $\text{Co}_2\text{FeAl}_{0.5}\text{Si}_{0.5}$  to be the best choice and this composition is the subject of many experimental investigations.

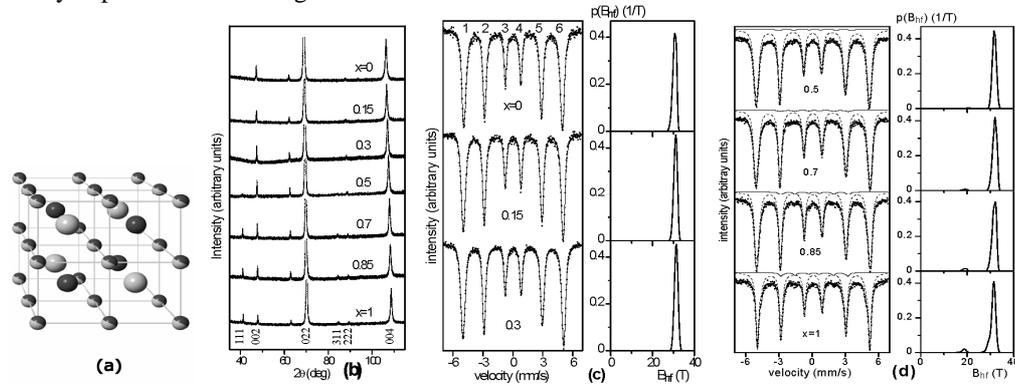


Fig. 1. a, The  $L2_1$ -type crystal structure: Co sits in the corner of the cubes, Fe and Z alternate in the center of the cubes; b, X-ray diffractograms of the  $\text{Co}_2\text{FeAl}_{1-x}\text{Si}_x$  samples; c and d, the respective room temperature Mössbauer spectra and hyperfine field distributions.

This picture is questioned by the x-ray measurements of G. Bortel (Fig. 1b). The  $\text{Co}_2\text{FeAl}$  has the B2 crystal structure (indicated by the absence of the  $\langle 111 \rangle$  superlattice reflection) and for the Al-Si substitution it changes into the  $L2_1$  structure between  $x = 0.3$  and  $0.5$ . The composition dependence of the Mössbauer parameters (Fig. 2) is in line with this structural change and significantly different from the theoretical expectations. It is worth mentioning that the comparison of the hyperfine fields measured at room temperature and 12 K indicates quite different temperature dependences of the magnetization for  $\text{Co}_2\text{FeAl}$  and  $\text{Co}_2\text{FeSi}$ , despite their rather high Curie temperatures (well above 1000K).

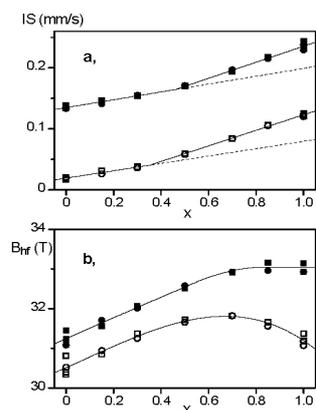


Fig. 2. Average isomer shift (a) and hyperfine field (b) of  $\text{Co}_2\text{FeAl}_{1-x}\text{Si}_x$  measured at room temperature (empty circles) and at 12 K (dots).

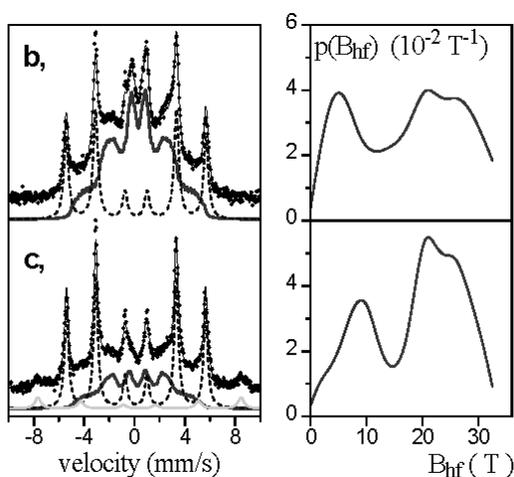


Fig. 3. CEMS spectra measured at 15 K for the following samples: (b) Si/5 nm B/2.5 nm  $^{57}\text{Fe}$ /5 nm B/10 nm Ag, and (c) Si/5 nm B/2.5 nm  $^{57}\text{Fe}$ /10 nm Ag. The subspectra of the crystalline Fe layer (dashed line) and the amorphous Fe-B interface (black solid line) are also indicated. In the case of (c), a small amount of oxide phase (gray solid line) can also be observed. The normalized hyperfine field distributions evaluated for the amorphous Fe-B interfaces are shown on the right panels. The difference of the HF distributions reveals that the Fe/B and the B/Fe interfaces are not equivalent.

## GRANTS

OTKA K101456 Mössbauer and magnetic study of intermetallic compounds (I. Vincze, 2012-2016)

TÉT 10-1-2011-0579 Magnetic interactions in multilayer heterostructures (J. Balogh, 2012-2014)

## PUBLICATIONS

### Articles

1. Balogh J, Bujdosó L, Kaptás D, Dézsi I, Nakanishi\* A; Top and bottom interfaces in Fe-B multilayers investigated by Mössbauer spectroscopy; *Phys Rev B*; **85**, 195429/1-6, 2012
2. Mihálk\* M, Zentková\* M, Antonak\* M; Arnold\* Z, Kamarád\* J, Skorokhod\* Y, Gritzner\* G, Kiss LF; Pressure effect on magnetic and insulator-metal transition of  $\text{La}_{0.67}\text{Pb}_{0.33}\text{Mn}_{0.9}\text{Co}_{0.1}\text{O}_{2.97}$  ceramic; *High Pressure Research*; **32**, 145-149, 2012
3. Caballero-Flores\* R, Franco\* V, Conde\* A, Kiss LF, Péter L, Bakonyi I; Magnetic multilayers as a way to increase the magnetic field responsiveness of magnetocaloric materials; *Journal of Nanoscience and Nanotechnology*; **12**, 7432-7436, 2012
4. Náfrádi\* B, Antal\* Á, Pásztor\* Á, Forró\* L, Kiss LF, Fehér\* T, Kováts É, Pekker S, Jánossy\* A; Molecular and spin dynamics in the paramagnetic endohedral fullerene  $\text{Gd}_3\text{N}@C_{80}$ ; *J Phys Chem Lett*; **3**, 3291–3296, 2012

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**S-F. X-RAY DIFFRACTION**

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*Gyula Faigel, Gábor Bortel, László Gránásy, Zoltán Jurek, Katalin Kamarás, Gyöngyi Klupp, Dorina Kocsis, #Éva Kováts, Katalin Németh, #Gábor Oszlányi, Áron Pekker, #Tamás Pusztai, László Rátkai, #Attila Szállás, Zsolt Szekrényes, #Gyula Tóth, György Tegze, Miklós Tegze*

**Carbon based systems.** — Lately various carbon based materials became the center of intensive research. Among them we studied fullerenes and related compounds, carbon nanotubes and graphene.

**Crystalline derivatives of fullerenes.** — Fullerenes are closed shell carbon molecules. The most abundant among them is  $C_{60}$ . The conjugated bond system makes  $C_{60}$  ideal precursor of ionic and covalent derivatives. In condensed state the rotation and the supramolecular interactions of the high-symmetry molecules enlarge the possibility of further structures. As a result of the above properties, fullerenes have unusually large number of solid state derivatives, like alkali metal salts, polymers, and cocrystals with a series of inorganic and organic molecules. In the group of  $A_3C_{60}$  compounds ( $A = Na, K, Rb,$  and  $Cs$ ) there are superconductors under ambient pressure ( $K_3C_{60}$  and  $Rb_3C_{60}$ ) but the cesium salts show a transition from an insulating to a metallic (superconducting at low temperature) state when applying moderate pressure. This transition has been identified as Mott localization of the electrons with the Jahn-Teller effect playing a key role in the mechanism. The very small molecular Jahn-Teller distortion is very difficult to detect, but we succeeded to prove its existence by temperature-dependent infrared spectroscopy through the symmetry reduction and subsequent changes in the spectra.

Most cocrystals of fullerenes are host-guest or donor-acceptor materials. An interesting example is the rotor-stator phases of fullerenes and cubanes. We studied two interesting questions connected to these materials: the orientational phase transition and the extension of this family with derivatives based on endohedral fullerenes.

Concerning the first point we used pressure-dependent infrared spectroscopy to detect the orientational phase transition in cubane-fullerene cocrystals. As for the second point, we extended the family by cubane and mesitylene cocrystals of the endohedral trimetallonitride compound of  $C_{80}$ ,  $Sc_3N@C_{80}\cdot C_8H_8$ . It has a rocksalt structure with static cubane and rotating fullerene molecules. At ambient temperature the  $Sc_3N$  unit also rotates inside the fullerene cage. We found that the Gd derivative has similar structure with interesting magnetic properties. Pairs of mesitylene molecules assemble in slightly distorted octahedra which form cubic cocrystals with  $C_{70}$  and also with  $Sc_3N@C_{80}$ . We prepared the latter material for the first time and started the structural studies.

**Carbon nanotubes and graphene.** — We studied carbon nanotubes and graphene, and hybrid materials based on these with other organic molecules. We detected the mechanism of the reaction of carbon nanotubes with the aromatic polycyclic hydrocarbon coronene, and found that besides the encapsulation of coronene molecules into the tubes, coronene also forms polymers in a side reaction. We determined the optimal conditions of monomer encapsulation. We characterized special nanopatterned graphene structures by Raman spectroscopy. Other supramolecular systems, hydrogen-bonded nucleic acid base-analogs,

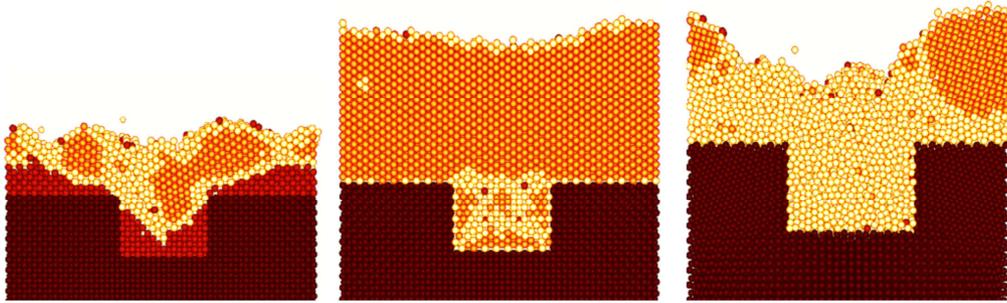
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# PhD student

were studied by infrared spectroscopy and molecular dynamics calculations, to detect the “melting” temperature of hydrogen bonds. Functionalized silicon carbide nanocrystals (with the purpose to be made biocompatible) were investigated by special surface-sensitive infrared methods (together with the group of A. Gali).

**Single molecule imaging.** — Using very short (10-100 fs) and intense x-ray pulse of an X-ray Free Electron Laser, scattering on a single particle can give useful information on its structure before the sample would eventually be destroyed. Single particles are injected into the x-ray beam and scattering patterns of single particles are collected by 2D detectors and stored individually. Evaluation of the very noisy patterns corresponding to particles of unknown orientation and solving the structure is a serious challenge. We developed a method to solve the orientation problem and build a consistent 3D data set from the detected patterns. We tested our method on synthetic noisy diffraction data of a large protein molecule. We have found the unknown orientations of the patterns, and solved the atomic structure of the molecule. The concept of our algorithm could be also applied to experiments where images of an object are recorded in unknown orientations and/or positions like in cryo-electron microscopy or tomography.

**Theory of phase transformations.** — A simple dynamical density functional theory is used to investigate freezing of an undercooled liquid in the presence of a crystalline substrate. We find that the adsorption of the crystalline phase on the substrate, the contact angle, and the height of the nucleation barrier are nonmonotonic functions of the lattice constant of the substrate. We show that the free-growth-limited model of particle-induced freezing by Greer et al. [Acta Mater. 48, 2823 (2000)] is valid for larger nanoparticles and a small anisotropy of the interface free energy. Faceting due to the small size of the foreign particle or a high anisotropy decouples free growth from the critical size of homogeneous nuclei. A complex behaviour has been observed when varying the lattice constant of an fcc substrate with a rectangular pit (Fig. 1).



*Fig. 1. Freezing on fcc substrate with a rectangular nanoscale pit. Spheres drawn around reduced density peaks larger than  $\Psi = 0.05$  are shown. Order parameters  $q_4$  and  $q_6$  are used for structural analysis. Hues from dark to light stand for the substrate and the (metastable) fcc, bcc, and (metastable) amorphous structures, respectively. From left to right the ratio of the interatomic distances for the substrate and the fcc crystal are 1.0, 1.098, and 1.42. For matching lattice constants, we observe fcc and bcc epitaxy, whereas at large mismatch amorphous phase mediated bcc solidification takes place. Half of the longitudinal-sections are displayed.*

We have reviewed the basic concepts and applications of the phase-field-crystal (PFC) method which is one of the latest simulation methodologies in materials science for problems

where atomic and microscales are tightly coupled. The PFC method operates on atomic length and diffusive time scales, and thus constitutes a computationally efficient alternative to molecular simulation methods. Its intense development in materials science started fairly recently following the work by Elder et al. [Phys. Rev. Lett. 88, 245701 (2002)]. Since these initial studies, dynamical density functional theory and thermodynamic concepts have been linked to the PFC approach. In a recent review, we have summarized these methodological development steps as well as the most important applications of the PFC method with a special focus on the physics of hard and soft matter.

#### **GRANTS AND INTERNATIONAL COOPERATION**

- OTKA K72954 Rotor-stator phases of the fullerene-cubane system and related supramolecular materials (S. Pekker, 2008-2012)
- OTKA K067980 New methods for solving the phase problem II. (G. Oszlányi, 2007-2012)
- OTKA T075813 Polymerization in carbon nanostructures (K. Kamarás, 2009-2012)
- OTKA K-81348 Ultrafast diffraction imaging of single particles (M. Tegze, 2010- 2014)
- Participation in COMET K2 project A1.1.: Numerical Investigations on Dendritic Mushy Zones (T. Pusztai, 2009–2012)
- Participation in EU FP7 NMP4-SL-2008/213669 ENSEMBLE Engineered Self-organised Multi-Component Structures with Novel Controllable Electromagnetic Functionalities (L. Gránásy, 2008–2012)
- ESA PECS Contract No. 4000104330/11/NL/KML: GRADECET-Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2011–2013).
- Participation in EU FP7 NMP-2011-LARGE-5/280421 EXOMET – Physical processing of molten light alloys under the influence of external fields (L. Gránásy, 2012–2016)
- NFÜ TECH-09-A2-2009-0134, FIBERSC2. Development of fiber integrated nonlinear microendoscope based on new fiber laser technology, for pharmacological and diagnostic investigations (2009-2012, consortium leader: R. Szipőcs, Scientist-in-charge for SZFI: K. Kamarás)
- EU FP7-Marie Curie Initial Training Network PITN-GA-2008-215399: Cavity-confined luminophores for advanced photonic materials: a training action for young researchers (FINELUMEN) (Coordinator: Nicola Armaroli, CNR-ISOF, Bologna, Italy, representative of contractor: K. Kamarás)
- MTA Infrastructure Grant. Laboratory for advanced structural studies (K. Kamarás 2012).

#### **LONG TERM VISITOR**

- M.-E. Füstös, Babeş-Bolyai University, Cluj-Napoca, Romania (Feb 1 – July 31, 2012, host: K. Kamarás)

**PUBLICATIONS***Articles*

1. Tegze M, Bortel G; Atomic structure of a single large biomolecule from diffraction patterns of random orientations; *J Struct Biol*; **179**, 41-45, 2012
2. Tóth GI, Tegze G, Pusztai T, Gránásy L; Heterogeneous crystal nucleation: The effect of lattice mismatch; *Phys Rev Lett*; **108**, 025502/1-4, 2012
3. Tegze G, Tóth GI; Osmotic convection-driven instability and cellular eutectic growth in binary systems; *Acta Mater*; **60**, 1689-1694, 2012
4. Szekrényes Zs, Kamarás K, Tarczay G\*, Llanes-Pallás A\*, Marangoni T\*, Bonifazi D\*, Björk J\*, Hanke F\*, Persson M\*; Melting temperature of hydrogen bonds probed by infrared spectroscopy and ab initio molecular dynamics; *J Phys Chem B*; **116**, 4626-4633, 2012
5. Klupp G, Matus P, Kamarás K, Ganin AY\*, McLennan A\*, Rosseinsky MJ\*, Takabayashi Y\*, McDonald MT\*, Prassides K\*; Dynamic Jahn-Teller effect in the parent insulating state of the molecular superconductor Cs<sub>3</sub>C<sub>60</sub>; *Nat Commun*; **3**, 912/1-6, 2012
6. Francis EA\*, Scharinger S\*, Németh K, Kamarás K, Kuntscher CA\*; Pressure-induced transition from the dynamic to static Jahn-Teller effect in (Ph4P)<sub>2</sub>IC<sub>60</sub>; *Phys Rev B*; **85**, 195428/1-10, 2012
7. Neumann PL\*, Tóvári E\*, Csonka S\*, Kamarás K, Horváth ZE\*, Biró LP\*; Large scale nanopatterning of graphene; *Nucl Instrum Meth B*; **282**, 130-133, 2012
8. Jurek Z, Thiele R\*, Ziaja B\*, Santra R\*; Effect of two-particle correlations on x-ray coherent diffractive imaging studies performed with continuum models; *Phys Rev E*; **86**, 036411, 2012
9. Náfrádi B, Antal Á, Pásztor Á, Forró L, Kiss L. F, Fehér T, Kovács É, Pekker S, Jánossy A; Molecular and Spin Dynamics in the Paramagnetic Endohedral Fullerene Gd<sub>3</sub>N@C<sub>80</sub>; *J Phys Chem Lett*; **3**, 3291-6; 2012
10. Emmerich\* H, Löwen\* H, Wittkowski\* R, Gruhn\* T, Tóth G I, Tegze G, Gránásy L; Phase-field-crystal models for condensed matter dynamics on atomic length and diffusive time scales: an overview; *Adv Phys*; **61**, 665-743, 2012

*Article in Hungarian*

11. Tegze Gy, Tóth Gy, Gránásy L; Kristályos önszerveződés határfelületeken: kétdimenziós kristályok (Crystalline self-organization on surfaces: two-dimensional crystals, in Hungarian); *Fizikai Szemle*; **62**, 185-187, 2012

*Book chapter*

12. Tóth GI, Pusztai T, Tegze G, Tóth\* G, Gránásy L; Phase-field crystal modeling of homogeneous and heterogeneous crystal nucleation; In: *Solidification of Containerless Undercooled Melts, Containerless Undercooling of Drops and Droplets*; Ed: D. M. Herlach and D. M. Matson, Wiley-VCH GmbH & KGaA, Weinheim, 2012, ISBN 978-3-527-33122-2, pp. 113-138, 2012

*See also: S-D.11, S-D.12, S-E.4*

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**S-G. COMPLEX FLUIDS**

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*Ágnes Buka, Tamás Bölcsönyi, Nándor Éber, Katalin Fodor-Csorba, Antal Jákli, István Jánossy, Péter Salamon,<sup>#</sup> Balázs Szabó,<sup>#</sup> Tibor Tóth-Katona, Anikó Vajda*

**Synthesis.** — New chiral banana compounds have been synthesized and characterized by polarizing microscopy, DSC and X-ray diffraction. These molecules have saturated alkyl tails (decyl and undecyl groups) as terminal groups. The self-organization of these molecules is different from their unsaturated analogues according to the electro-optical investigations. New cunean derivatives have also been characterized, which all exhibit  $B_x$  phase.

**Measurement of material constants.** — The effect of director pretilt on the dielectric and optical responses of a nematic liquid crystal at the twist magnetic Fréedericksz transition was analyzed for a planar cell. As a result a novel dielectric measurement method was introduced for determining the elastic constant  $K_{22}$ , which was first applied for the determination of the elastic constants of a bent-core nematic material.

**Electric field driven pattern formation.** — The influence of the combined action of a dc and an ac electric field on electroconvection (EC) was studied in a nematic liquid crystal with high, positive dielectric anisotropy (5CB). Pattern morphologies were identified; the thresholds and critical wave numbers were measured and analyzed as a function of frequency, dc-to-ac voltage ratio, and thickness. The current-voltage characteristics were simultaneously detected.

The temporal evolution of patterns within the driving period  $T$  of the ac voltage was studied in the 10 mHz–250 Hz frequency range. The stationary EC pattern of the conductive regime was shown to transform into a flashing one at ultralow frequencies (Fig. 1a). Furthermore a transition between EC (Fig. 1b) and flexoelectric domains (FD, Fig. 1c) was detected which is repeating in each half period. The two patterns are well separated in time and in Fourier space. The experimental findings are in good agreement with the theoretical predictions based on an extended standard model including flexoelectricity.

**A book** reviewing flexoelectricity in liquid crystals was published. The volume addresses the molecular theory of flexoelectricity, the various experimental methods for measuring the flexoelectric coefficients, the role of flexoelectricity in pattern formation and in forming chiral smectic subphases, as well as the display applications based on flexoelectricity.

**Liquid crystal composite materials.** — The behaviour of magnetic nanoparticle-doped nematics was reviewed depending on the host liquid crystal, on the type, shape, size and concentration of the magnetic particles. It was shown that in such doped systems a magnetic field induced shift of the isotropic-to-nematic phase transition temperature is detectable.

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<sup>#</sup> PhD student

S-G. Complex fluids

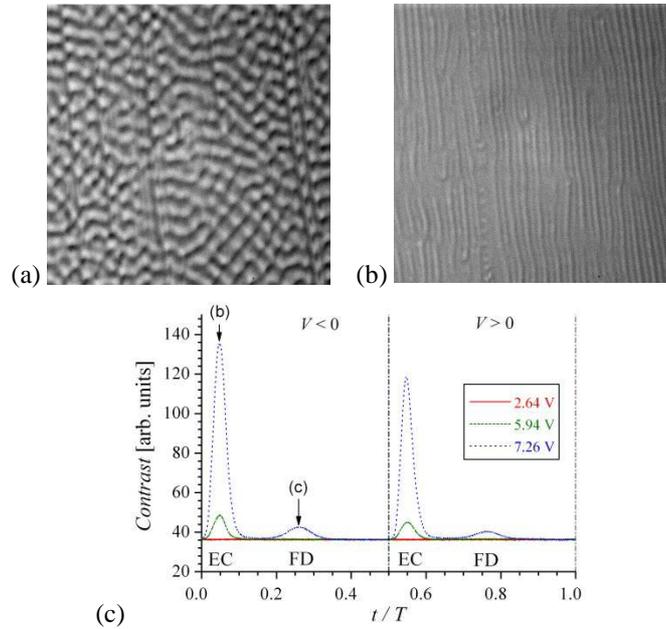


Fig. 1. (a) EC pattern; (b) flexoelectric domains; (c) pattern contrast vs. time at 30 mHz.

**Granular dynamics.** — Shear induced alignment of elongated particles was studied experimentally and numerically. We showed that shear alignment of ensembles of macroscopic particles is comparable even on a quantitative level to simple molecular systems, despite the completely different types of particle interactions. We demonstrated that for dry elongated grains the preferred orientation forms a small angle with the streamlines, independent of shear rate across three decades. For a given particle shape, this angle decreases with increasing aspect ratio of the particles. The shear-induced alignment results in a considerable reduction of the effective friction of the granular material (Fig. 2).

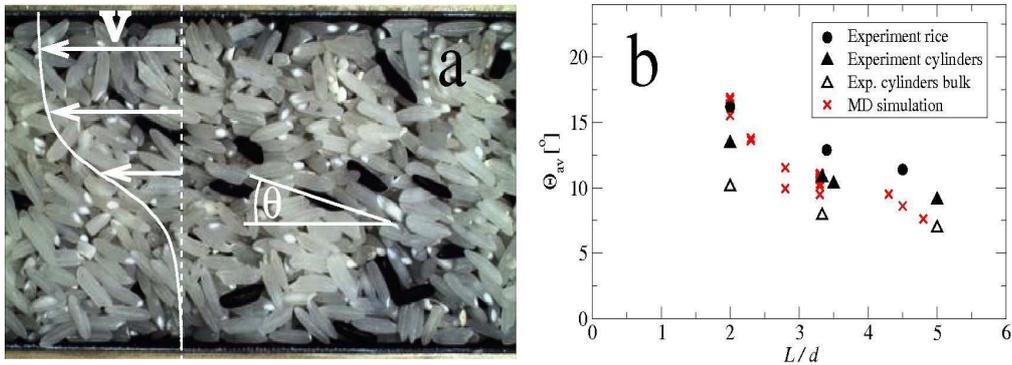


Fig. 2. (a) Shear induced alignment of elongated grains; (b) the alignment angle decreases with increasing particle length.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA K81250	Electro and photomechanical effects in organic soft materials (Jánossy I, 2010-2014)
NKTH TÉT	AR-3/2008 (Hungarian-Argentinian bilateral) Transient and metastable states (Buka Á, 2009-2012)
MTA-ASCR	(Hungarian-Czech bilateral) Synthesis and characterization of reactive mesogenic monomers, and their utilization in crosslinked systems (Tóth-Katona T, 2010-2012)
MTA-INSA	(Hungarian-Indian bilateral) Experimental and Theoretical Studies on Soft Condensed Matter (Éber N, 2010-2012)
MTA-SASA	(Hungarian-Serbian bilateral) Structural studies of liquid crystalline mixtures (Éber N, 2010-2012)
MTA-SAS	(Hungarian-Slovak bilateral) Anisotropic magnetic fluids (Éber N, 2010-2012)
MÖB-DAAD	(Hungarian-German bilateral) From anisotropic liquids to anisotropic granular material (Börzsönyi T., 2012-2013)

## LONG TERM VISITORS

- Laura Olivia Palomares: Instituto de Física, Universidad Nacional Autónoma de México, Mexico D.F., Mexico, January 02 – December 31, 2012 (host: Jánossy I)
- Prof. David Statman: Allegheny College, Meadville, USA, June 15 – August 01, 2012 (host: Jánossy I)
- Brianne Lee Zins: Allegheny College, Meadville, USA, June 15 – August 01, 2012 (host: Jánossy I)
- Nicholas Engel Romano: Allegheny College, Meadville, USA, June 15 – August 01, 2012 (host: Börzsönyi T)
- Marla Ashley Sacks: Allegheny College, Meadville, USA, June 15 – August 01, 2012 (host: Éber N)

## PUBLICATIONS

### Articles

1. Novotná\* V, Mieczkowska\* K, Hamplová\* V, Domján\* A, Pocięcha\* D, Kašpar\* M, Fodor-Csorba K; Non-symmetrical bent-shaped compounds containing a chiral moiety; *Liq Cryst*; **39**, 1252-1260, 2012
2. Aguirre\* E, Anordo\* E, Éber N, Buka Á; Regular structures in 5CB liquid crystals under the joint action of ac and dc voltages; *Phys Rev E*; **85**, 041703/1-9, 2012
3. Salamon P, Éber N, Lehmann\* M, Gleeson\* JT, Sprunt\* S, Jáklí A; Dielectric technique to measure the twist elastic constant of liquid crystals - The case of a bent-core material; *Phys Rev E*; **85**, 061704/1-9, 2012
4. Éber N, Palomares\* LO, Salamon P, Krekhov\* A, Buka Á; Temporal evolution and alternation of mechanisms of electric field induced patterns at ultra-low-frequency driving; *Phys Rev E*; **86**, 021702/1-9, 2012

5. Buka Á, Éber N, Fodor-Csorba K, Jákli A, Salamon P; Physical properties of a bent-core nematic liquid crystal and its mixtures with calamitic molecules; *Phase Transit*; **85**, 872-887, 2012
6. Börzsönyi T, Szabó B, Törös\* G, Wegner\* S, Török\* J, Somfai\* E, Bien\* T, Stannarius\* R; Orientational order and alignment of elongated particles induced by shear; *Phys Rev Lett*; **108**, 228302/1-5, 2012
7. Wegner\* S, Börzsönyi T, Bien\* T, Rose\* G, Stannarius\* R; Alignment and dynamics of elongated cylinders under shear; *Soft Matter*; **8**, 10950-10958, 2012

#### **Article in Hungarian**

8. Szabó B; Hogyan török a szemcsés anyag? Avagy egy különös analógia az optikával (How does a granular material deform? - A peculiar analogy with optics, in Hungarian); *Természet Világa*; **143** (11), 500-503, 2012

#### **Conference proceedings**

9. Éber N, Salamon P, Buka Á; Competition between electric field induced equilibrium and non-equilibrium patterns at low frequency driving in nematics; In: *Proceedings of the 13th Small Triangle Meeting on Theoretical Physics (Stará Lesná, November 14-16, 2011)*; Eds.: Buša J, Hnatič M, Kopčanský P; IEP SAS, Košice, pp. 56-63, 2012
10. Obadović\* D.Ž, Stojanović\* M, Cvetinović\* M, Vajda A, Éber N, Fodor-Csorba K; Mesophase behaviour of binary mixtures of bent-core and calamitic compounds; In: *Proceedings of the 11th International Conference on Fundamental and Applied Aspects of Physical Chemistry*, (September 24-28, 2012, Belgrade, Serbia); Eds.: Anić S and Čupić Ž; Society of Physical Chemists of Serbia, Belgrade, pp. 423-425 (2012)

#### **Books, book chapters**

11. Buka Á, Éber N (Eds.); *Flexoelectricity in Liquid Crystals. Theory, Experiments and Applications*; Imperial College Press, London, ISBN: 978-1-84816-799-5; 2012
12. Jákli A, Harden\* J, Éber N; Chapter 3, Flexoelectricity of bent-core molecules; In: *Flexoelectricity in Liquid Crystals. Theory, Experiments and Applications*; Eds.: Buka Á, Éber N, ISBN: 978-1-84816-799-5; Imperial College Press, London; pp. 61-99, 2012
13. Buka Á, Tóth-Katona T, Éber N, Krekhov\* A, Pesch\* W; Chapter 4, The role of flexoelectricity in pattern formation; In: *Flexoelectricity in Liquid Crystals. Theory, Experiments and Applications*; Eds.: Buka Á, Éber N, ISBN: 978-1-84816-799-5; Imperial College Press, London; pp. 101-135, 2012
14. N. Éber; Appendix A. Measured flexoelectric coefficients of nematic liquid crystals; In: *Flexoelectricity in Liquid Crystals. Theory, Experiments and Applications*; Eds.: Buka Á, Éber N, ISBN: 978-1-84816-799-5; Imperial College Press, London; pp. 249-265, 2012
15. Tomašovičová\* N, Kopčanský\* P, Éber N; Magnetically Active Anisotropic Fluids Based on Liquid Crystals; In: *Anisotropy Research: New Developments*; Ed.: Lemu\* HG, ISBN: 978-1-62081-987-6; Nova Science Publishers (ebook), pp. 253-281, 2012

## S-H. RADIOFREQUENCY SPECTROSCOPY

György Kriza, Péter Bánki, Mónika Bokor, Péter Matus, Bernadette Sas, Kálmán Tompa, Tamás Verebéli,<sup>#</sup> Francis Ian Bickford Williams

**Structural status of a protein as seen by wide-line  $^1\text{H}$  NMR.** — Human nucleolar phosphoprotein p140 (hNopp 140) is a highly phosphorylated protein inhibitor of casein kinase 2 (CK2). As in the case of many kinase-inhibitor systems, the inhibitor has been described to belong to the family of intrinsically disordered proteins (IDPs), which often utilize transient structural elements to bind their cognate enzyme. We investigated the structural status of this protein. The overall disordered state of hNopp140 is underlined *inter alia* by the hydration data measured by wide-line NMR. Measurement of the thermal evolution of the hydration in aqueous protein solutions below  $0^\circ\text{C}$  provides information on the globular or disordered nature of a protein. The hydration vs. temperature curve of globular proteins is approximately constant in a wide (a few tens of degrees) temperature range (see, e.g., BSA in Fig.1). The temperature variation of hydration in disordered proteins is considerably stronger (see ERD10 in Fig.1). The hydration curves of hNopp140 and ERD10 are nearly identical and differ dramatically from that of BSA, providing evidence for the disordered nature of the first material.

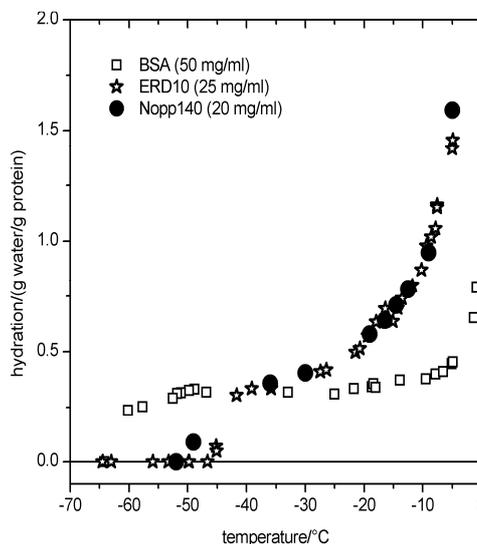


Fig. 1. Hydration data for hNopp140 (black circles), the intrinsically disordered ERD10 (stars) and the globular BSA (open squares) are shown.

Although some methods show no stable structure of hNopp140, with other techniques some helical tendencies and preformed structural elements were found. The analysis of the compactness of hNopp140 indicates that the protein falls somewhere between the premolten globule and the random coil type of disordered proteins, but it is closer to the premolten globule type. This observation is also supported by the wide-line NMR measurements, as judged from the ratio of the variances of the wide-line NMR spectra measured at room temperature and at low temperature ( $T < -200^\circ\text{C}$ ). This number is related to the mobile/rigid state of the protein molecule and we find that this ratio increases from globular proteins to IDPs. Since the measured ratio for hNopp140 falls between these limits, we conclude that hNopp140 is in a partly disordered, partly ordered state.

**Collective excitations in graphene.** — Edge magneto-plasmon excitations are a dynamic manifestation of the (quantum) Hall effect (QHE). Localised along the sample boundary, they provide a means of probing the nature of the edge and the emergence of the Landau levels responsible for the QHE. We have done, in graphene, a picosecond time of flight experiment

<sup>#</sup> Ph.D. student (ELTE)

## S-H. Radiofrequency spectroscopy

to determine their propagation velocity from which it is possible to separate the Hall effect contribution from the drift velocity in the edge potential of quantum origin which lifts the QHE Landau level above the Fermi level. We show these edge excitations to be chiral, to have quantized propagation velocity and very low attenuation, all excellent attributes for chiral plasmonics.

### GRANTS AND INTERNATIONAL COOPERATION

SPEC – Saclay: Collaboration agreement with Service de Physique de L'Etat Condensé (SPEC, CEA-Saclay, France) on electron crystals and nano-electronics (2005-2013); principal investigator: F.I.B. Williams.

Joint Project supported by the Korean Research Council of Fundamental Science & Technology (KRCF) and MTA (Hungarian project leader: P. Tompa, Institute of Enzymology, BRC, MTA; participating RISSPO scientists: K. Tompa, M. Bokor, 2011-2012)

### PUBLICATIONS

#### *Book chapter*

1. Tompa K; Bokor M; Tompa P\*; Chapter 13. Wide-line NMR and protein hydration; In: *Intrinsically Disordered Protein Analysis: Vol. 1, Methods and Experimental Tools, Methods in Molecular Biology*; Eds: V.N. Uversky, A.K. Dunker, Springer Science+Business Media, LLC, New York, NY, USA, 2012; Vol. 895, Part 2, pp. 167-196, DOI: 10.1007/978-1-61779-927-3\_13

See also: S-F.5

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**S-I. ELECTRODEPOSITED NANOSTRUCTURES**

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*László Péter, Imre Bakonyi, Kata Berkesi, Júlia Dégi, Katalin Neuróhr, Lajos Pogány, Bence Tóth*

**Depth profile analysis.** — In cooperation with MTA's Institute of Nuclear Research, we developed earlier a reverse depth profile analysis technique to reveal the near-substrate composition depth profile of thin films. The technique was now extended for studying the thickness evolution of the composition in d.c.-plated and pulse-plated Fe-Ni alloys. We found that the pulsed deposition mode leads to an even composition profile, especially if the duty cycle is below 0.2.

**Electrodeposition.** — We investigated the electrochemical codeposition of Co and Pb. Although these elements are immiscible in equilibrium, the codeposition from an acetate-type bath was possible. In the case of d.c. plating, either pure Pb or a Co-rich deposit could be obtained in a compact form, but in the intermediate Co-content range the deposits were very rough. However, compact deposits could be obtained in the entire composition range by using two-pulse plating. X-ray diffraction patterns recorded for the two-pulse plated deposits revealed a nanocrystalline structure with grain sizes in the range 5–20 nm. The XRD peaks could be well indexed to pure face-centered cubic Co and Pb, indicating that the Pb codeposited with Co is not dissolved in Co but is segregated. The segregation of Co and Pb in the deposit was also shown in the polarization curves recorded during the electrochemical dissolution of the deposits and in the simultaneously recorded electrochemical quartz crystal microbalance data. Both the d.c.-plated and the two-pulse plated deposits exhibited anisotropic magnetoresistance without any indication of a noticeable giant magnetoresistance contribution. This means that the observed magnetoresistance arises from spin-dependent electron scattering events dominantly within the sufficiently large Co regions and not along electron paths between two Co regions via the Pb regions. Low-temperature resistivity measurements revealed a superconducting transition slightly below that of pure Pb, indicating a proximity effect due to the presence of ferromagnetic Co regions.

**Magnetoresistance and surface roughness.** — The magnetoresistance and the surface roughness of electrodeposited Co-Ni/Cu multilayers were studied in the light of the optimization of the electrodeposition procedure. We reported earlier [L. Péter et al., *Electrochim. Acta* **49** (2004) 1513] that the single-bath electrodeposition process used for the preparation of Co/Cu multilayers can be optimized from an electrochemical point of view in order to avoid unwanted Co dissolution. We have now extended this study for electrodeposited Co-Ni/Cu multilayers to establish if the same optimization method is appropriate when two magnetic elements are present. Several Co-Ni/Cu multilayers were prepared by varying the deposition potential of the Cu layer. The composition analysis of the deposits showed that the Ni:Co ratio exhibits a minimum as a function of the Cu deposition potential, which can be explained by considering both the dissolution of Co and the mass transport of the reactants. The magnetoresistance had a maximum at a fairly positive Cu deposition potential where Co dissolved during the deposition of the Cu layer. The surface roughness of the Co-Ni/Cu multilayer samples increased as the Cu deposition potential becomes more negative. No similar effect was found when either of the magnetic elements was absent. Both the saturation magnetoresistance value and the intensity of the satellite peaks in the X-ray diffractograms were highly correlated to rather the resulting surface roughness of the deposits than to the Cu deposition potential itself. The results draw attention

to the complexity of the optimization procedure of the deposition of multilayers with several alloying components.

#### GRANTS AND INTERNATIONAL COOPERATION

- OTKA K75008 Giant magnetoresistance (GMR) in electrodeposited multilayers (I. Bakonyi, 2009-2012)
- OTKA NN79943 Formation mechanism, microstructure evolution and reactivity of simplectites created during garnet breakdown processes (Principal investigator: K. Török, Eötvös Loránd Geophysical Institute of Hungary; SZFKI participant: J. Dégi; 2010–2014)
- OTKA K104696 Electrodeposition of special magnetic materials from nonaqueous solutions (L. Péter, 2012-2015)
- NIH TÉT 10-1-2011-0555 (Hungarian-Greek bilateral project) Magnetotransport phenomena in ferromagnetic/semimetal nanowires (Hungarian project leader: L. Péter, 2012-2014)
- MÖB-DAAD PROJECT #14533 Electrochemical Synthesis of Magnetic Nanowires and their Thermoelectric Effects under Magnetic Fields (Hungarian project leader: L. Péter, 2011-2012)

#### LONG-TERM VISITOR:

- N. Rajasekaran, Ph.D. student, Central Electrochemical Research Institute, Karaikudi, India, Oct. 2012 - April 2013 (hosts: L. Péter and I. Bakonyi)

#### PUBLICATIONS

##### *Articles*

1. Bakonyi I; Relevance of Fe atomic volumes for the magnetic properties of Fe-rich metallic glasses; *J Magn Magn Mater*; **324**, 3961-3965, 2012
2. Esmaili\* S, Bahrololoom\* ME, Péter L; Magnetoresistance of electrodeposited NiFeCu alloys; *Thin Solid Films*; **520**, 2190-2194, 2012
3. Jafari Fesharaki\* M, Nabiyouni\* GR, Dégi J, Pogány L, Bakonyi I, Péter L; Anomalous codeposition of cobalt and ruthenium from chloride-sulfate baths; *J Solid State Electrochem*; **16**, 715-722, 2012
4. Jafari Fesharaki\* M, Péter L, Schucknecht\* T, Rafaja\* D, Dégi J, Pogány L, Neuróhr K, Széles\* É, Nabiyouni\* G, Bakonyi I; Magnetoresistance and structural study of electrodeposited Ni-Cu/Cu multilayers; *J Electrochem Soc*; **159**, D162-D171, 2012

5. Neuróhr K, Dégi J, Pogány L, Bakonyi I, Ungvári\* D, Vad\* K, Haki\* J, Révész\* Á, Péter L; Composition, morphology and electrical transport properties of Co-Pb electrodeposits; *J Alloy Comp*; **545**, 111-121, 2012
6. Révész\* Á, Péter L, Szabó\* PJ, Szommer\* P, Bakonyi I; Microstructure and morphology of electrodeposited Ni-P alloys treated by high-energy surface mechanical attrition; *Curr Appl Phys*; **12**, 109-114, 2012
7. Szász K, Bakonyi I; Modeling the magnetoresistance versus field curves of GMR multilayers with antiferromagnetic and/or orthogonal coupling by assuming single-domain state and coherent rotations; *J Spintron Magn Nanomater*; **1**, 157-167, 2012

*See also: S-E.3., S-J.5.*

## S-J. METALLURGY AND MAGNETISM

*Lajos Károly Varga, István Balogh, Éva Fazakas, Gábor Gulyás, Pawel Kamasa, György Kovács<sup>+</sup>*

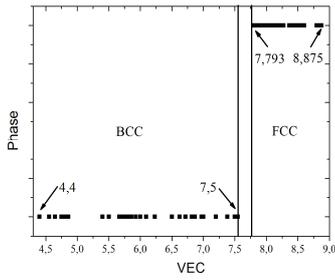
**Metallurgy.** — Recent developments in materials engineering have generated interest in equimolar multicomponent late transition element (Cu-, Fe-, Ni-Co) and early transition element (Ti-, Zr-, V-, Ta) based alloys which retain a single-phase crystalline state in bulk form via conventional ingot casting. These materials are known as high-entropy alloys, or HEA's. We have established a database of the existing experimental data for high-entropy alloys with the aim of identifying possible correlations between their mechanical properties and some easily accessible alloy characteristics. These alloy characteristics can be obtained by using tabulated data of the alloy components like atomic radius, number of valence electrons, etc. The atomic mismatch is calculated conventionally as

$$\delta = 100 \sqrt{\sum_i^n c_i \left(1 - \frac{r_i}{\bar{r}}\right)^2}.$$

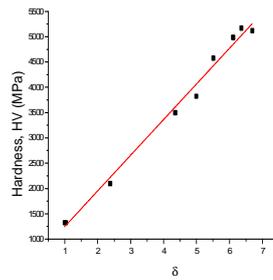
The average valence electron concentration (VEC) is defined as

$$\text{VEC} = \sum_{i=1}^n c_i (\text{VEC})_i,$$

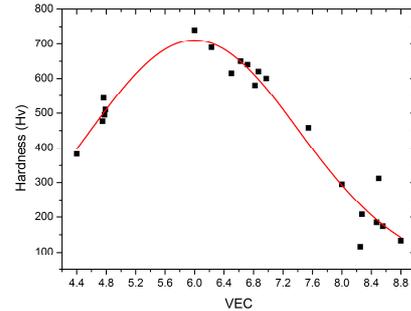
where  $(\text{VEC})_i$  is the VEC of the  $i$ 'th component. VEC counts for the total electrons including the  $d$ -electrons in the valence band. We have found the correlations shown in Figs. 1 to 3.



*Fig. 1. Crystallographic phase versus VEC for single-phase HEA's*



*Fig. 2. Hardness versus  $\delta$  for single-phase HEA's*



*Fig. 3. Hardness versus VEC for single-phase HEA's*

Based on these correlations, one can design optimal high entropy alloys possessing desired strength, thermal stability, and corrosion properties.

**Soft magnetic nanocrystalline alloys.** — An internal demagnetizing factor was introduced as  $N_{di} = \mu_0 H_c / B_s$  in order to properly describe the commutation magnetization curve within the  $\tanh$  model of the hysteresis loop. A shearing factor  $N_s$  was introduced as a function of the

<sup>+</sup> Permanent position: ELTE, Budapest

external demagnetizing factor ( $N_{de}$ ) as  $N_s = 1/(1+N_{de}\mu_i)$  in order to obtain the static initial permeability and remanence values of a toroidal sample (with  $N_{de} = 0$ ) from the data of a rodlike sample (with  $N_{de} \neq 0$ ) within the framework of the *tanh* model.

**Simultaneous DTA and TMAG measurements.** — Our home-made instrumentation for simultaneous DTA and TMAG measurements was further improved by redesigning the protecting gas and air flow around the current-heated platinum boat where the piece of ribbon sample is situated (see Fig.4). The magnetic and thermal changes are recorded against the same sample temperature, avoiding the uncertainties connected with measurements carried out in separate equipments. These patterns (see Fig.5) have been used to characterize Finemet type amorphous ribbons of different provenance in order to rule out those which are not suitable for costly heat treatments in mass production of inductive elements made of toroidal ribbon windings by the company Magnetec-Ungarn.

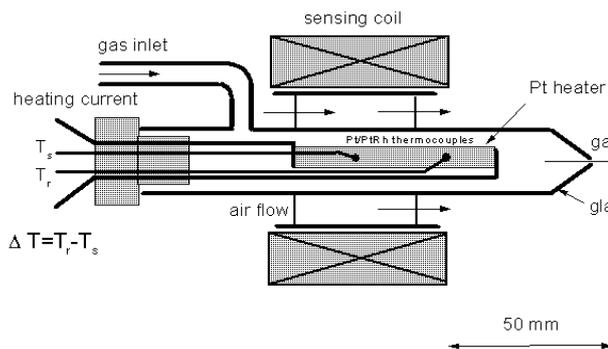


Fig.4. Probe head for DTA and TMAG measurements

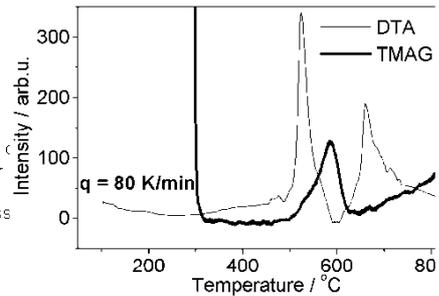


Fig.5. DTA and TMAG crystallization patterns.

**Spin-off activity.** — Former undergraduate students of the Magnetism and metallurgy group have established two spin-off companies under the scientific supervision of the Wigner Research Centre for Physics:

1. O. Temesi, G. Gulyás and A. Huszár have established H-Ion Ltd. for “Research and development on the preparation and investigation of soft magnetic amorphous alloys.” They receive support from Hungarian Government Grant No GOP2011111\_D4C53315.
2. Z. Posgay has established his micro business for “Development of a catalytic hydrolysis process for recycling the aluminum wastage” supported by Hungarian “Start-up” grant.

**GRANTS AND INTERNATIONAL COOPERATION**

- OTKA K73451 Preparation and investigation of Al- and Ti-based bulk amorphous and nanostructured composites (L.K. Varga, 2008-2012).
- MTA-BAS Hungarian-Bulgarian Academy Exchange Programme: Glass forming ability, structural relaxation and (nano)crystallization (L.K. Varga, 2009-2012).
- MTA-SAS Hungarian-Slovakian Academy Exchange Programme: Study of physical properties of special magnetic materials (L.K. Varga, 2010-2012).
- MTA-PAS Hungarian-Polish Academy Exchange Programme: Investigation of thermophysical properties of coatings (P. Kamasa, 2008-2013).

- MTA-RAS Hungarian-Russian Academy Exchange Programme: Calorimetric study of phase transformations (P. Kamasa, 2008-2013).
- MTA-RAS Hungarian-Romanian Academy Exchange Programme: Structure, thermal and mechanical properties of amorphous and nanocrystalline Al-base alloys (É. Fazakas, 2008-2012).
- WATT 22 Ltd. Research and development activity for the preparation and investigation of soft magnetic amorphous alloys (L.K. Varga, 2012).
- MAGNETEC-UNGARN Ltd. Development of measuring system for studying the thermal behaviour of soft magnetic amorphous alloys (L.K. Varga, 2012).

## PUBLICATIONS

### Articles

1. Fazakas É, Erős\* A, Csanády\* Á, Gulyás G, Kamasa P, Varga LK; Formation of amorphous state by ball milling and mechanical crystallization in Al-Ti-Ni alloy system; *IOP Conf. Series: Mater Sci Eng*; **27**, 012081/1-4, 2011
2. Kane\* SN, Singh\* K, Ghodke\* N, Gupta\* A, Varga LK; On the optimization of soft magnetic properties of high B<sub>s</sub> Fe<sub>83.7</sub>B<sub>14.8</sub>Cu<sub>1.5</sub> nanocrystalline alloy; In: Proc. International Conference on Recent Trends in Physics (ICRTP 2012), *J Phys: Conf Series*; **365**, 012015/1-4, 2012
3. Kane\* SN, Tripathi\* S, Coisson\* M, Olivetti\* ES, Tiberto\* P, Vinai\* F, Baricco\* M, Fiore\* G, Apolinário\* A, Sousa\* CT, Araujo\* JP, Varga LK; Microstructure and magnetic properties of (Fe<sub>100-x</sub>Co<sub>x</sub>)<sub>84.5</sub>Nb<sub>5</sub>B<sub>8.5</sub>P<sub>2</sub> alloys; *J All Comp*; **536**, Suppl. 1, S337-S341, 2012
4. Kuzmann\* E, Stichleutner\* S, Sági\* A, Varga LK, Havancsák\* K, Skuratov\* V, Homonnay\* Z, Vértes\* A; Mössbauer study of FINEMET type nanocrystalline ribbons irradiated with swift heavy ions; *Hyperf Int*; **207**, 73-79, 2012
5. Révész\* Á, Kis-Tóth\* Á, Varga LK, Schafner\* E, Bakonyi I, Spassov\* T; Hydrogen storage of melt-spun amorphous Mg<sub>65</sub>Ni<sub>20</sub>Cu<sub>5</sub>Y<sub>10</sub> alloy deformed by high-pressure torsion; *Int. J Hydr Energy*; **37**, 5769-5776, 2012
6. Stojanova\* L, Russew\* K, Fazakas E, Varga LK; Thermo-mechanical study of rapidly solidified amorphous alloys Al<sub>85</sub>Ni<sub>5</sub>Co<sub>2</sub>RE<sub>8</sub>; *J All Comp*; **540**, 192-197, 2012
7. Takács\* J, Kovács\* Gy, Varga LK; The external demagnetizing factor and the static characteristic loop; *Physica B*; **407**, 2434-2437, 2012
8. Varga\* B, Fazakas E, Varga LK; Analysis of quasicrystal generation in conventionally solidified Al-Cu-Fe alloys; *Metalurgia International*; **17**, 27-30, 2012
9. Varga\* B, Fazakas E, Varga LK; Prediction guide for a multi-component alloy structure; *Metalurgia International*; **17**, 53-57, 2012
10. Varga LK, Kovács\* Gy; Effect of transversal applied bias field on the longitudinal soft magnetic properties of nanocrystalline Finemet cores; *IEEE Trans Magn*; **48**, 1360-1362, 2012
11. Takács\* J, Kovács\* Gy, Varga LK; The static characteristic loop and the external demagnetizing factor; *Materials Sciences and Applications*; **3**, 684-689, 2012

12. Takács\* J, Kovács\* Gy, Varga LK; Internal demagnetizing factor in ferrous metals; *Journal of Metallurgy*; **2012**, 752871/1-5, 2012; DOI: 10.1155/2012/752871

***Conference proceedings***

13. Modak\* SS, Mazaleyra\* F, Lo Bue\* M, Varga LK, Kane\* SN; Effective anisotropy field distribution of soft magnetic nanocrystalline  $\text{Fe}_{84}\text{Zr}_{3.5}\text{Nb}_{3.5}\text{B}_8\text{Cu}_1$  ribbons; *AIP Conf Proc*; **1447**, 1163-1164 (2012)

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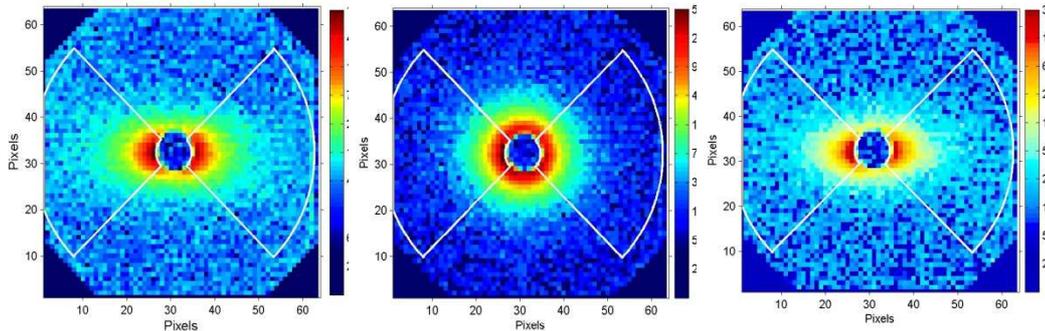
**S-K. NEUTRON SPECTROSCOPY IN CONDENSED MATTER**


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*László Rosta, László Almásy, László Cser, Gergely Eszenyi,<sup>#</sup> Margit Fábrián, János Füzi, György Káli, Zoltán László,<sup>#</sup> Adél Len, Márton Markó, Ferenc Mezei, Gergely Nagy, János Orbán,<sup>#</sup> G. Pépy,<sup>+</sup> Alex Szakál,<sup>#</sup> Gyula Török, Renáta. Ünneper,<sup>#</sup> Tamás Veres*

**Research with neutrons.** — One of the key and largest installations of the research infrastructure in Hungary is the 10-MW Budapest Research Reactor (BRR) with its experimental stations. It is the base for a domestic and international user community to serve for exploratory and applied research in many fields of science and technology as well as for methodological developments in neutron beam techniques. We operate a number of neutron scattering instruments (small angle scattering spectrometer, diffractometers, reflectometers, three-axis spectrometers); nearly 150 experiments were performed during this year by using these devices. Here we selected two topics to be presented as typical projects both for scientific and industrial application relevance.

**Wool fiber structure.** — The nanoscale structure of various filaments attracts particular interest in their technical applications. Small angle neutron scattering (SANS) is an ideal tool for the investigation of such anisotropic systems. Recently we have performed pioneering experiments on wool and mohair fibers. They have a variety of properties that influence the texture and feel of the final woven textile products. Chemical treatment, washing and drying, moreover repeated stress procedures can considerably influence the fiber properties. In wool, individual polypeptide chains are joined together to form proteins by a variety of covalent chemical bonds, called cross-links, and non-covalent physical interactions. To improve the physical properties, for instance shrink resistance of textiles, they are often treated with environmentally unfriendly chemicals, so here we present a set of SANS measurements to compare the effect of various chemical treatments (solution of chlorine, caraoat – potassium monopersulphate, enzyme and chlorine and enzyme and caraoat). The SANS facility at BNC was used with neutron wavelengths between 3.9 and 16 Å. The wool samples were packed



*Fig. 1a. Chlorine*

*Fig. 1b. Caraoat*

*Fig. 1c. Enzyme*

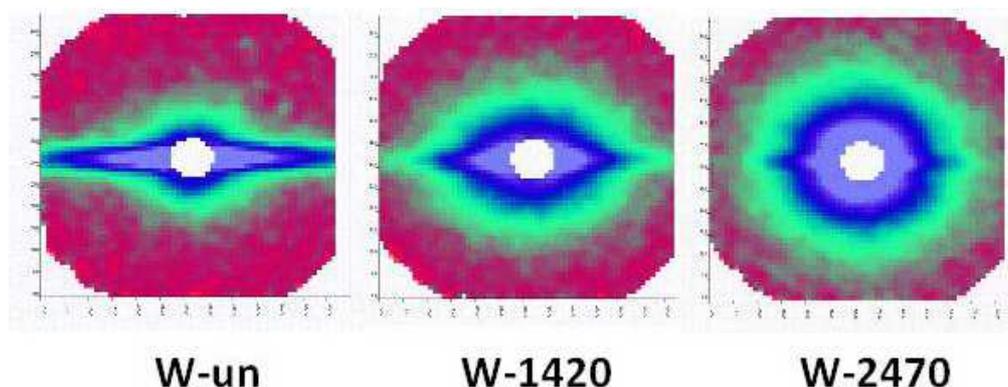
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<sup>#</sup> PhD student

<sup>+</sup>Permanent position: Laboratoire Léon Brillouin (LLB), CEA Saclay, 91191 Gif Sur Yvette, Cedex, France

into Al containers with the fibers aligned vertically. The results of SANS measurements are shown in Fig.1 in the form of 2D spectra.

The alignment of fibers, which is reflected in the scattering patterns due to the anisotropic nanoscale structure, tells about the treatment effect. The enzyme and chlorine treatments appeared to have the least disruptive effect on the fiber since the spectra were isotropic, whereas just the chlorine treatment had the greatest influence. In the dry wool structure we observed a density fluctuation with spherical gyration radius  $\sim 7-9$  nm corresponding to the physical diameter of long cylindrical samples. This can be identified as the micro-fibril size of the studied wool filaments. Wetting experiments on samples of mohair with mean diameter  $25.3 \mu\text{m}$  and  $37.3 \mu\text{m}$  were also performed. 2D SANS spectra were measured on dry samples and on samples with  $\text{D}_2\text{O}$ . These results gave an indication of where and how the water molecules are attached to and detached from the wool fiber. This new knowledge will go as far as developing an understanding, at the molecular level, the influence of the wetting and drying process of wool and mohair fibers. This project was performed as a science and technology collaboration between Hungary and South-Africa.



*Fig.2. 2D SANS scattering intensities of the 0.5 mm diameter tungsten samples taken from the different steps of the wire production. Temperatures of annealing: not annealed, 1420 K and 2470 K*

**Nanoscale morphology of tungsten wires.** — Another filament structure study was related to the morphology of doped tungsten used in lighting industry. Tungsten research has a long tradition in Hungary owing to GE TUNGSRAM – a leading manufacturer of lighting products worldwide. Our SANS study focused on the nanoscale structure of wires and, in particular, on the structure-stabilizing feature of potassium doping. We investigated the potassium bubbles present in the tungsten matrix of the drawn wires to understand several qualitative and quantitative characteristics of the potassium-tungsten complex system. During the mechanical and thermal processing the potassium bubbles form a specific texture that delays the break of the wire and prolongs its life. During the wire drawing the sphere-like bubbles get elongated along the axis of the wire forming ellipsoidal and cylinder-like bubbles. With further deformation the aspect ratio of a bubble reaches a critical value and becomes unstable: the ellipsoid splits into a row of elongated bubbles with a smaller aspect ratio. In the further steps of annealing the degree of the elongation decreases until all the bubbles adopt spherical shape. These rows of bubbles guide the grain boundary migration allowing the growth of elongated grains along the axis of the wire. This structure gives a good tensile

strength of the wires. Analyzing the 2D SANS maps (Fig.2) of series of samples annealed at different temperatures we can determine the elongation ratio and give an accurate description of the maturation of the bubble system inside the wire during the production. Using a sophisticated 2D data treatment method we obtained the anisotropy of the scattering in a large  $Q$  range ( $10^{-5} \text{ \AA}^{-1}$ -  $10^{-1} \text{ \AA}^{-1}$ ) enabling us to determine the size and shape of potassium bubbles. This lead us to understand that micro-crack formation during manufacturing of thin tungsten wires has always been presumed, and here it was finally demonstrated experimentally.

## GRANTS AND INTERNATIONAL COOPERATION

EU-FP7-CP-CSA-INFRA-2008-1.1.1 No. 226507-NMI3 – Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (J. Füzi, 2009-2012)

EU-FP7 – CHARISMA – Cultural Heritage Advanced Research Infrastructures: Synergy for a multidisciplinary approach to conservation/restoration (L. Rosta, 2009-2013)

EU-FP7-INFRASTRUCTURES-2011-1-283883, NMI3-II —Neutron Scattering and Muon Spectroscopy Integrated Initiative (L.Rosta, 2012-2015)

NAP VENEUS05 OMFB-06482/2008 Visegrád Cooperation for Development and Application of Neutron Spectroscopy Techniques in Multidisciplinary Research (L. Rosta, 2008-2011)

OTKA-A08-3 OMFB-00590/2010 Structure and dynamics of self-organized lamellar molecular systems (Mezei F. 2010-2012)

Research and Development Agreement between Wigner RCP and Helmholtz-Zentrum Berlin on Time-of-Flight Neutron Spectroscopy Techniques (L.Rosta, 2012-2014)

International Atomic Energy Agency: Project No. CRP1575, Development, Characterization and Testing of Materials of Relevance to Nuclear Energy Sector Using Neutron Beams (Gy. Török 2012-2013)

NFÜ- MAG ZRt. TÉT-0018 South-Africa, Structural Analysis of Treated Textile Fibres (Gy. Török 2011-2013)

## PUBLICATIONS

### Articles

1. Nagy G, Pieper\* J, Krumova\* SB, Kovács\* L, Trapp\* M, Garab\* G, Peters\* J; Dynamic properties of photosystem II membranes at physiological temperatures characterized by elastic incoherent neutron scattering. Increased flexibility associated with the inactivation of the oxygen evolving complex; *Photosynth Res*; **111**, 113-124, 2011
2. Rosta L, Len A, Pépy G, Harmat\* P, Nano-scale morphology of inclusions in tungsten wires – a complex SANS study; *Neutron News*; **23**, 13-16, 2011
3. Szakál A, Czifrus\* S, Marko M, Füzi J, Rosta L, Cser, L; Optimization of focusing supermirror neutron guides for low gamma-background; *Nucl Instr Meth A*; **634**, S130-S133, 2011

4. Cser L, Krexner\* G, Markó M, Szakál A; Neutron holography – a brief history and overview; *Neutron News*; **23**, 17-20, 2012
5. Fábián M, Sváb E; Uranium surrounding in borosilicate glasses from neutron- and X-ray diffraction and reverse Monte Carlo modeling; *Neutron News*; **23**, 9-12, 2012
6. Kasztovszky\* Zs, Rosta L; How can neutrons contribute to Cultural Heritage Research?; *Neutron News*; **23**, 25-28, 2012
7. Mezei F, Russina\* M, Káli Gy; Neutron diffraction for long pulse neutron sources; *Neutron News*; **23**, 29-31, 2012
8. Nagy G, Szabó\* M, Ünneper R, Káli Gy, Miloslavina\* Y, Lambrev\* PH, Zsiros\* O, Porcar\* L, Rosta L, Garab\* G; Modulation of the multilamellar membrane organization and of the chiral macrodomains in the diatom *Phaeodactylum tricornutum* revealed by small-angle neutron scattering and circular dichroism spectroscopy; *Photosynth Res*; **110**, 71-79, 2012
9. Posselt\* D, Nagy\* G, Kirkensgaard\* JJK, Holm\* JK, Aagaard\* TH, Timmins\* P, Rétfalvi\* E, Rosta L, Kovács\* L, Garab\* Gy; Small-angle neutron scattering study of the ultrastructure of chloroplast thylakoid membranes – periodicity and structural flexibility of the stroma lamellae; *Biochim Biophys Acta – Bioenergetics*; **8**, 1220-1228, 2012
10. Saerbeck\* T, Klose\* F, Le Brun\* AP, Füzi J, Brule\* A, Nelson\* A, Holt\* SA, James\* M; Polarization "Down Under": The polarized time-of-flight neutron reflectometer PLATYPUS; *Rev Sci Instr*; **83**, 081301/1-12, 2012
11. Török Gy, Lebedev\* V, Vinogradova\* L; Structural and conformational properties of polymeric stars with fullerene centre in solutions by SANS; *Procedia Chemistry*; **4**, 154-163, 2012

#### *Articles in Hungarian*

12. Rosta L, Nyolcvan éves a neutron (Eighty years from the discovery of neutron, in Hungarian); *Nukleon*; **5**(4), 1-5, 2012
13. Rosta L, Neutronkutatások Magyarországon (Neutron research in Hungary, in Hungarian); *Nukleon*; **5**(5), 1-5, 2012

#### *Conference proceedings*

14. Franklyn\* CB, Török Gy; Use of small angle neutron scattering to study various properties of wool and mohair fibres; In: *Proc. Applications of Nuclear Techniques Eleventh International Conference (12–18 June 2011 Crete, Greece)*; *AIP Conf Proc*; **1412**, 93-97, 2011
15. Russina\* M, Mezei F, Káli Gy; First implementation of novel multiplexing techniques for advanced instruments at pulsed neutron sources; *J Phys Conf Ser*; **340**, 2012

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**S-L. NEUTRON SCATTERING**

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*László Pusztai, Ildikó Harsányi, Pál Jóvári, László Kőszegi, György Mészáros, Viktória Mile, Szilvia Pothoczki, Erzsébet Sváb, László Temleitner*

**Electrolyte solutions.** — A detailed study of the microscopic structure of two electrolyte solutions, cesium fluoride (CsF) and cesium iodide (CsI) in water, has been conducted. For revealing the influence of salt concentration on the structure, CsF solutions at concentrations of 15.1 and 32.3 and CsI solutions at concentrations of 1.0, 3.9 molar % were investigated. For each concentration, total scattering structure factors from neutron and x-ray diffraction and 10 partial radial distribution functions from molecular dynamics simulations have been combined in one single structural model generated by Reverse Monte Carlo (RMC) modeling. The average angle of X...H-O (X: F, I) particle arrangements, characteristic to anion-water hydrogen bonds, is closer to 180° than that found for O...H-O arrangements (water-water hydrogen bonds) at higher concentrations. In Fig.1, simulation boxes for the highest concentrations are shown with the ions emphasized. Concerning concentrated lithium chloride solutions, new neutron and x-ray diffraction experiments have been performed that have been shown to be of superior quality to existing literature data. The cations were shown to possess an environment in which water oxygens and anions partially occupy octahedral sites. Surprisingly, some chloride ions seem to have some of their coordinated water molecules oriented symmetrically.

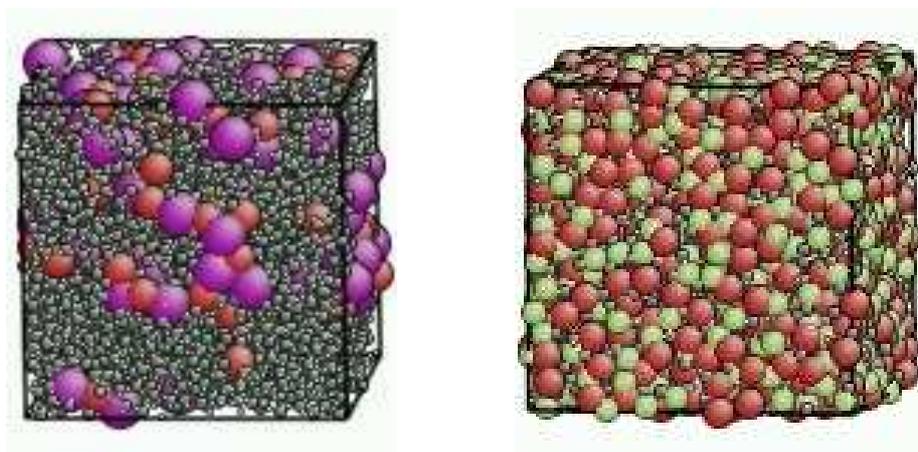
**Molybdate glasses.** — Mo-rare earth oxides are widely used due to their large ion and electron conductivities, catalytic activity, non-linear optical properties and good mechanical resistance. MoO<sub>3</sub> is well-known as a conditional network former and it is not able to form a glass itself at slow cooling rates. The aim of our work was to characterise some new molybdate glasses containing Nd<sub>2</sub>O<sub>3</sub> and B<sub>2</sub>O<sub>3</sub> and to verify their effect on the molybdate glass network. Nd<sub>2</sub>O<sub>3</sub> is an appropriate component due to its specific optical properties but it increases the melting temperature. By introducing B<sub>2</sub>O<sub>3</sub> it is possible to obtain low melting point materials over a wider concentration range. We performed both neutron and high energy x-ray diffraction experiments. For the Mo-O network the first neighbour distance at 1.8 Å was obtained with 4-fold oxygen coordination. For the B-O network two characteristic first neighbour distances were obtained at 1.40 Å and 1.60 Å, corresponding to the 3-fold trigonal and 4-fold tetrahedral B-O coordination. We concluded that the basic network is formed by mixed MoO<sub>4</sub>-BO<sub>4</sub> and MoO<sub>4</sub>-BO<sub>3</sub> units.

**Methodological developments.** — We have developed and tested a new Reverse Monte Carlo algorithm and the corresponding software RMC\_POT. In RMC\_POT, molecules are held together and the molecular geometry is maintained via a direct inclusion of bonding and non-bonding (including dihedral contributions) interactions. Potentials acting between atoms belonging to different molecules may also be used. RMC\_POT has been shown to be superior to previous molecular RMC algorithms on the example of liquid dimethyl-trisulfide.

**Amorphous chalcogenides.** — We investigated the amorphous chalcogenide GeCu<sub>2</sub>Te<sub>3</sub> with x-ray diffraction and extended x-ray absorption fine structure measurements at the Ge, Cu and Te K-edges. Structural models were obtained by fitting the four experimental datasets simultaneously by RMC modelling. We found that Ge-Ge and Cu-Cu bondings are both significant. The average coordination numbers of Cu and Te, as well as of Ge, are close to four. Thus, unlike for Ge-Sb-Te alloys, in case of GeCu<sub>2</sub>Te<sub>3</sub> the coordination numbers are

similar in the amorphous and crystalline phases. The high average coordination number of the network contributes to the enhanced thermal stability of amorphous  $\text{GeCu}_2\text{Te}_3$ .

The structure of  $\text{Ge}_5\text{As}_x\text{Se}_{95-x}$  ( $x = 10, 20, 30, 38$  at.%) and  $\text{Ge}_{15}\text{As}_x\text{Se}_{85-x}$  ( $x = 10, 25, 34$  at.%) glasses has been investigated by high-energy x-ray diffraction and extended x-ray absorption fine structure measurements. The experimental datasets have been fitted using the RMC technique. We find that the homonuclear Ge–Ge, As–As, Se–Se and heteronuclear Ge–As bonds play an important role in the structure formation of the Ge–As–Se glasses. The total number of these bonds decreases quite slowly with the mean coordination number similarly to the nonlinear refractive index.



(a) Concentrated CsI solution.

(b) Concentrated CsF solution.

*Figure 1 Snapshots taken from molecular dynamics simulation of (a) the 3.9 molar % CsI solution and (b) the 32.3 molar % CsF solution. Grey (small) balls: atoms of water molecules; red balls: Cs+ ions; magenta balls: I- ions; light green balls: F- ions. (Ball sizes are according to the van der Waals radii.). The pictures illustrate that although both solutions are at their saturated concentrations, the ion/water ratios are very different.*

## GRANTS AND INTERNATIONAL COOPERATION

OTKA K083529 Investigations concerning the structure of complex liquids (L. Pusztai, 2011-2014)

TÉT\_10-1-2011-0004 (Hungarian-Japanese bilateral): Investigations of structural disorder in liquids, as well as in amorphous and crystalline solids, via combining diffraction and EXAFS experiments with Reverse Monte Carlo modelling (L. Pusztai, 2012-2013)

MTA-BAS (Hungarian-Bulgarian bilateral): Structure studies of crystalline and amorphous materials by neutron diffraction (E. Sváb, 2010-2012)

MTA-BAS (Hungarian-Bulgarian bilateral): Investigation of disordered materials based on Se-Te chalcogenide glasses by means of neutron diffraction and IR spectrophotometry (E. Sváb, 2010-2012)

**PUBLICATIONS***Articles*

1. Vrhovšek\* A, Gereben\* O, Jamnik\* A, Pusztai L; Hydrogen bonding and molecular aggregates in liquid methanol, ethanol and propanol; *J Phys Chem B*; **115**, 13473-13488, 2011
2. Harsányi I, Bopp\* PA, Vrhovšek\* A, Pusztai L; On the hydration structure of LiCl aqueous solutions: a Reverse Monte Carlo based combination of diffraction data and Molecular Dynamics simulations; *J Mol Liq*; **158**, 61-67, 2011
3. Fábíán M, Sváb E, Pamukchieva\* V, Szekeres\* A, Vogel\* S, Ruett\* U; Study of As—Se—Te glasses by neutron-, X-ray diffraction and optical spectroscopic methods; *J Non-Cryst Solids*; **358**, 860-868, 2012
4. Temleitner L, Pusztai L, Rubio-Arroyo\* MF, Aguilar-Lopez\* S, Klimova\* T, Pizio\* O; Microscopic and mesoscopic structural features of an activated carbon sample, prepared from sorghum via activation by phosphoric acid; *Materials Research Bulletin*; **47**, 4409-4413, 2012
5. Sváb E, Beregi E, Fábíán M, Mészáros Gy; Neutron diffraction structure study of Er and Yb doped  $YAl_3(BO_3)_4$ ; *Optical Materials*; **34**, 1473–1476, 2012
6. Harsányi I, Temleitner L, Beuneu\* B, Pusztai L; Neutron and X-ray diffraction measurements on highly concentrated aqueous LiCl solutions; *J Mol Liq*; **165**, 94-100, 2012
7. Ohara\* K, Temleitner L, Sugimoto\* K, Kohara\* S, Matsunaga\* T, Pusztai L, Ito\* M, Ohsumi\* H, Kojima\* R, Yamada\* N, Usuki\* T, Fujiwara\* A, Takata\* M; The roles of the Ge-Te core network and the Sb-Te pseudo network during rapid nucleation-dominated crystallization of amorphous  $Ge_2Sb_2Te_5$ ; *Advanced Functional Materials*; **22**, 2251-2257, 2012
8. Gereben\* O, Kohara\* S, Pusztai L; The liquid structure of some food aromas: joint X-ray diffraction, all-atom Molecular Dynamics and Reverse Monte Carlo investigations of dimethyl sulfide, dimethyl disulfide and dimethyl trisulfide; *J Mol Liq*; **169**, 63-73, 2012
9. Pothoczki Sz, Temleitner L, Pusztai L; Determination of molecular orientational correlations in disordered systems from diffraction data; *Advances in Chemical Physics*; **150**, 143-168, 2012
10. Antipas\* GSE, Temleitner L, Karalis\* K, Kohara\* S, Pusztai L, Xenidis\* A; A containerless study of short-range order in high-temperature Fe-Si-Al-Ca-Mg-Cr-Cu-Ni oxide systems; *J Mol Struct*; **1019**, 151-158, 2012
11. Steinczinger\* Zs, Pusztai L; An independent, general method for checking consistency between diffraction data and partial radial distribution functions derived from them: the example of liquid water; *Condensed Matter Physics*; **15**, 23606/1-6, 2012
12. Gereben\* O, Pusztai L; Molecular conformations and the liquid structure in bis(methylthio)methane and diethyl sulfide: diffraction experiments vs molecular dynamics simulations; *J Phys Chem B*; **116**, 9114-9121, 2012

13. Mile V, Gereben<sup>\*</sup> O, Kohara<sup>\*</sup> S, Pusztai L; On the structure of aqueous cesium fluoride and cesium iodide solutions: Diffraction experiments, Molecular Dynamics simulations and Reverse Monte Carlo modeling; *J Phys Chem B*; **116**, 9758-9767, 2012
14. Gereben O, Pusztai L; RMC\_POT, a computer code for Reverse Monte Carlo modeling the structure of disordered systems containing molecules of arbitrary complexity; *Journal of Computational Chemistry*; **33**, 2285–2291, 2012
15. Voleska<sup>\*</sup> I, Akola<sup>\*</sup> J, Jóvári P, Gutwirth<sup>\*</sup> J, Wagner<sup>\*</sup> T, Yannopoulos<sup>\*</sup> SN, Jones<sup>\*</sup> RO; Structure, electronic, and vibrational properties of glassy Ga<sub>11</sub>Ge<sub>11</sub>Te<sub>78</sub>: Experimentally constrained density functional study; *Phys Rev B*; **86**, 094108/1-9, 2012
16. Kaban<sup>\*</sup> I, Jóvári P, Wang<sup>\*</sup> R-P, Luther-Davies<sup>\*</sup> B, Mattern<sup>\*</sup> N, Eckert<sup>\*</sup> J; Structural investigations of Ge<sub>5</sub>As<sub>x</sub>Se<sub>95-x</sub> and Ge<sub>15</sub>As<sub>x</sub>Se<sub>85-x</sub> glasses using x-ray diffraction and extended x-ray fine structure spectroscopy; *J Phys: Condensed Matter*; **24**, 385802:1-7, 2012
17. Chrissanthopoulos<sup>\*</sup> A, Jóvári P, Kaban<sup>\*</sup> I, Gruner<sup>\*</sup> S, Kavetsky<sup>\*</sup> T, Borc<sup>\*</sup> J, Wang<sup>\*</sup> W, Ren<sup>\*</sup> J, Chen<sup>\*</sup> G, Yannopoulos<sup>\*</sup> SN; Structure of AgI-doped Ge–In–S glasses: Experiment, reverse Monte Carlo modelling, and density functional calculations; *J Solid State Chem*; **192**, 7-15, 2012

**Articles in Hungarian**

18. Fábrián M., Sváb E; Boroszilikát üvegek szerkezetvizsgálata neutrondiffrakcióval (Neutron diffraction study of borosilicate glasses, in Hungarian); *Nukleon*; **V(119)**, 1-6, 2012

**See also: S-K.5.**

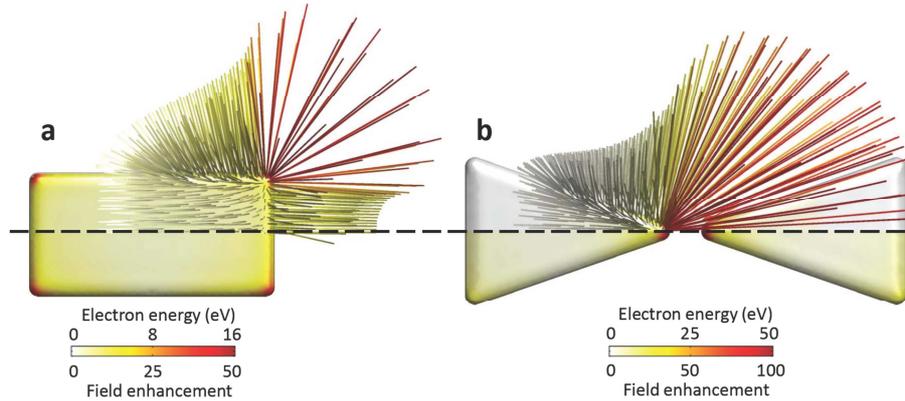
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**S-M. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER**


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*Győző Farkas, Balázs Bódi, Péter Dombi, Júlia Fekete, Norbert Kroó, Péter Rácz, Sándor Varró*

**Experimental research.** — We carried out experimental investigations on ultrafast photoemission from tailored metallic nanostructures. We could define structures where the femtosecond photoemission process and electron acceleration was significantly enhanced thanks to hot spots on the nanoparticles. We established that the electron acceleration process in these nanoparticle fields is ponderomotive in its nature and we found clear correlation between the nanolocalized field enhancement and the electron spectrum measured with a retarding field analyzer. Theory and nanoparticle fabrication support for these experiments were provided by the University of Graz in a close collaboration (Fig. 1).



*Fig. 1. Spatial distribution of electrons in photoemission from metallic nanoparticles, including (a) nanorods and (b) bowtie-type structures. The electron energy is encoded in the colour and length of the trajectories.*

With the help of the hELIOS grant of the National Development Agency, we set up a multifunctional attosecond laboratory. Based on an amplified Ti:sapphire laser system delivering 4-mJ 35-fs pulses with 1 kHz repetition rate, we set up multiple workstations for high harmonic generation, XUV spectroscopy, ultrafast photoemission and optical damage threshold testing. Research at these workstations on various subjects is under way and further developments and upgrades are also planned.

We took part also in experiments related to the diffraction efficiency of gratings etched into fused silica. We successfully modelled the diffraction efficiency of gratings fabricated with the use of two-beam interferometric laser-induced backside wet etching (TWIN-LIBWE).

**Theory of strong-field phenomena and quantum optics.** — The generation of broad-band radiation and short pulses rely on highly nonlinear processes induced by intense laser fields. In general, the magnitudes of these nonlinearities depend on the target. Besides, carrier-envelope phase difference effects may also be important concerning short pulses. Depending on various parameters, intense fields may cause relatively modest effects, and moderately intense lasers may induce very high-order processes. We discussed an example for the latter situation, and we showed that the collective radiation back-reaction of relativistic surface

currents of graphene electrons driven by a laser field can cause a violent distortion in the scattered radiation (Fig. 2).

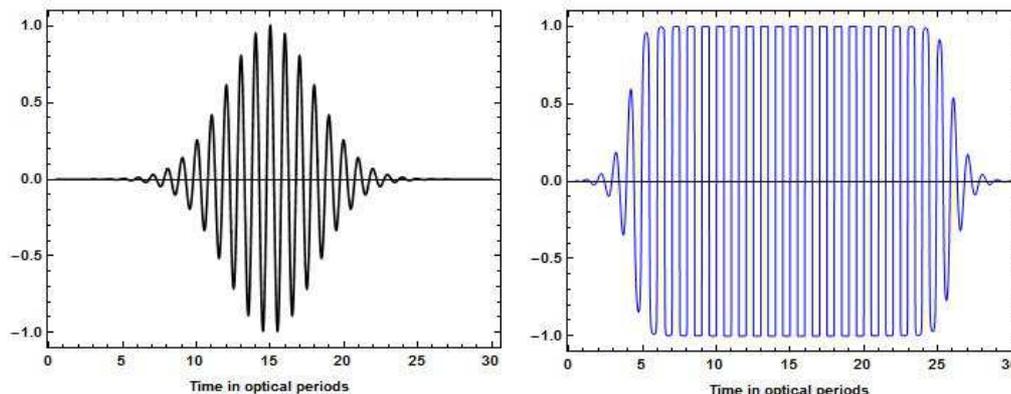


Figure 2. Distortion of a five-cycle *p*-polarized Gaussian laser pulse (left) impinging at Brewster angle on a graphene layer. The reflected component is nonzero (right). Its existence cannot be explained by the usual Fresnel formulae. The rectangular (Rademacher function) shape stems from the “clipping effect.”

A high spatial resolution surface plasmon near field scanning tunneling microscope (STM) was used to study the properties of localized surface plasmons (SPO) in so-called hot spots on a gold surface, where the local electromagnetic field is extremely high. A CW semiconductor laser and a femtosecond Ti:Sa laser were used to excite the plasmons and the SPO excited tunnel current was used as the detector. When scanning the STM from negative to positive bias and reversed, hysteresis in the tunnel signal was found. By taking into account a multiple image charge induced double-well potential our experimental findings were theoretically explained.

We have calculated the characteristics of the synchrotron radiation emitted by ultrarelativistic electrons in the interior of a coaxial cylindrical mirror. This is an unconventional geometrical arrangement, where the “superradiance” may be realized in two dimensions. This scheme may also serve as a possibility to reduce radiation losses.

A mathematical analysis of the fractional part of energy (that is  $x = \{E/E_0\}$ , or “round-off error”) in energy measurements of chaotic radiation has been carried out. We represent the realizations of this quantity by binary sequences like  $x = 0.001011000010\dots$  and discuss their “digital randomness.” On the basis of the statistics of 0’s and 1’s, we have derived the probability distribution of  $x$ . We have proved that if the digits are independent and have the same distribution, then  $x$  has zero-point fluctuations.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA 73728      Attosecond dynamics of matter in ultra-high laser fields with sub-cycle temporal and sub-wavelength, nanometer-scale spatial resolution (S. Varró, 2008-2012)

OTKA K104260      Particles and intense fields (T. S. Bíró and S. Varró, 2012-2016)

## S-M. Interactions of intense laser fields with matter

- DAAD A/12/01761 Phase-space distribution of elementary quantum systems and the radiation problem in nano-electrodynamics. Deutsche Akademische Austauschdienst. Research stay in Germany, 3 months, 2012. (DAAD A/12/01761, S. Varró, 2012)
- NFÜ, hELIOS Grant for the foundation of the Budapest ELI Laser Laboratory (P. Dombi, 2011-2013)
- NFÜ Grant No. ELI\_09-1-2010-0010, Helios Project (P. Dombi, Gy. Farkas, P. Rácz, S Varró, 2011-2013)
- TÉT ES7/2008 Ultrafast laser-solid interaction dynamics in the field of intense, few-cycle laser pulses (P. Dombi, P. Rácz, J. Fekete, 2009-2012).
- INSTITUTE FOR QUANTUM PHYSICS, University of Ulm (Ulm, Germany); Wigner functions in optics. (S. Varró).
- INSTITUTE FOR QUANTUM OPTICS, University of Ulm (Ulm, Germany); Radiation properties of Nitrogen-Vacancy centers in diamond (S. Varró); Surface plasmon research. (S. Varró and N. Kroó).
- INSTITUTE FOR APPLIED PHYSICS, Technical University of Darmstadt (Darmstadt, Germany); Quantum phase-space: Statistical properties of hybrid light. (S. Varró).
- PHYSICS DEPARTMENT, University of Connecticut (Storrs, Connecticut, USA); Gauge-invariant Wigner functions. (S. Varró).
- MAX PLANCK INSTITUTE for Quantum Optics (Garching, Germany); Surface plasmon research using STM (N. Kroó); Ultrafast photoemission from metallic nanotips (P. Dombi).
- UNIVERSITY OF ALBERTA, Edmonton, Canada, Field-enhanced electron acceleration with few-cycle laser pulses (P. Dombi).
- INSTITUTE FOR PHOTONIC SCIENCES, Barcelona, Ultrafast electron acceleration experiments with mid-infrared lasers (P. Dombi, P. Rácz).
- KARL-FRANZENS-UNIVERSITÄT, Graz, Investigation of femtosecond photoemission from nanostructures (P. Dombi).

## PUBLICATIONS

### *Articles*

1. Rácz P, Dombi P; Non-ponderomotive electron acceleration in ultrashort surface plasmon fields; *Phys Rev A*; **84**, 063844/1-5, 2011
2. Kiss\* B, Vass\* C, Heck\* P, Dombi P, Osvey\* K; Fabrication and analysis of transmission gratings produced by the indirect laser etching technique; *J Phys D: Applied Physics*; **44**, 415103/1-5, 2011
3. Balogh\* E, Dombi P, Varjú\* K; Terahertz pulses enhance generation of attosecond light bursts; *SPIE Newsroom*; 6 February 2012, pp. 1-2, 2012;  
DOI: 10.1117/2.1201201.003988.

***Conference proceedings***

4. Varró S; Graphene-based carrier-envelope phase difference meter. In: Proc. Light at Extreme Intensities (Szeged, Hungary, 14–18 November 2011); Eds.: K. Osvay, P. Dombi, JA. Fülöp, K. Varjú; AIP Conf Proc; 1462, 128-131, 2012. Books, book chapters
5. Varró S; Interference phenomena and whispering-gallery modes of synchrotron radiation in a cylindrical wave-guide; In: *Free Electron Lasers, Chapter 7*; Ed.: Varró S, Rijeka, InTech; pp. 175-186, 2012
6. Osvay\* K, Dombi P, Fülöp\* JA, Varjú\* K (eds.); Proc. Light at Extreme Intensities (Szeged, Hungary, 14–18 November 2011); *AIP Conf Proc*; **1462**, pp. 1-262, 2012.

***See also: S-O.1***

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**S-N. GAS DISCHARGE PHYSICS**

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*Péter Hartmann, Aranka Derzsi, Zoltán Donkó, Zoltán György Horváth, Ihor Korolov, Anikó-Zsuzsa Kovács,<sup>#</sup> Kinga Kutasi, Pál Mezei, Károly Rózsa*

**Physics of electric discharges.** — We have developed an improved analysis method to evaluate data of infrared laser absorption measurements of the density of metastable atoms in low-pressure discharges. Our measurements and data analysis resulted in unexpectedly high metastable atom densities near the cathode surfaces, which can only be explained by – to-date unclarified – production processes at the surface. We have carried out particle-in-cell simulations to analyze the behaviour of dust particles suspended in a dual-frequency gas discharge, where changing the excitation waveform allows transport manipulation of dust particles. Similar simulations were used to uncover the effects of the operation frequency of radiofrequency discharges. These investigations have shown that the control range of ion properties (under dual frequency excitation) gets more restricted towards low frequencies. We developed an experimental Franck-Hertz cell operated on the basis of photoemission and have analyzed the complex electron kinetics in this device by a Monte Carlo stochastic simulation.

**Strongly coupled plasma research.** — We further developed our molecular dynamics simulations (including codes for GPU architectures) and different theoretical approaches (lattice summation and quasilocalized charge approximation). We applied these techniques to the study of collective and transport processes in strongly coupled plasmas. We demonstrated the enhancement of two-stream instabilities due to strong coupling. We established the connection between the Maxwell relaxation time and the crossover of the elastic and dissipative components of the frequency dependent complex viscosity in strongly coupled Yukawa liquids. Wave dispersions of two component 2D and 3D Yukawa liquids were computed and analyzed, showing the validity of the virtual atom approximation in the strongly coupled regime.

**Surface wave microwave discharge systems for biomedicine and nanostructuring.** — Surfatron generated surface wave microwave discharges produced in small diameter tubes contain high density of active species. When the discharge is created in flowing gas the active species can be transported into different size and configuration reactors that can be used for different applications, such as sterilization of medical tools, surface treatment and functionalization, and synthesis of nanostructures. The density of active species downstream of an Ar-O<sub>2</sub>-N<sub>2</sub> discharge was determined both experimentally and by means of modeling. Calculations were conducted in order to understand the role of active species in surface functionalization and their interaction with bacteria (attachment of active atoms to the bacteria) during the sterilization process.

**Electrolyte cathode atmospheric pressure glow discharge (ELCAD).** — The analytical characteristics of a capillary design of the electrolyte cathode atmospheric glow discharge (ELCAD), operated with a W-rod anode at a discharge current of 70 mA and a discharge voltage of 950 V, were exploited through spatially resolved atomic absorption spectrometry (AAS) experiments. For this purpose, the ELCAD cell, placed on a platform adjustable with micrometer screws, was inserted into the optical path of a commercial line-source AAS

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<sup>#</sup> PhD student

instrument. A flow injection system was developed and applied to introduce 3 mL of aqueous standards of a set of environmentally relevant metals (Ca, Cd, Cr, Cu, Na, Pb and Zn) into the plasma. The analyte atom distribution along the vertical axis of the conically-shaped ELCAD plasma (height: 3.5 mm) is element specific. All the absorbance maxima are observed in the near cathode region (e.g., in the range of 0.5-1.0 mm from the cathode), while the AA signal smoothly fades towards the anode. Several spectrochemical buffers (citric acid, EDTA, chlorides of Ca, Cs, La, Li, and Na) were studied for improving the sensitivity of the AAS determinations for Cr. A significant increase in the sensitivity (20 %) was found only with the addition of 0.55 % (m/v) La solution. The limit of detection data for Cd, Cu, Na and Zn are 3.4, 4.2, 9.2 and 0.9 mg l<sup>-1</sup>, respectively. The AAS calibration curves for Cd, Cu, Na and Zn are linear up to 75, 200, 100 and 25 mg l<sup>-1</sup>, respectively.

#### GRANTS AND INTERNATIONAL COOPERATION:

- OTKA K-77653 High performance modeling and simulation of low-temperature and strongly coupled plasmas (Z. Donkó, 2009–2013)
- OTKA PD-75113 Phase transition and collective dynamics of two-dimensional many-particle systems (P. Hartmann, 2009–2012)
- OTKA NN-103150 Dusty plasma: a laboratory for classical many-particle physics (P. Hartmann, 2012–2015)
- OTKA K-68390 Investigations of atomization processes in an electrolyte cathode atmospheric glow discharge (P. Mezei, 2007-2012)
- OTKA-K-104531 High and low-frequency discharges for biomedical applications and nanostructuring (K. Kutasi 2012-2016)
- MTA-SASA (Hungarian-Serbian bilateral) Hybrid models for gas breakdown and formation of plasmas (K. Kutasi 2010-2013)
- TÉT\_10-1-2011-0717 (Hungarian-French bilateral) Study of Ar-O<sub>2</sub> surface-wave microwave discharges and their pos-discharges (K. Kutasi 2011-2012)
- TÉT\_10-1-2011-0717 (Hungarian-Slovenian bilateral) Investigation of microwave discharges applicable in biomedicine and nanotechnology (K. Kutasi 2012-2013)
- COST Action MP1101 Biomedical Applications of Atmospheric Pressure Plasma Technology (K. Kutasi 2012-2015)

#### PUBLICATIONS

##### Articles

1. Mezei P, Cserfalvi\* T; A critical review of published data on the gas temperature and the electron density in the electrolyte cathode atmospheric glow discharges; *Sensors*; **12**, 6576-6586, 2012
2. Schulze\* J, Derzsi A, Dittmann\* K, Hemke\* T, Meichsner\* J, Donkó Z; Ionization by drift and ambipolar electric fields in electronegative capacitive radio frequency plasmas; *Phys Rev Lett*; **107**, 275001/1-5, 2011

3. Korolov I, Bánó\* G, Donkó Z; Experimental investigation of the asymmetric charge exchange reaction in the Ar+–Ni system in the afterglow of a pulsed glow discharge; *Spectrochimica Acta Part B: Atomic Spectroscopy*; **66**, 706-711, 2011
4. Stano\* M, Pinhao\* N, Loffhagen\* D, Kucera\* M, Donkó Z, Matejcik\* S; Effect of small admixtures of N<sub>2</sub>, H<sub>2</sub> or O<sub>2</sub> on the electron drift velocity in argon: experimental measurements and calculations; *Eur Phys J D*; **65**, 489-498, 2011
5. Iwashita\* S, Uchida\* G, Schulze\* J, Schüngel\* E, Hartmann P, Shiratani\* M, Donkó Z; Sheath-to-sheath transport of dust particles in a capacitively coupled discharge; *Plasma Sources Sci Technol*; **21**, 032001/1-5, 2012
6. Bánó\* G, Donkó Z; On the high argon metastable atom density measured near the cathode surface of a hollow cathode discharge; *Plasma Sources Sci Technol*; **21**, 035011/1-10, 2012
7. Magyar\* P, Korolov I, Donkó Z; Photoelectric Franck-Hertz experiment and its kinetic analysis by Monte Carlo simulation; *Phys Rev E*; **85**, 056409/1-10, 2012
8. Rosenberg\* M, Kalman\* G J, Hartmann P; Instabilities in Yukawa liquids; *Contrib Plasma Phys*; **52**, 70-73, 2012
9. Budea\* Á, Derzsi A, Hartmann P, Donkó Z; Shear viscosity of liquid-phase Yukawa plasmas from Molecular Dynamics simulations on graphics processing units; *Contrib Plasma Phys*; **52**, 194-198, 2012
10. Golden\* K I, Kalman\* G J, Hartmann P, Donkó Z; Collective modes in classical mass-asymmetric bilayers; *Contrib Plasma Phys*; **52**, 130-134, 2012
11. Kovács A, Hartmann P, Donkó Z; Dynamic shear viscosity in a 2D Yukawa system; *Contrib Plasma Phys*; **52**, 199-202, 2012
12. Kalman\* G J, Kyrkos\* S, Golden\* K I, Hartmann P, Donkó Z; The roton minimum: Is it a general feature of strongly correlated liquids?; *Contrib Plasma Phys*; **52**, 219-223, 2012
13. Kalman\* G J, Donkó Z, Hartmann P, Golden\* K I, Kyrkos\* S; Collective modes in strongly coupled binary liquids; *Contrib Plasma Phys*; **52**, 234-237, 2012
14. Goree\* J, Donkó Z, Hartmann P; Cutoff wave number for shear waves and Maxwell relaxation time in Yukawa liquids; *Phys Rev E*; **85**, 066401/1-7, 2012
15. Kutasi K, Sá\* P A, Guerra\* V; O<sub>2</sub> dissociation in Ar-O<sub>2</sub> surface-wave microwave discharges; *J Phys D: Appl Phys*; **45**, 195205/1-8, 2012
16. Donkó Z, Hartmann P, Shukla\* P K; Consequences of an attractive force on collective modes and dust structures in a strongly coupled dusty plasma; *Physics Letters A*; **376**, 3199-3203, 2012
17. Korolov I, Donkó Z, Czarntzki\* U, Schulze\* J; The effect of the driving frequencies on the electrical asymmetry of dual-frequency capacitively coupled plasmas; *J Phys D: Appl Phys*; **45**, 465205/1-9, 2012

#### **Conference proceedings**

20. Donkó Z; Electron kinetics in air studied by Monte Carlo simulation; In: *Proc. of 18th Symposium on Application of Plasma Processes and Workshop on Plasmas as a*

*Planetary Atmosphere Mimics (January 15-20, 2011, Hotel Boboty, Vrátna, Malá Fatra, Slovakia); pp. 53-56*

***Other***

21. Z. Gy. Horváth; Beyond the Beam: A History of Multidimensional Lasers; *Optics and Photonics News*; July/August, 36-41, 2012

***See also: S-R.4.***

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**S-O. LASER APPLICATIONS**

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*Aladár Czitrovsky, László Himics,<sup>#</sup> Péter Jani, Attila Kerekes,<sup>#</sup> Margit Koós, Attila Nagy, Dániel Oszetzky, Sára Tóth, Lénárd Vámos, Miklós Veres, Júlia Fekete*

**Optical measuring techniques.** — As the coordinator of a consortium of 5 institutions within the ELI\_09-1-2010-0010 NFÜ project we started the development of a laser system, new optical coatings, and measurement methods related to ELI ALPS (Extreme Light Infrastructure Attosecond Light Pulse Source). In the frame of this project we established an Attosecond Laser Laboratory (ALL) with clean room area and an Optical Metrology Laboratory (OML). In ALL we developed a laser system with 35 fs pulse duration, 1 kHz repetition rate, and 4 mJ pulse energy. We generated high harmonics and registered an attosecond pulse train. In OML we implemented a measurement system for high resolution optical surface testing with a vertical resolution of  $\sim 0.1$  nm for surfaces up to  $102 \times 102$  mm<sup>2</sup>. In OML using femtosecond laser pulses we are developing an optical damage threshold testing system for characterization of optical coatings and a high dynamic range light scattering measurement system for control of the purity of substrates and quality of optical materials. For clean room monitoring at ALL, we use our previously developed airborne particle counter.

We used our formerly developed pulmonary waveform generator and laser Doppler anemometer for in vitro testing and measurement of the aerosol flow in transparent hollow human airway models to determine the velocity distribution and drug delivery in realistic hollow airway models. We performed a numerical modeling of flow dynamics and flow profiles (which determines aerosol deposition) in the stochastic lung model and applied the computational fluid dynamics (CFD) code for various respiratory tracts. The results of the simulations were compared with experimental data.

The newly developed prototype of Nano-LDA photon correlation system was tested in Cambridge University and Clausthal Technical University where different nano-particles in the  $\sim 100$  nm size range were measured. The measured data were compared to results of other methods (e.g. Differential Mobility Analyzer, Optical particle sizer) and a good agreement was observed.

**Amorphous carbon layers.** — Formation, investigation and tailored engineering of color centers is one of the most intensely studied areas of current diamond and nanodiamond research. Silicon vacancy (Si-V) center, for example, has an intense photoluminescence feature around 738 nm, which is well within the wavelength window of highest optical transparency of organic tissues and it has a small width of about 10 nm. For this reason, nanodiamonds with Si-V defects are promising candidates for in vivo sensing applications. Such applications, however, require well-controlled preparation methods and detailed understanding of the properties of the defects.

One of the simplest ways of producing nanodiamonds with Si-V centers is to incorporate Si atoms into the growing diamond structure during the deposition process. Obviously, preparation conditions have important effect on the properties of the forming structures. Analysis of the light emission from Si-V centers in nanodiamond sample series prepared in a

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<sup>#</sup> PhD student

wide range of methane concentrations and substrate temperatures allowed us to determine the optimal conditions leading to diamond structures with efficiently emitting Si-vacancy centers.

Figure 1 shows the evolution of the Si-V photoluminescence peak parameters with methane concentration for different substrate temperatures used during nanodiamond film growth. It can be seen that higher methane concentrations and temperatures both cause blueshift and narrowing of the Si-V peak. Intense light emission was observed in samples prepared at low substrate temperatures and relatively high methane concentrations.

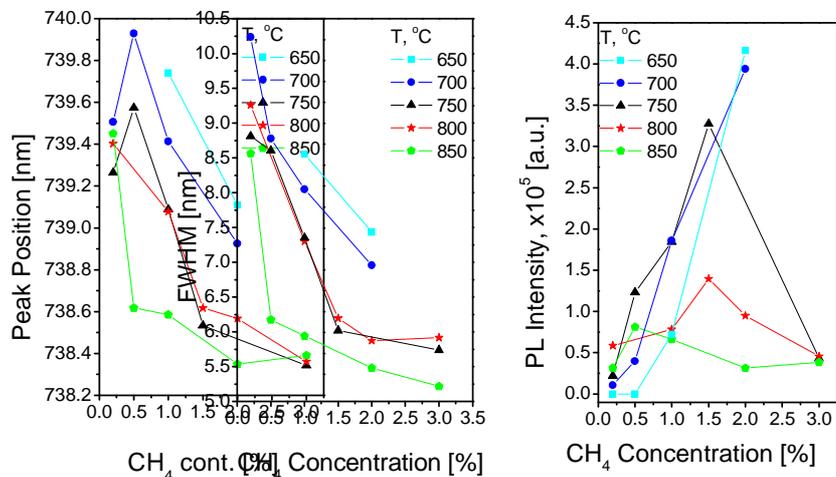


Fig. 1 Evolution of Si-V photoluminescence peak parameters with methane content of the feed gas in sample sets prepared at different substrate temperatures.

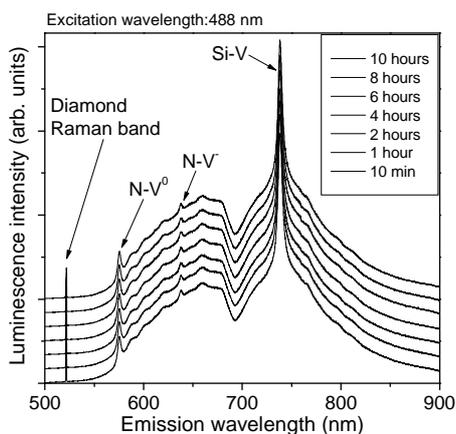


Fig. 2 Photostability of color centers in nanodiamond at power density of 12 kW/cm<sup>2</sup>.

Photostability of color centers under intense and long-time illumination is essential for their practical application. We found that both N-V and Si-V color centers have excellent stability over time when irradiated with light power densities of up to 12 kW/cm<sup>2</sup> (Fig. 2). In addition, photostability of Si-V was demonstrated at elevated temperatures (up to 373 K) and higher power densities of 144 kW/cm<sup>2</sup>.

## GRANTS AND INTERNATIONAL COOPERATION

ELI\_09-1-2010-0010 NFÜ Establishing Budapest Research Centre for ELI Laser Technology - hELIos project (A. Czitrovsky, 2010-2013)

MTA Research Infrastructure Grant No. 072/2011 (A. Czitrovsky, 2011-2012)

HOYA-SZFI IG Contract No. 279/2011, Measurement and analysis of air pollution at HOYA Corporation, Mátészalka (A. Czitrovsky, 2010-2012)

IAEA-15455 Porous polymer drug-eluting coating prepared by radiation induced polymerization (M. Veres, 2009-2012)

TÉT KR-6/2009 Hungarian-Korean bilateral: Surface modification of nanodiamond by conductive polymer (M. Veres, 2010-2012)

OTKA PD-106130 Generation of highly luminescent color centers in nanocrystalline diamond (S. Tóth, 2012-2015).

Gi3989/2008 Technoorg-Linda - SZFKI, Development of nanoparticle measurement system, (P. Jani, 2009-2012)

## LONG TERM VISITOR

— Prof. Mitsa Vladimir, Uzhgorod State University, Uzhgorod, Ukraine, August 15 – September 15, 2012 (host: M. Koós)

## PUBLICATIONS

### Articles

1. Varró S, Kroó N, Oszetzky D, Nagy A, Czitrovsky A; Hanbury Brown–Twiss type correlations with surface plasmon light, *J Modern Optics*, **58**, 2049-2057, 2011
2. Gopalan\* AI, Ko\* KR, Lee\* SH, Shanmugasundaram\* K, Veres M, Lee\* KP; Radiation induced preparation of new multifunctional nanobiowebs; *Rad Phys Chem*; **81**, 1407-1410, 2012.
3. Gyollai\* I, Gucsik\* A, Veres M, Koós M, Nagy\* Sz, Bérczi\* Sz; A Combined Petrographic and Micro-Raman Study of Meteoritic Microdiamond in ALH-77257 Ureilite and ALH-78113 Aubrite; *Spectroscopy Letters*; **45**, 151-155, 2012.
4. Karmenyan\* AV, Perevedentseva\* E, Veres M, Cheng\* CL; Simultaneous photoluminescence and SERS observation of nanodiamond at laser deposition on noble metals; *Plasmonics online*; pp. 1-9, 2012; DOI 10.1007/s11468-012-9393-x, 2012.

### Patent

5. Vámos L, Jani P, Schlosser P, Szigethy\* D; Data evaluation procedure for determination of the size of nano-particles in photon-correlation anemometer; Hungarian Patent P 12 00403, 2012

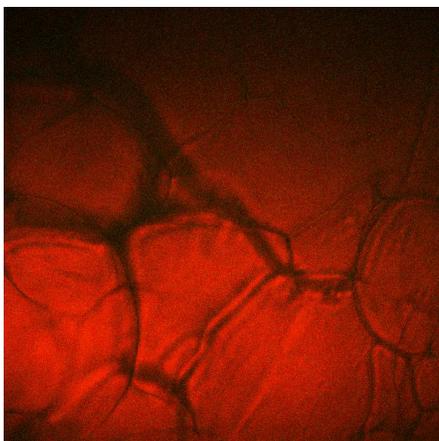
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**S-P. FEMTOSECOND LASERS**


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*Róbert Szipőcs, Péter Antal,<sup>#</sup> Zoltán Várallyay, Dániel Csáti, Attila Kolonics*

**Nonlinear 3D microscopy.** — We performed a high number of experiments related to *in vivo* optical disease diagnosis, such as basalioma detection, or *in vivo* drug monitoring, in collaboration with our scientific partners at Semmelweis University, Department of Dermatology and a pharmaceutical company, Genetic Immunity, respectively. For these measurements, we upgraded our standard scanning two-photon absorption fluorescence microscope (*Axio Examiner LSM 7 MP*, product of Carl Zeiss) by a second harmonic generation (SHG) detection unit, which could be efficiently used for label-free detection of the collagen network of the skin for instance. Beside auto-fluorescence and SHG detection, coherent anti-Stokes Raman scattering (CARS) allows for label-free imaging of tissue with chemical contrast and high spatial and temporal resolution as well. In CARS, laser beams at two frequencies, called the pump ( $\omega_p$ ) and Stokes ( $\omega_s$ ), are used to illuminate the sample. When the difference frequency between the two beams is tuned to match an intrinsic molecular vibrational frequency in the sample,  $\omega_{\text{vib}}$ , a nonlinear interaction occurs: new light is generated at the anti-Stokes frequency,  $\omega_{\text{as}} = 2\omega_p - \omega_s$ , by the CARS process. CARS imaging offers chemical selectivity, high spatial resolution imaging *in vivo* in living animals and humans.



*Fig. 1 CARS-image of murine white adipose tissue.*

Last year we developed a prototype of a simple wavelength extension unit for our tunable Ti:sapphire lasers comprising a two stage Yb-fiber amplifier unit, which allows CARS measurements practically on the same microscope and lasers setup that is used for single wavelength 3D microscopic imaging. In collaboration with our industrial partner, R&D Ultrafast Lasers Ltd, this year we have constructed a closed box, fully automated, turn-key version of this novel CARS unit, and applied this system for 3D CARS microscopic measurements on different biological samples, such as for murine ear treated by mineral oil, white adipose tissue, and murine brain slices. As an example, we show a CARS image recorded for murine white adipose tissue in Fig.1.

**Optical fiber theory.** — Dispersive properties of optical fibers play an important role in long distance, high speed optical data transmission systems and in ultrashort (ps or fs) pulse optical fiber laser systems. Recently we showed that reversed or flat dispersion functions in a wide wavelength range can be obtained by introducing resonant structures in the fiber cladding in hollow-core air-silica photonic bandgap fibers or in solid-core Bragg fibers with step-index profile. This year we investigated the physics behind the operation of “dispersive” optical fibers, i.e., optical fibers designed for dispersion (D) or dispersion slope (S) compensation to the second or third order. In general, we showed that the group delay ( $\tau$ ) of a relatively

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<sup>#</sup> PhD student

narrowband optical pulse transmitted through a piece of optical fiber of unit length is proportional to the energy ( $U$ ) stored by the standing wave electromagnetic field at the same (central) frequency, as far as the confinement loss is small. This strong relationship between these two physical quantities is not surprising at all, but has not been emphasized and used for the design of “dispersive” optical fibers. We are convinced that having this relationship in mind we can construct higher performance “dispersive” optical fibers, such as high-order mode (HOM) fibers, and hollow or solid core photonic bandgap (PBG) fibers.

Among others, we performed simulations for solid-core photonic bandgap fibers of two different kinds. The results of these simulations are summarized in Fig. 2.

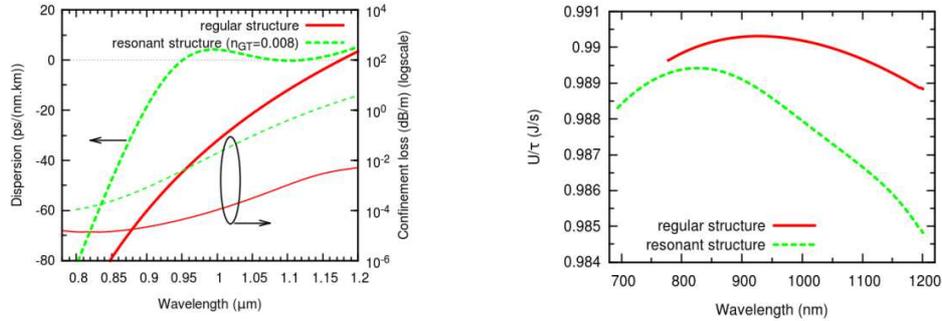


Fig. 2 Computed dispersion and confinement loss(left) and computed stored energy-group delay ratio (right) in solid core PBG fibers of two different designs having a unit length of 1 m (incident power is 1W).

We found that the  $U/\tau$  ratio is very close to unity all over the fiber transmission band, furthermore, the lower confinement loss increases the energy-group delay ratio close to 1, as expected. Since the stored energy in the fiber is derived from the electric field distributions at each wavelength, we can say that modifications in the dispersion function of any optical fiber always result in a change in the mode field distributions at each wavelength, and *vice versa*. From this relationship, it also follows that surface modes appearing in hollow core PBG fibers for instance seriously affect the dispersion profile of these optical fibers. In conclusion, we can say that having this relationship in mind one can construct higher performance “dispersive” optical fibers for nonlinear wavelength conversion (e.g., FOPO) or pulse compression applications for instance.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA 76404 Design and application of photonic crystal fibers for femtosecond pulse optical fiber lasers, laser amplifiers and optical parametric oscillators (R. Szipőcs, 2009-2013)

TECH-09-A2-2009-0134 National Technology Program, – Development of fiber integrated nonlinear microendoscope for pharmacological and diagnostic examinations based on novel fiber laser technology (Coordinator: R. Szipőcs, 2009-2013)

ELI\_09-1-2010-0010 ELI Laser Center Budapest (Helios) project (Participant: R. Szipőcs (2011-2013)

## CONTRACT

SZFKI-SZTE: Development of nonlinear microscopy for brain imaging (R. Szipőcs, 2011-2012)

## PUBLICATIONS

### *Articles*

1. Antal P, Szipőcs R; Tunable, low-repetition-rate, cost-efficient femtosecond Ti:sapphire laser for nonlinear microscopy; *Appl Phys B*; **107**; 17–22, 2012
2. Antal P, Szipőcs R; Relation between group delay, energy storage and loss in dispersive dielectric mirrors; *Chinese Optics Letters*, **10**, 053101/1-4, 2012

### *Conference proceedings*

3. Csáti D, Antal P, Szipőcs R; An inherently synchronized Yb fiber laser extension unit for broadly tunable, femtosecond pulse Ti-sapphire lasers for CARS microscopy, In: *Proc. FILAS Fiber Lasers and Applications, (San Diego, California, February 1-3, 2012)*; *OSA Technical Digest Series*; JTh2A.29/1-3, 2012
4. Csáti D, Szipőcs R; Noise Characterization of a Mode-Locked, All-Fiber, All Normal-Dispersion Ytterbium Ring Oscillator Using Two-Channel Polarization Control by a Computer; In: *Proc. FILAS Fiber Lasers and Applications, (San Diego, California, February 1-3, 2012)*; *OSA Technical Digest Series*; FTh3.1A.1/1-3, 2012
5. Kolonics A, Csáti D, Antal P, Szipőcs R; A simple, cost efficient fiber amplifier wavelength extension unit for broadly tunable, femtosecond pulse Ti-sapphire lasers for CARS microscopy; In: *Proc. BIOMED Biomedical Optics and Digital Holography and Three Dimensional Imaging (Miami, Florida, United States, April 28-May 2 2012)*; *OSA Technical Digest Series*; BSu3A.28 /1-3, 2012

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**S-Q. OPTICAL THIN FILMS**

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*Kárpát Ferencz*

**Optical thin film structures consisting of nanoscale laminated layers.** — We have continued our research concerning the development of optical thin film structures consisting of nanooptically thin layers for advanced applications in laser physics and measurement technology. Using multiple target thin film optimisation methods and our electron-beam deposition technology, we have developed many new kinds of optical coatings. Some examples:

- High damage threshold beamsplitter coating type “BS67pHD” consisting of 12 layers ( $\text{Ta}_2\text{O}_5/\text{SiO}_2$ ) for high power Ti:Sa laser applications
- High damage threshold beamsplitter coating type “BS600S” consisting of 15 layers ( $\text{Ta}_2\text{O}_5/\text{SiO}_2$ ) having  $R_s = 50 \pm 5\%$  in the wavelength range 350 – 800 nm at  $45^\circ$  angle of incidence.
- Optical mirror and beamsplitter set for a new type holocamera (Laser-FALCONEYE/H multi-functional holographic gage-camera (partner: Technoorg Linda Ltd.).
- Custom designed laser mirror having from the polarization state independent high reflectance and phase change in the wavelength range 770 – 850 nm at angle of incidence  $45^\circ$  useful for light manipulation without changing the phase information (partner Austrian Institute of Technology GmbH).
- Deposition technology of HR 800 nm/ $0^\circ$  and HR 800 nm/ $45^\circ$  laser mirrors on 76,2 mm and 101,6 mm diameter, flat or concave BK7 glass substrates.
- Electrically conductive fused silica window partially transparent for UV irradiation and highly transparent for the excited fluorescence light in the visible range.

Our indium-tin-oxide (ITO) layers with prescribed electrical resistance and visible optical transmittance were successfully applied as heatable windows or in integrated optical biological sensors.

**Superpolishing technology.** — We have further refined our optical superpolishing technology by adding special chemical materials to the polishing slurry for reducing the probability of aggregation. The result of the technological modification is the improved quality of laser mirror substrates (lowest scratch/dig values) and higher yield of the polishing process. We have routinely produced 25.4 mm diameter BK7 glass laser mirror substrates with an rms surface roughness of 0.2 nm.

The above summarized results will have high importance in the production of high quality laser optical elements for femtosecond petawatt laser facilities planned in the frame of the European project ELI.

These results were obtained in the frame of the scientific cooperation between the Institute and Optilab Ltd.

**CONTRACT**

OPTILAB-SZFKI No. 936/2011

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**S-R. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS**

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*István Földvári,<sup>#</sup> László Bencs, Elena Beregi, Gabriella Dravecz, Krisztina György,<sup>#</sup> Nikolett Laczai,<sup>#</sup> Ágnes Péter, Katalin Polgár, Zsuzsanna Szaller, Éva Tichy-Rács<sup>#</sup>*

**Growth and study of nonlinear borate crystals.** — Eu+Tb doped  $\text{GdAl}_3(\text{BO}_3)_4$  (GAB) single crystals were grown by the top-seeded flux technique (TSSG). Besides the regular Huntite type rhombohedral crystals ( $R32$ ,  $Z=3$ ) a new polytypic modification was discovered at high Eu+Tb concentrations ( $\text{Eu+Tb} = 0.14 - 0.37$ ). The structure of the new monoclinic phase ( $C2/c$ ,  $Z=8$ ) was determined by single crystal x-ray diffraction methods, including the coordination, symmetry and bonding distances of the characteristic structural units; the distorted  $\text{AlO}_6$  octahedra,  $\text{RO}_6$  trigonal prisms, and  $\text{BO}_3$  triangles. This structure was theoretically predicted for GAB but never experienced before. Within the applicable dopant concentration range, the starting crystallization temperature was the major factor in formation either the  $R32$  or the  $C2/c$  phases, and the higher temperatures belonged to the monoclinic modification.

**Growth and study of scintillator crystals.** — Pure and rare earth doped  $\text{Li}_6\text{Y}(\text{BO}_3)_3$  (Er, Yb) and  $\text{Li}_6\text{Gd}(\text{BO}_3)_3$  (Ce) single crystals were grown by Czochralski method in different concentrations using sintered material. The quality of the crystals was demonstrated by spectroscopic method.

Yttrium oxy-orthosilicate and lutetium–yttrium oxy-orthosilicate phases were prepared in nanocrystalline form by different wet chemical methods, like as sol-gel preparation, mechano-chemical method and hydrothermal synthesis. The different intermediate and final reaction products were identified by x-ray phase analysis, FTIR and Raman spectroscopy. The characteristic morphology of the final products was also determined.

**Growth and study of niobate crystals.** — Ferroelectric  $\text{K}_3\text{Li}_2\text{Nb}_5\text{O}_{15}$  (KLN-1) crystals were grown by the top-seeded solution method from pure and  $\text{Na}^+$ ,  $\text{Rb}^+$  and  $\text{Cs}^+$  doped melt. The impact of alkali additives was assessed all over the entire pulling range investigating the variation of structural and physical properties by spectroscopic and dielectric methods. Alkali additives played dual role in the growth process by affecting the crystallization temperature and promoting the K and Li site occupancies. By decreasing the crystallization temperature,  $\text{Cs}_2\text{O}$  additive reduced the concentration both of antisite Nb ions at Li site and alkali vacancies. Thus it can be considered as an ideal fluxing agent for growth of KLN crystals.

Faceted growth is a dominant factor reducing the quality of the Z-axis pulled stoichiometric  $\text{LiNbO}_3$  crystals (cracks, domain inversion, twinning, etc.). In the top seeded solution growth (HTTSG) technique the faceting was related to the convex growth interface. Gradually variable rotation rate technique was worked out to assure near planar interface during the whole growth process. Optimal crystal quality was achieved under conditions  $Gr/Re^2 > 1$  (mixed convection interaction parameter), where  $Gr$  and  $Re$  are the Grashof and rotational Reynolds numbers, respectively.

**Development of analytical methods for materials science and environmental control.** — Electrolyte cathode atmospheric glow discharge (ELCAD) cell was inserted into a commercial atomic absorption spectrometer (AAS). A flow injection system was developed to introduce aqueous standards of some environmentally relevant metals into the plasma. By

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<sup>#</sup> PhD student

## S-R. Growth and characterization of optical crystals

using these AAS calibration curves, the detection limit for Cd, Cu, Na and Zn were 3.4, 4.2, 9.2 and 0.9 mg/l, respectively.

## GRANTS AND INTERNATIONAL COOPERATION

MTA-Polish Acad. Sci. program. Growth and spectroscopic studies of rare-earth doped nonlinear optical crystals for applications (I. Földvári, 2011-2013). Partner: Institute of Low Temperature and Structure Research, PAS, Wrocław

MTA-Russian Acad. Sci. program. No.22. Growth of single crystals with wide band-gap and investigation of their crystal lattice defects by spectroscopic methods (J. Janszky, K. Polgár, 2011-2013). Partner: Joffe Phys. Techn. Institute, RAS, St. Petersburg.

MTA-Russian Acad. Sci. program. No.23. Preparation and investigation of media for solid state lasers and stimulated Raman emission (K. Polgár, 2011-2013). Partner: General Physics Institute, RAS, Moscow.

## PUBLICATIONS

### Articles

1. Erdei\* G, Berze\* N, Péter Á, Játékos\* B, Lőrincz\* E; Refractive index measurement of cerium-doped  $\text{Lu}_x\text{Y}_{2-x}\text{SiO}_5$  single crystal; *Opt Mater*; **34**, 781-785, 2012
2. Beregi E, Sajó\* I, Lengyel K, Bombicz\* P, Czugler\* M, Földvári I; Polytropic modifications in heavily Tb and Eu doped gadolinium aluminum borate crystals; *J Crystal Growth*; **351**, 72-76, 2012
3. Szaller Zs, Péter Á, Polgár K, Szabó Gy; High temperature top seeded solution growth of stoichiometric lithium niobate  $\text{LiNbO}_3$  (sLN) with planar interface; *J Crystal Growth*; **360**, 181-184, 2012
4. György K, Bencs L, Mezei P, Cserfalvi\* T; Novel application of the electrolyte cathode atmospheric glow discharge: Atomic absorption spectrometry studies; *Spectrochim Acta B*; **77**, 52-57, 2012
5. Bencs L, György K, Kardos M, Osán\* J, Alföldy\* B, Varga\* I, Szoboszlai\* N, Ajtony\* Zs, Stefánka\* Zs, Széles\* É, Kovács L; Determination of trace elements in lithium niobate crystals by solid sampling and solution-based spectrometry methods; *Anal Chim Acta*; **726**, 1-8, 2012
6. Péter Á, Polgár K, Tóth\* M; Synthesis and crystallization of Lithium-Yttrium orthoborate  $\text{Li}_6\text{Y}(\text{BO}_3)_3$  phase; *J Crystal Growth*; **346**, 2012, 69-74

See also: S-L.5, S-O.4, S-S.2, S-S.5

## S-S. CRYSTAL PHYSICS AND NONLINEAR OPTICS

László Kovács, István Bányász, Gábor Corradi, Ivett Hajdara,<sup>#</sup> Ervin Hartmann, Krisztián Lengyel, Gábor Mandula

**OH<sup>-</sup> defects in congruent LiNbO<sub>3</sub> crystals.** — The incorporation of OH<sup>-</sup> ions into nearly congruent LiNbO<sub>3</sub> was studied by the density-functional theory (DFT) method using the SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code. A supercell consisting of 810 atoms containing one antisite Nb<sup>5+</sup>, one H<sup>+</sup> ion and 4 Li<sup>+</sup> vacancies was used in the calculation of free and Fermi energies. The free energies in 4 of the 6 investigated configurations are in the same range as determined from temperature dependent OH<sup>-</sup> absorption measurements. The calculated Fermi energies ( $\approx 3.7$  eV) are smaller than that for stoichiometric LiNbO<sub>3</sub> (4.2 eV) in agreement with UV absorption measurements.

**Transient holograms on small polarons in LiNbO<sub>3</sub> single crystals.** — Small-polaron based holograms suitable for real time holography in the visible ( $\lambda_{\text{probe}}=488$  nm) have been produced in thermally reduced LiNbO<sub>3</sub>. The phase gratings appear upon irradiation by a non-collinear pair of single ns-laser pulses, have a lifetime in the ms region, and can be assigned to spatially modulated densities of small bound electron polarons and bipolarons, and O<sup>-</sup> hole polarons.

**Phase transition of potassium lithium niobate (KLN) crystals.** — The phase transition of KLN crystals has been studied by measuring the temperature dependence of the dielectric constant ( $\epsilon$ ). The transition's broad temperature range and the frequency dependence of  $\epsilon$  indicate a relaxor type ferroelectric behaviour for KLN crystals containing more than 52 mol % niobium. During the phase transition Li<sup>+</sup> ion displacement may occur.

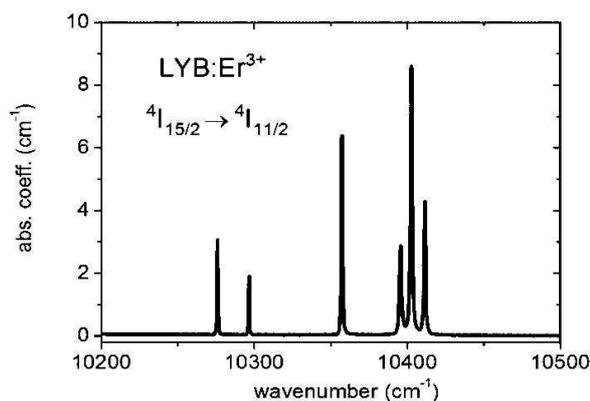


Fig.1. Crystal field splittings of the  $^4I_{11/2}$  level of  $Er^{3+}$  in  $Li_6Y(BO_3)_3$  crystal at 8 K

fully resolved hyperfine structure due to the  $^{167}Er$  isotope. A series of transitions from the

### Luminescence of Ag and Mn centres in lithium tetraborate single crystals.

— The luminescence yield of the tissue-equivalent thermo-luminescent dosimeter and neutron detector material  $Li_2B_4O_7:Cu$  could be enhanced by additional dopants like Ag and Mn, the co-dopants serving along with Cu as traps during irradiation and as recombination centers.

### Spectroscopy of $Li_6Y(BO_3)_3:Er$ single crystals.

— EPR spectra show the presence of a dominant  $Er^{3+}$  centre apparently substituted at a Y site, with

<sup>#</sup> PhD student

$^4I_{15/2}$  ground state and their crystal field splittings were measured using high resolution absorption and luminescence spectroscopies. 90 Stark components of 20 multiplets (from the  $^4I_{15/2}$  ground state to the  $^4D_{7/2}$  excited state) could be identified in the spectrum up to  $40.000\text{ cm}^{-1}$  (Fig.1).

**Coherent radiative processes in rare earth doped single crystals.** — The homogeneous linewidth of the optical transitions around 980 nm have been measured in Yb or Er doped  $\text{LiNbO}_3$  and  $\text{Li}_6\text{Y}(\text{BO}_3)_3$  crystals. Dipole relaxation times of  $\approx 33$  and 13 ns, and population relaxation times of  $\approx 0.35$  and  $0.38\ \mu\text{s}$  have been determined for ytterbium and erbium doped  $\text{LiNbO}_3$  samples, respectively. In LYB:Yb $^{3+}$  a thick (40-50MHz) and a narrow (2-3MHz) line are superimposed. The temperature dependence of the homogeneous linewidth and the population relaxation time have also been measured for LYB: Yb $^{3+}$  and LYB:Er $^{3+}$ .

**Design and fabrication of diffractive optical elements and waveguides by ion implantation.** — Slab and channel waveguides were obtained in sillenite and eulytine type bismuth germanate samples via single- and two-energy implantation of  $\text{N}^+$  ions. Ellipsometric measurements proved the existence of relatively broad implanted barrier layers. Planar waveguides have been formed via irradiation with 25 MeV  $\text{C}^{5+}$  ions at low fluences ( $10^{13}$  -  $10^{15}$  ions/cm $^2$ ). Optical phase diffraction gratings have been realized in Pyrex glass samples using focused  $\text{C}^{3+}$  and  $\text{C}^{5+}$  microbeams of 6 and 11 MeV. Quasi-sinusoidal refractive index profiles have been achieved by modulation of the irradiated fluence. Channel waveguides have also been fabricated in Er doped tungsten-tellurite oxide glass samples using  $\text{C}^{3+}$  and  $\text{C}^{5+}$  ions (Fig.2.).

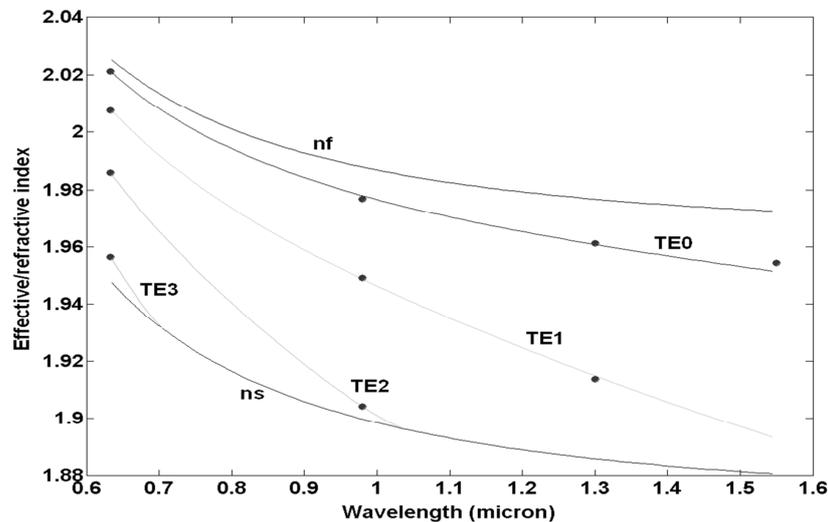


Fig.2. Multispectral reconstruction of the refractive index of the guiding and barrier layer as a function of the wavelength in a 3.5 MeV  $\text{N}^+$  ion irradiated planar waveguide in Er: Te glass. Sample was irradiated with  $8 \times 10^{16}$  ions/cm $^2$ . Calculated effective indices (nf and ns) of the modes are also shown.

## GRANTS AND INTERNATIONAL COOPERATION

OTKA K68688 Fabrication of waveguides and diffractive optical elements via ion implantation (T. Lohner, MTA Research Institute for Technical Physics)

- and Materials Science, contributors I. Bányász and A. Watterich, 2007 – 2012)
- OTKA CK 80896 Scintillator materials for medical imaging purposes (L. Kovács, 2010-2013)
- OTKA K83390 Resonant optical processes in solids (L. Kovács, 2011-2015)
- OTKA K101225 Fabrication of integrated optical elements via ion beam implantation and irradiation for telecommunication applications (I. Bányász, 2012-2014)
- Hungarian – German project (MÖB 29696 and DAAD 54377942) Small polarons in Er or Yb doped oxide crystals (G. Corradi, 2012-2013)
- MTA – CNR Application of ion implantation to the fabrication of integrated optical devices (I. Bányász, 2010-2012) Italian partner: MDF Laboratory, IFAC, Sesto Fiorentino
- MTA – Estonian Academy of Sciences joint project: Radiation induced effects in pure and doped wide-gap borate crystals (G. Corradi, 2010-2012)
- MTA – Bulgarian Academy of Sciences joint project: Growth and spectroscopy of ferroelectric and multiferroic materials (L. Kovács, 2010-2012)

## PUBLICATIONS

### Articles

1. Kovács L, Lengyel K, Gospodinov\* M; Optical spectroscopy of multiferroic rare-earth manganites; *Ferroelectrics*; **428**, 82-86, 2012
2. Hajdara I, Lengyel K, Kovács L, Péter Á, Szaller Zs; Effect of alkali doping on the Raman spectra of potassium lithium niobate crystals; *Ferroelectrics*; **428**, 57-63, 2012
3. Bruening\* H, Dieckmann\* V, Schoke\* B, Voit\* KM, Imlau\* M, Corradi G, Merschjann\* C; Small-polaron based holograms in LiNbO<sub>3</sub> in the visible spectrum; *Opt Express*; **20**, 13326-13336, 2012
4. Bányász I, Berneschi\* S, Bettinelli\* M, Brenci\* M, Fried\* M, Khanh\* NQ, Lohner\* T, Nunzi Conti\* G, Pelli\* S, Petrik\* P, Righini\* GC, Speghini\* A, Watterich A, Zolnai\* Z; MeV energy N<sup>+</sup> - implanted planar optical waveguides in Er-doped tungsten-tellurite glass operating at 1.55 μm; *IEEE Photonics Journal*; **4**, 721-727, 2012
5. Bányász I, Berneschi\* S, Khanh\* NQ, Lohner\* T, Lengyel K, Fried\* M, Péter Á, Petrik\* P, Zolnai\* Z, Watterich A, Nunzi-Conti\* G, Pelli\* S, Righini\* GC; Formation of slab waveguides in eulytine and sillenite type BGO and CaF<sub>2</sub> crystals by implantation of MeV nitrogen ions; *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*; **286**, 80–84, 2012

### Articles in Hungarian

6. Hartmann E; Tarján Imre a magyar kristályfizikában (I. Tarján and crystal physics in Hungary, in Hungarian); *Fizikai Szemle*; **62**, 230-233, 2012

*Conference proceedings*

7. Bányász I, Zolnai\* Z, Pelli\* S, Berneschi\* S, Nunzi Conti\* G, Fried\* M, Lohner\* T, Petrik\* P, Brenci\* M, Righini\* GC; Fabrication of barrier-type slab waveguides in Er<sup>3+</sup>-doped tellurite glass by single- and double energy MeV N<sup>+</sup> ion implantation; *Conference Integrated Optics: Devices, Materials, and Technologies XVI (OE110), part of Symposium Photonics West 2012, 21–26 January 2012, San Francisco, California, USA; Proc. of SPIE; 8264, 826406, 2012*

See also: S-R.3, S-R.6

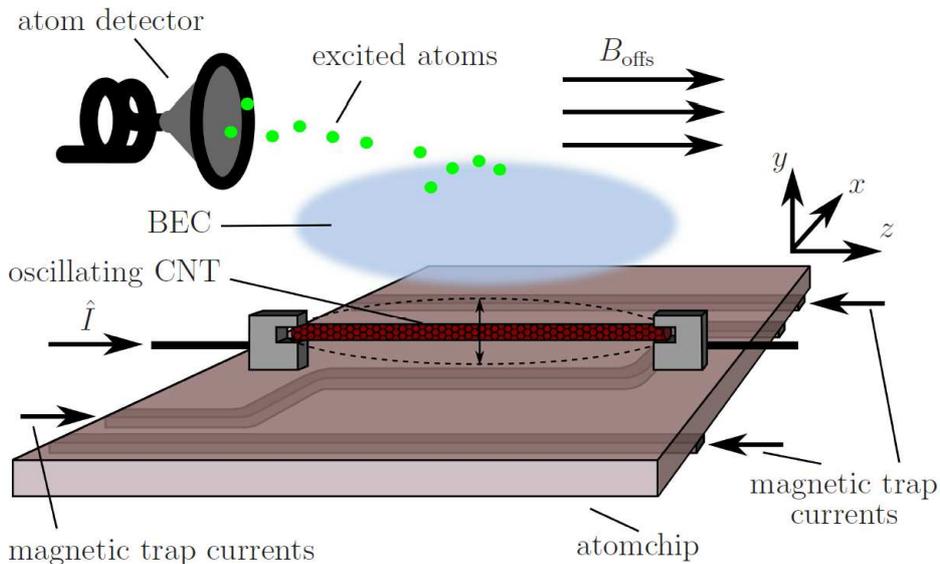
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**S-T. QUANTUM OPTICS AND QUANTUM INFORMATION**


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*Péter Domokos, Péter Ádám, János Asbóth, Zoltán Darázs,<sup>#</sup> András Dombi,<sup>#</sup> Aurél Gábris,<sup>#</sup> József Janszky,<sup>#</sup> Orsolya Kálmán, László Kecskés,<sup>#</sup> Zsolt Kís, Tamás Kiss, Bálint Kollár,<sup>#</sup> Gábor Kónya,<sup>#</sup> Zoltán Kurucz, Dávid Nagy, Péter Sinkovicz,<sup>#</sup> Viktor Szalay, Gergely Szirmai, Géza Tóth, András Vukics*

**Cavity QED, Bose-Einstein condensates, many-body physics.** — We evaluate the coupling of a Bose-Einstein condensate of ultracold paramagnetic atoms to the magnetic field of the current in a mechanically vibrating carbon nanotube within the frame of a full quantum theory. We find that the interaction is strong enough to sense quantum features of the nanowire current noise spectrum by means of hyperfine-state-selective atom counting. Such a non-destructive measurement of the electric current via its magnetic field corresponds to the classical galvanometer scheme, extended to the quantum regime of charge transport. The calculated high sensitivity of the interaction in the nanowire-BEC hybrid systems opens up the possibility of quantum control, which may be further extended to include other relevant degrees of freedom (Fig.1).



*The quantum galvanometer on an atom chip. A BEC is loaded into the magnetic microtrap created by the classical electric currents through integrated conductors on a dielectric substrate (represented on the bottom of the chip). A suspended carbon nanotube is also part of the electric circuit and transports the quantum current. The oscillating CNT creates a magnetic field in the 10 MHz range interacting with the hyperfine transitions of the atoms. Atoms transferred to untrapped states are detected by a single-atom detector.*

**Resonant nonlinear optics in doped crystals.** — We theoretically analyze pulse propagation in a medium of inhomogeneously broadened two-level quantum systems which have a vibrational degree of freedom with respect to the center-of-mass coordinate. This system mimics local mode oscillations of rare-earth-metal-ion dopants in dielectric crystals that are

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<sup>#</sup> PhD student

coupled to electronic transitions. We show the emergence of various nonlinear optical phenomena, such as self-induced transparency or the nonlinear interaction between two pulses coupling to different electrovibrational transitions. Interaction between the pulses makes it possible to generate various Raman sidebands of the incident fields and to tune the location where they are generated. We also demonstrate controlled population transfer between electrovibrational states of the ions at specific points along the propagation axis. Similarities and differences between our results and other pulse propagation phenomena of few-level quantum systems are discussed.

**Quantum information processing, quantum walks, chaotic dynamics of entangled qubits.** Quantum walks obey unitary dynamics: they form closed quantum systems. The system becomes open if the walk suffers from imperfections represented as missing links on the underlying basic graph structure, described by dynamical percolation. Openness of the system's dynamics creates decoherence, leading to strong mixing. We present a method to analytically solve the asymptotic dynamics of coined, percolated quantum walks for a general graph structure. For the case of a circle and a linear graph we derive the explicit form of the asymptotic states. We find that a rich variety of asymptotic evolutions occur: not only the fully mixed state, but other stationary states; stable periodic and quasiperiodic oscillations can emerge, depending on the coin operator, the initial state, and the topology of the underlying graph.

Multidimensional quantum walks can exhibit highly nontrivial topological structure, providing a powerful tool for simulating quantum information and transport systems. We present a flexible implementation of a two-dimensional (2D) optical quantum walk on a lattice, demonstrating a scalable quantum walk on a nontrivial graph structure. We realized a coherent quantum walk over 12 steps and 169 positions by using an optical fiber network. With our broad spectrum of quantum coins, we were able to simulate the creation of entanglement in bipartite systems with conditioned interactions. Introducing dynamic control allowed for the investigation of effects such as strong nonlinearities or two-particle scattering. Our results illustrate the potential of quantum walks as a route for simulating and understanding complex quantum systems.

**Molecular dynamics.** — A variational finite basis representation/discrete variable representation (FBR/DVR) Hamiltonian operator has been introduced. By calculating its matrix elements exactly one obtains, depending on the choice of the basis set, either a variational FBR or a variational DVR. The domain of grid points on which the FBR/DVR is variational has been shown to consist of the subsets of the set of grid points one obtains by diagonalizing commuting variational basis representations of the coordinate operators. The variational property implies that the optimal of the subsets of a fixed number of points, i.e., the subset which gives the possible highest accuracy eigenpairs, gives the DVR of the smallest trace. The symmetry properties of the variational FBR/DVR Hamiltonian operator are analyzed and methods to incorporate symmetry into FBR/DVR calculations are discussed. It is shown how the Fourier-basis FBR/DVR suitable to solving periodic systems arise within the theory presented. Numerical examples are given to illustrate the theoretical results. The use of variational effective Hamiltonian and coordinate operators has been instrumental in this study. They have been introduced in a novel way by exploiting quasi-Hermiticity.

## GRANTS AND INTERNATIONAL COOPERATION

- OTKA K83858 Quantum optical and quantum information processing networks and their nonclassical properties (T. Kiss, 2011-2015)
- OTKA PD 104652 Realization of strongly correlated matter by ultracold atoms (G. Szirmai, 2012-2015)
- Momentum Program, Quantum Measurement Theory in Hybrid Mesoscopic Couplers and Networks (P. Domokos, 2011-2015)
- NKTH ERC\_HU\_09 OPTOMECH: Optomechanical coupling: extending Cavity Quantum Electrodynamics (P. Domokos, 2010-2014)
- FP7 Initial Training Network, CCQED Circuit and Cavity Quantum Electro-Dynamics (P. Domokos, 2011-2014)
- TéT, Hungarian-Czech Bilateral Intergovernmental S&T Cooperation (CZ-11/2009): Quantifying non-classicality in quantum walks and quantum optical networks (T. Kiss, 2010-2012)
- MÖB – DAAD, Quantum measurement in the hybrid system of coupled Bose-Einstein condensate and carbon nanotubes (P. Domokos, MÖB/18-1/2012)

## PUBLICATIONS

### Articles

1. Koniorczyk\* M, Szabó\* L, Adam P; Hardy's paradox and entangled structure of forward scattered waves, *Phys Rev A*; **84**, 044102/1-4, 2011
2. Zamora\* A, Szirmai G, Lewenstein\* M; Layered quantum Hall insulators with ultracold atoms; *Phys Rev A*; **84**, 053620, 2011
3. Ádám P, Szabó\* L, Mechler\* M, Koniorczyk\* M; Forward-scattered wave analysis of an optical Hardy-like setup; *Phys Scr*; **T147**, 014001/1-4, 2012
4. Demeter\* G, Kis Z, Hohenester\* U; Nonlinear pulse propagation phenomena in ion-doped dielectric crystals; *Phys Rev A*; **85**, 033819, 2012
5. Hyllus\* P, Pezzé\* L, Smerzi\* A, Tóth G; Entanglement and extreme spin squeezing for a fluctuating number of indistinguishable particles; *Phys Rev A*; **86**, 012337/1-11, 2012
6. Kálmán O, Kiss T, Fortágh\* J, Domokos P; Quantum galvanometer by interfacing a vibrating nanowire and cold atoms; *Nano Letters*; **12**, 435-439, 2012
7. Kollár B, Kiss T, Novotny\* J, Jex\* I; Asymptotic dynamics of coined quantum walks on percolation graphs; *Phys Rev Lett*; **108**, 230505/1-5, 2012
8. Kónya G, Nagy D, Szirmai G, Domokos P; Finite-size scaling in the quantum phase transition of the open-system Dicke mode; *Phys Rev A*; **86**, 013641/1-11, 2012
9. Moroder\* T, Hyllus\* P, Tóth G, Schwemmer\* C, Niggelbaum\* A, Gaile\* S., Gühne\* O, Weinfurter\* H; Permutationally invariant state reconstruction; *New J Phys*; **14**, 105001/1-25, 2012
10. Schreiber\* A, Gábris A, Rohde\* P.P, Laiho\* K, Štefaňák\* M, Potoček\* V, Hamilton\* C, Jex\* I, Silberhorn\* Ch; A 2D quantum walk simulation of two-particle dynamics; *Science*; **336**, 55-58, 2012

11. Szalay V, Szidarovszky\* T, Czakó\* G, Császár\* AG; A paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements; *J Math Chem*; **50**, 636–651, 2012
12. Szalay V, Ádám P; Variational properties of the discrete variable representation: Discrete variable representation via effective operators; *J Chem Phys*; **137**, 064118/1-21, 2012
13. Szirmai G, Szépfalussy P; Three-fluid hydrodynamics of spin-1 Bose-Einstein condensates; *Phys Rev A*; **85**, 053603/1-9, 2012
14. Tóth\* G; Multipartite entanglement and high-precision metrology; *Phys Rev A*; **85**, 022322/1-10, 2012
15. Vitagliano\* G, Hyllus\* P, Egusquiza\* IL, Tóth G; Spin squeezing inequalities for arbitrary spin; *Phys Rev Lett*; **107**, 240502/1-4, 2011
16. Vukics A; C++QEDv2: The multi-array concept and compile-time algorithms in the definition of composite quantum systems; *Comp Phys Comm*; **183**, 1381-1396, 2012
17. Xuereb\* A, Domokos P; Dynamical scattering models in optomechanics: going beyond the ‘coupled cavities’ model; *New Journal of Physics*; **14**, 095027/1-12, 2012
18. Vukics A, Domokos P; Adequacy of the Dicke model in cavity QED: A counter-no-go statement; *Phys Rev A*; **86**, 053807/1-8, 2012
19. Nyitray\* G, Kis Z; Self-confining waves; *J Mod Optics*; **59**, 1558-1568, 2012
20. Asbóth JK; Symmetries, topological phases, and bound states in the one-dimensional quantum walk; *Phys Rev B*; **86**, 195414/1-9, 2012



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**SUPPLEMENTARY DATA**

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**EDUCATION**


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**GRADUATE AND POST-GRADUATE COURSES***Eötvös Loránd University, Budapest*

- Advanced Experimental Particle Physics (G. Vesztergombi)
- Algebraic Bethe Ansatz and its applications (F. Woynarovich)
- Cavity Quantum Electrodynamics (P. Domokos, J. Asbóth)
- Cognitive Neuroscience (L. Négyessy)
- Completely integrable many body systems (F. Woynarovich)
- Computational Neuroscience (Z. Somogyvári)
- Electrodeposition of metals (L. Péter)
- Electrons in solids (I. Tüttő)
- Electrons in solids (J. Sólyom)
- Inner structure of compact stars (G.G. Barnaföldi and M. Vasúth)
- Introduction to Experimental Particle Physics (G. Vesztergombi)
- Introduction to general relativity, (I. Rácz)
- Introduction to general relativity, (M. Vasúth)
- Introduction to gravitational theory and high energy physics (G.G. Barnaföldi and M. Vasúth)
- Jet physics (P. Lévai)
- Liquid crystals, their chemistry and chemical physics (K. Fodor-Csorba)
- Macromolecules I. (S. Pekker)
- Many-body physics I. (G. Szirmai)
- Many-body physics II. (G. Szirmai)
- Nanomagnetism (J. Balogh)
- Neural Modelling (Z. Somogyvári, M. Bányai, D. Cserpán)
- Nuclear Solid State Physics I (D.L. Nagy)
- Nuclear Solid State Physics II (D.L. Nagy)
- Open Quantum System Theory (L. Diósi)
- Pattern formation in complex systems (Á. Buka and T. Börzsönyi)
- Phase structure of strongly interacting matters (P. Lévai)
- Physics of liquid crystals and polymers (Á. Buka and N. Éber)
- Physics of the heliosphere (G. Erdős)
- Plasma physics of the Solar System (K. Szegő)
- Relativistic heavy ion collisions (P. Lévai)
- Renormalization methods for strongly correlated systems (Ö. Legeza)
- Superconductivity (I. Tüttő)
- Topological insulators (J. Asbóth)

*Budapest University of Technology and Economics*

- Advanced thermodynamics (P. Ván)
- Coherent control of quantum systems (Z. Kis)
- Group theory in solid state research (G. Kriza)

## Education

- Infrared and Raman spectroscopy (K. Kamarás)
- Infrared vibrational spectroscopy, part of the course Experimental methods in materials science (L. Kovács)
- Interacting spin systems (K. Penc)
- Introduction to theoretical plasma physics (A. Bencze)
- Investigation methods in materials science (M. Bokor and K. Tompa)
- Ion beam analysis, part of the course Experimental methods in materials science (E. Szilágyi)
- MHD in low-dimensional systems (A. Bencze)
- Neutron scattering I, part of the course Experimental methods in material science (B. Nagy, L. Bottyán)
- Nuclear Solid State Physics I (D.L. Nagy)
- Nuclear Solid State Physics II (D.L. Nagy)
- Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres)
- Spectroscopy and structure of matter (K. Kamarás)
- Superconductivity (G. Kriza)

### ***Semmelweis University, Budapest***

- Neuroinformatics (L. Négyessy, F. Bazsó, Z. Somogyvári, L. Zalányi, M. Bányai)

### ***Szent István University, Gödöllő***

- Biophysics (Z. Szókefalvi-Nagy, SZIE AOTK)
- Computer Aided Engineering (L. Zoltan)
- Machine elements I. (L. Zoltan)
- Machine elements II. (L. Zoltan)

### ***University of Szeged***

- Analytical mechanics (L. Fehér)
- Application of statistical physics (F. Iglói)
- Experimental methods of nuclear physics (T. Csörgő)
- Fundamental processes in nonlinear laser-matter interactions (S. Varró)
- Introduction to theoretical physics I. (L. Fehér)
- Nuclear and Particle Physics I (T. Csörgő)
- Physics of amorphous matter I-II (M. Koós)
- Quantum field theory (L. Fehér)
- Selected topics in mathematical physics (L. Fehér)
- Statistical physics (F. Iglói)

### ***University of Pécs***

- Calculus I. (K. Szlachányi)
- Calculus II. (K. Szlachányi)
- Control theory (J. Füzi)
- Digital Control (J. Füzi)
- Electronics (J. Füzi)

- Mathematical methods in physics IV. (P. Ádám)
- Numerical methods (P. Ádám)
- Operating systems (B. Kollár)
- Probability theory (P. Ádám)
- Quantum mechanics I. (J. Janszky)
- Quantum mechanics II. (J. Janszky)
- Quantum mechanics II. (P. Ádám)
- Statistical physics (K. Szlachányi)
- Theoretical physics III. (P. Ádám)

***University of Debrecen***

- Particle Physics, MSc Course (D. Horváth)
- Quantum Field Theory (T.S. Biró)
- Structure and Experimental Test of the Standard Model, PhD Course (D. Horváth)

***Óbuda University, Budapest***

- Chemistry and Physics of Polymers (S. Pekker)

***Rolls-Royce University Technology Centre, Cambridge University, UK***

- Phase field modelling and solidification (L. Gránásy, T. Pusztai, G. I. Tóth, G. Tegze)

***National University of Public Service, Budapest***

- Mathematical analysis – theory and practice (B. Tóth)

**LABORATORY PRACTICES AND SEMINARS**

***Eötvös Loránd University, Budapest***

- Experiments on liquid crystals (Á. Buka, N. Éber, T. Tóth-Katona)
- Laboratory for solid state physics, Preparation and crystallization of metallic glasses (I. Vincze)
- Laboratory practice (T. Pusztai)
- Laboratory practice in solid state physics and materials science (K. Tompa and M. Bokor)
- Physical chemistry laboratory practice (L. Péter, B. Tóth)
- RBS and ERDA analysis, extended practice for physics student (E. Kótai).
- Solar-terrestrial relation for astrophysics students (M. Tátrallyay)
- Solid-state physics seminar (I. Tüttő)
- Solid-state physics seminar (J. Sólyom)

***Budapest University of Technology and Economics***

- Infrared and Raman spectroscopy (K. Kamarás)
- Infrared vibrational spectroscopy, part of the course Experimental methods in materials science (K. Lengyel)

## Education

- Laboratory practice on investigation methods in materials science (M. Bokor and K. Tompa)
- Practice course in experimental physics for engineer-physicists (A. Szakál)
- Practice course in electrodynamics for energy-engineers (A. Szakál)
- Problem solving courses in thermodynamics (T. Fülöp)
- Problem solving course in heat exchange (P. Ván)
- Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres)
- Seminar to the Physics 2 course for bachelor students in electrical and software engineering (B. Nagy)

### *University of Pécs*

- Control theory seminar (J. Füzi)
- Electronics laboratory practice (J. Füzi)
- Operating systems (B. Kollár)

## DIPLOMA WORKS

### *Eötvös Loránd University, Budapest*

- Z.A. Boldizsár, Investigation of the plasma environment around the orbit of Titan (MSc, Supervisor Z. Németh).
- Á. Budea, Application of graphics processing units for simulations of many-particle systems (MSc, Supervisor Z. Donkó).
- D. Kálmán, Applied methods by cosmic muon detection (BSc, Supervisor G.G. Barnaföldi).
- G. Kónya, Bose-Einstein condensates in optical resonators (MSc, Supervisor P. Domokos).
- Zs. Kovács, Flow phenomena in granular materials (MSc, Supervisor T. Börzsönyi).
- I. Márton, Experimental investigation of ultrafast electron acceleration in the vicinity of metallic nanostructures (MSc, Supervisor P. Dombi).
- D. Molnár, Plasma spectroscopic measurements by the Cassini space mission in the magnetosphere of Saturn (BSc, Supervisor K. Szegő).
- G. Monostori, Fast method for determination of feed-down corrections in particle physics experiments (MSc, Supervisors Á. Fülöp and G. Vesztegombi).
- N. Német, Modelling ultrafast photoemission from metallic nanostructures (BSc, Supervisor P. Dombi).
- L. Oláh, Investigation of large-scale Inhomogeneities using cosmic particles (MSc, Supervisor GG Barnaföldi).
- P. Sinkovicz, Detection and simulation of spin liquid phases with ultracold atoms (MSc, Supervisor G. Szirmai).
- M. Vargyas, Analysis of the PHENIX dilepton spectrum in 200 GeV Au+Au collisions at RHIC (MSc, Supervisor T. Csörgő).
- A.J. Zsigmond, Measurement of the inelastic proton-proton cross section in the CMS experiment (Supervisors G.I. Veres\* and F. Siklér)

*University of Szeged*

- A. Házi, Investigation of the stochastic Schrödinger equation in white-noise (MSc, Supervisor L. Diósi)

**PH.D. STUDENTS***Eötvös Loránd University, Budapest*

- Á. Agócs, Database management for large particle physics experiments at CERN LHC (Supervisors A. Benczur and G. Vesztegombi)
- A.G. Agócs, Interaction between high-pT hadrons and quark-gluon plasma in CERN LHC ALICE experiment (Supervisor P. Lévai)
- G. Barcza, Development and application of the non-local density matrix renormalization group (non-local DMRG) method to low-dimensional spin and fermionic models (Supervisors Ö. Legeza and F. Gebhard\*)
- Gy. Bencédi, Identification of high-pT particles in CERN LHC ALICE experiment (Supervisor P. Lévai)
- D. Berényi, Particle production in time-dependent strong fields in the ELI and the CERN LHC experiments (Supervisor P. Lévai)
- G. Cseh, Investigation of transient processes in hot plasmas (Supervisor G. Kocsis)
- G. Csire, Quasiparticle spectra of the metal-superconducting heterostructure.
- Z. Darázs, Quantum control with measurements (Supervisors T. Kiss and A. Csordás)
- M. Dolgos, Metastable structures in stratified systems (Supervisor L. Bottyán)
- A. Dombi, Quantum dynamics of atomic motion in multimode optical resonator fields (Supervisor P. Domokos)
- K. György, Study on solid sampling spectrochemical methods for the characterization of the impurity and dopant content of optical crystals (Supervisor L. Bencs)
- I. Hagymási, Heavy-fermion behavior in the periodic Anderson model (Supervisor J. Sólyom)
- D. Kocsis, Spectroscopy on filled carbon nanotube systems (Supervisor K. Kamarás)
- G. Kónya, Many-body physics in cavity QED (Supervisor P. Domokos)
- N. Laczai, Fabrication of nano-scintillator materials for medical imaging purposes (Supervisor L. Bencs)
- K. Lukács, Investigation of the evolution of the interplanetary magnetic field (Supervisor G. Erdős)
- K. Márton, Ultrarelativistic hadron-nucleus collisions at CERN SPS energies (Supervisors A. László and D. Varga\*)
- F. Máté Nagy, Numerical study of gravitational wave generation.
- K. Németh, Chemical functionalization of carbon nanotubes (Supervisor K. Kamarás)
- K. Neuróhr, Electrochemical preparation of multilayers with giant magnetoresistance (Supervisor L. Péter)
- L. Oláh, Analysis of identified particles by ALICE HMPID (Supervisor G.G. Barnaföldi)
- M. Pápai, Modelling the electronic, structure of transition metal compounds (Supervisor G. Vankó)
- T.N. Papp, Open quantum systems (Supervisor L. Diósi)

## Education

- S. Pochybova, High energy quark and gluon jets in proton-proton and heavy ion collisions (Supervisor P. Lévai)
- L. Rátkai, Phase-field modelling of columnar to equiaxed transition with fluid flow (Supervisor T. Pusztai)
- P. Salamon, Flexoelectricity in liquid crystals (Supervisor N. Éber)
- B. Szabó, Experimental investigations of granular flows (Supervisor T. Börzsönyi)
- É. Tichy-Rács, Synthesis, crystallization and spectroscopy of rare-earth-alkaline orthoborates (Supervisor K. Polgár)
- B. Tóth, Giant magnetoresistance (GMR) in multilayers (Supervisors I. Bakonyi and L. Péter)
- R. Ünnep, Study of self-assembly functional nano particles by neutron scattering (Supervisor F. Mezei)
- K. Ürmösy, Advanced statistical methods in high energy physics (Supervisor T.S. Biró)
- T. Verebélyi, NMR and DSC study of protein solutions (Supervisor K. Tompa)
- A.J. Zsigmond, Study of high density QCD matter in Pb+Pb and p+Pb collisions in the CMS experiment at the LHC (Supervisors F. Siklér and G.I. Veres\*)

### ***Budapest University of Technology and Economics***

- M. Bányai, Data circulation and random walks on weighted directed graphs and the cerebral cortex (Supervisor F. Bazsó)
- B. Botka, Raman spectroscopy of carbon nanotube peapods (Supervisor K. Kamarás)
- D. Cserpán, Doctoral School of Informatics (Supervisor Z. Somogyvári)
- M. Lajkó, Theoretical studies of strongly frustrated spin and charge systems (Supervisor K. Penc)
- M. Lampert, Study of plasma turbulence and zonal flows on various tokamak devices (Supervisor S. Zoletnik)
- J. Orbán, Investigation and development of signal processing electronics for position sensitive particle counters (Supervisors L. Rosta and Cs. Sükösd\*)
- J. Romhányi, Bond and plaquette ordering in interacting electron systems (Supervisor K. Penc)
- A. Szakál, Investigation of the structure and dynamics of metal-hydrogen systems with neutron scattering (Supervisor L. Cser)
- Zs. Szekrényes, Infrared spectroscopy of self-assembled structures on surfaces (Supervisor K. Kamarás)
- B. Tál, Measurements of fast transients in a tokamak plasma (Supervisor G. Veres)
- Gyula I. Tóth, Budapest University of Technology and Economics, supported by grant No. EU FP7 NMP4-SL-2008/213669 ENSEMBLE Engineered Self-organised Multi-Component Structures with Novel Controllable Electromagnetic Functionalities, (Supervisor L. Gránásy)
- P. Rácz, Development of femtosecond light and electron sources for high resolution methods (Supervisor P. Dombi)

### ***Semmelweis University, Budapest***

- M. Ashaber, Wiring functional tactile cortical representations, combined optical imaging, light- and electron microscopic track tracing studies in the primate somatosensory cortex (Supervisor L. Négyessy)

- E. Pálfi, The role of somatosensory cortical inhibition in tactile functions (Supervisor L. Négyessy)

***Pázmány Péter Catholic University, Budapest***

- B. Jákli, Control of biomechatronic robotic arm (Supervisor L. Négyessy)

***University of Szeged***

- A. Barna, Stability and contrast improvement of ultrashort KrF laser pulses for laser-plasma experiments (Supervisor I. Földes)
- L. Himics, Nanocrystalline diamonds for advanced applications (Supervisor M. Koós)
- H-M. Tóháti, Optical spectroscopy of confined luminescent materials (Supervisor K. Kamarás)

***University of Pécs***

- M. Aladi, Generation of high-harmonics from gases, clusters and solids (Supervisor I. Földes)
- I. Hajdara, Spectroscopy of ferroelectric oxide crystals (Supervisor L. Kovács)
- L. Kecskés, Complex chaos in the dynamics of qubits (Supervisor T. Kiss)
- A. Kerekes, Development of optical instrumentation for environmental measurements (Supervisor A. Nagy)
- B. Kollár, Quantum information in quantum-optical networks (Supervisor T. Kiss)
- Z. László, Magnetic bearings for neutron beam phase space tailoring (Supervisors J. Nagy, J. Füzi)
- N. Sándor, Optical information writing and coherent processing using metastable quantum states (Supervisor G. Dzsotjan)
- P. Sinkovicz, Spin liquid phases (Supervisor G. Szirmai)
- Á. Varga, Quantum state discrimination (Supervisor P. Ádám)

***University of Pannonia, Veszprém***

- K. Berkesi, Investigation of radioactive contamination on smooth and increased surfaces of noble metal electrodes (Supervisor L. Péter)

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**DISSERTATIONS**

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***Ph.D.***

- P. Antal, Development of a tunable, long-cavity, femtosecond pulse Ti:sapphire laser, and group delay dependent loss in dielectric mirrors (Eötvös Loránd University, Supervisor R. Szipócs)
- Zs. Huhn, The role of place cells and grid cells in spatial navigation (Eötvös Loránd University, Supervisors, P. Érdi and Z. Somogyvári)
- M. Markó, Atomic resolution neutron holography (Budapest University of Technology and Economics, Supervisor L. Cser)
- D. Merkel, Development and modification of magnetic thin films (Eötvös Loránd University, Supervisor L. Bottyán)
- M. I. Nagy, New exact solutions of relativistic hydrodynamics (Eötvös Loránd University, Supervisor T. Csörgő)
- P. Rácz, Investigation of electron beams generated by femtosecond surface plasmons, (Budapest University of Technology and Economics, Supervisor P. Dombi)
- J. Romhányi, Exotic ordering and multipole excitations in anisotropic systems (Budapest University of Technology and Economics, Supervisor K. Penc)
- E. Simon, Theoretical study of the interaction of the surface magnetic impurities (Eötvös Loránd University, Supervisor B. Újfalussy)
- Gy. Tóth, Phase-field analysis of nucleation phenomena, (Budapest University of Technology and Economics, Supervisor L. Gránásy)

***D.Sc.***

- G. Erdős, Magnetic field measurements in the heliosphere
- P. Mezei, The investigation of the electrolyte cathode atmospheric pressure d.c. current glow discharge

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**MEMBERSHIP**


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- I. Bakonyi — Elected Member of the General Assembly of MTA (2010-2012)  
 — Member of the Solid State Physics Committee of MTA (2011-2014)  
 — Member of the Editorial Advisory Board (from 2005), Journal of Materials Science and Technology (Bulgaria, Sofia)  
 — Member of the European Board (from 2006), European Academy of Surface Technology (EAST)  
 — Member, International Advisory Board, INTERFINISH 2012 – Green Emerging Metal Finishing Technologies and New Developments, XVIII World Interfinish Congress and Exhibit (Milan, Italy, 2012)  
 — Member, Organizing Committee, 9th International Conference on Physics of Advanced Materials (ICPAM-9, Iasi, Romania, 2012)  
 — Member, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
- J. Balogh — Int. Board on the Application of the Mössbauer Effect (IBAME), 2007-2012
- G.G. Barnaföldi — Hungarian Representative in EU ESF CompStar 2008-2013.  
 — Editor of The European Physics Journal A: Hadrons and Nuclei Topical Issue on Relativistic Hydro- and Thermodynamics in Nuclear Physics  
 — Member of Physics PhD School at Eötvös Loránd University, Budapest
- F. Bázsó — Programme Committee Member, International Conference on Artificial Neural Networks ICANN 2012 Sept. 11-14, Lausanne
- L. Bencs — Editorial Board member of Environmental Monitoring and Management  
 — Editorial Board member of ISRN Analytical Chemistry
- T.S. Biró — Member of the Scientific Advisory Committee of the European Physical Journal (representing MTA and ELFT, until August 31, 2012)  
 — Co-Editor of the European Physical Journal A: Hadrons and Nuclei;

## Membership

- Chairman of Wigner FK RMI TT (Scientific Advisory Board)
  - Member of International Advisory Board for Strangeness in Quark Matter conferences; (Birmingham UK 2013)
  - Member of Physics PhD School Advisory Board at TU Budapest (BME)
  - Member of Physics PhD School, Eötvös Lorád University, Budapest
  - Editor of The European Physics Journal A (Hadrons and Nuclei) Topical Issue on Relativistic Hydro- and Thermodynamics in Nuclear Physics
- Á. Buka
- Electronic-Liquid Crystal Communications, Editorial Board
  - International Liquid Crystal Conference, International Advisory Board
  - National Scientific Research Fund (OTKA), Physics Panel Member
  - Solid State Physics Committee of MTA, Member
  - ERC Starting Grant, Condensed Matter Panel Member
- L. Cser
- International Scientific Advisory Council of BNC (Budapest Neutron Centre)
- T. Csörgő
- Academia Europaea (London), elected member (2011-)
  - Member, physics PhD School, ELTE, Budapest
  - Member, Institutional Board, PHENIX Experiment, BNL
  - Member, Executive Council, TOTEM Experiment, CERN LHC
  - Member, CERN LHC Resource Review Board
  - Member, International Advisory Committee, WPCF conference, Frankfurt am Main, Germany
  - Member, International Advisory Committee, ISMD, Kielce, Poland
  - Principal Investigator, PHENIX - Hungary sub-collaboration
  - Principal Investigator, TOTEM - Hungary sub-collaboration
- A. Czitrovsky
- Chairman of the Working Group Instrumentation in EAA
  - Member of the Board of International Aerosol Association
  - Member of Gesellschaft für Aerosolforschung
  - President of the Hungarian Aerosol Society
  - Member of the ELI\_ALPS Scientific Advisory Committee
  - President of the Hungarian Branch of the European Optical Society

- Head of the Optical Chapter of the Scientific Society for Optics, Acoustics, Motion Pictures and Theatre Technology (Budapest)
  - Member of the Editorial Board of “Fizikai Szemle”
  - Chairman of the Optical Chapter of Roland Eötvös Physical Society
  - Chairman of the Committee for the Lasers Physics and Spectroscopy in MTA
  - Member of the Int. Organizing Committee of the European Aerosol Conference (Granada, 2011)
  - Member of the Int. Program Committee of Int. Conf. on Advanced Laser Technologies (Thun, Switzerland, 2012)
- L. Diósi
- Management Committee, EU COST Action Fundamental Problems in Quantum Physics
  - Member of Editorial Advisory Board, The Open Nuclear & Particle Physics Journal
- P. Domokos
- Editor of the European Physical Journal D
  - Liaison Committee representative of the International Union of Pure and Applied Physics (IUPAP)
- Z. Donkó
- Conference series “Symposium of the Phenomena in Ionized Gases”, Member of International Scientific Committee, from 2006
  - Conference series “Strongly Coupled Coulomb Systems”, Member of International Advisory Board, 2007-
  - Conference series “Symposium on Application of Plasma Processes,” Member of International Scientific Committee, from 2008
- G. Erdős:
- Chairman of the Committee on Astronomy and Space Physics of MTA
  - National Representative of COSPAR
- N. Éber
- Member of The Open Crystallography Journal, Editorial Board
  - Member of the Journal of Research in Physics, Editorial Board
- P. Érdi
- Co-Director: Budapest Semester in Cognitive Sciences
  - Program co-Chair, International Conference on Artificial Neural Networks ICANN 2012 Sept. 11-14, Lausanne
  - Member of the Editorial and Programme Advisory Board of the Springer Complexity publishing program
  - Member of the Executive Committee of the European Neural Network Society

## Membership

- Member of the Editorial Board of the Journal of Applied System Studies
- Member of the Editorial Board of the Cognitive Neurodynamics
- Associate Editor of Neurobiology
- Member of the Editorial Board of the Nonlinear Biomedical Physics Open Access Journal
  
- G. Faigel — XFEL In-kind Review Committee member
- XFEL SAC member
  
- K. Fodor- — ESF COST D35, Management Committee
- Csorba — Open Organic Chemistry Journal, Board Member
  
- T. Fülöp — Member of the Organizing Committee of 6th Finno-Ugric International Conference of Mechanics with Special Symposia (Ráckeve, 2013)
  
- L. Gránásy — Member of the ESA Topical Team “Solidification of Containerless Undercooled Melts”, SOL – EML
- Member of The Minerals, Metals, and Materials Society, USA
- Solid State Physics Committee of MTA
- Mathematics and Science Committee of AKT
  
- P. Hartmann — Conference series "Europhysics Conference on the Atomic and Molecular Physics of Ionized Gases" Member of International Scientific Committee, 2008-2014
  
- J. Janszky — Member of the Editorial Board of Nonlinear and Quantum Optics
- Member of the Editorial Board of Problems in Physics
  
- I. Jánossy — electronic-Liquid Crystal Communications, Editorial Board
  
- K. Kamarás — Editorial Board Member, European Physical Journal B
- Z. Kis — Member of the Editorial Board of the Physical Review A
- T. Kiss — Member of the Commission on Quantum Electronics (C17) of the International Union of Pure and Applied Physics (IUPAP)
  
- G. Kriza — Member of the Solid State Physics Committee of MTA (from 2007)
- Elected Member of the General Assembly of MTA (2007-2012)
- Member of Ph.D. School of Physics, BME (from 2008)
- Member of Bolyai Fellowship Board, MTA (from 2010)

- N. Kroó
  - Member of MTA Domus Hungarica Scientiarum et Artium Fellowship Board (from 2008)
  - Member of the Presidium of MTA
  - Chairman of the Research Infrastructure Committee of MTA
  - Chairman of the Committee of International Relations of MTA
  - Chair of the Governing Council of the Hungarian Research Infrastructure Program
  - Chair of the Rátz High School Prize
  - Member of the Hungarian UNESCO Committee
  - Chair of the Dennis Gabor International Prize Committee
  - Member of the Scientific Council of the European Research Council
  - Chairman of the Research Infrastructure Expert Group of ERA (EC)
  - Member of the High Level Expert Group on Digital Libraries and Scientific Publications (EC)
  - Member (former Chair) of the Section of Physical and Engineering Sciences of Academia Europaea
  - Member of the Advisory Group on ESOF
  - Member of the ELI\_ALPS Scientific Advisory Committee
- K. Kutasi
  - Conference series “International Workshop on Non-equilibrium Processes in Plasma Physics and Studies of Environment,” member of International Scientific Committee, from 2006
- Ö. Legeza
  - Member of the Statistical Physics Scientific Committee, MTA
  - Member of the Young Researcher Committee, MTA
  - Secretary of the Statistical Physics Section of Roland Eötvös Physical Society (ELFT)
- P. Lévai
  - Member of the Physics PhD. School, ELTE
  - Member of the Hungarian CERN Committee
  - Member of the CERN Council
  - Member of the ESFRI (European Strategy Forum on Research Infrastructure)
  - Member of the Committee on Research Infrastructure.
  - Member of the Committee on Nuclear Physics.
  - Member of the Committee on Particle Physics.
  - Member of the IAC of the Quark Matter 2012 Conference (Washington, 2012. 08.13-18)
  - Member of the IAC of the 7th International Workshop on

## Membership

- High-pT Physics at LHC, (Frankfurt, 2012.03.26-30)
- Member of the IAC of the 8th International Workshop on High-pT Physics at LHC, (Wuhan, 2012.10.21-24)
- F. Mezei
- International Scientific Advisory Council of BNC (Budapest Neutron Centre)
  - European Neutron Scattering Association (ENSA) Committee
  - Scientific Advisory Council of SNS (Spallation Neutron Source), Oak Ridge National Laboratory, USA
- D.L. Nagy
- Common Coordination Committee of the Hungarian Academy of Sciences and the Joint Institute for Nuclear Research, Dubna, MTA Representative
  - Joint Institute for Nuclear Research, Dubna, Scientific Council, Member
  - European XFEL, Council, Member
  - Budapest Neutron Centre (BNC), International Scientific Advisory Committee, Member
  - FP7 Research Infrastructures Programme Committee, expert
  - International Board of the Applications of the Mössbauer Effect, Chair
  - European Synchrotron Radiation Facility, Consortium CENTRALSYNC, Steering Committee, Member
  - Hyperfine Interactions, Editorial Board, Member
  - International Union of Pure and Applied Physics (IUPAP), Commission on Physics for Development (C13), Member
  - European Physical Society, Council, Member
  - C-ERIC consortium, Working Group, Member
  - European Strategy Forum on Research Infrastructures, Working Group on Regional Issues, Member
  - European Science Foundation, Member Organisation Forum on Research Infrastructures, Member
  - Program Advisory Committee for Condensed Matter Physics, Joint Institute for Nuclear Research, Dubna, Member
- L. Péter
- Secretary, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
  - Representative for Hungary, International Society of Electrochemistry (2011-2013)
  - Council Member of Graduate School of Chemistry, ELTE

- (2009-)
- Editor for Electrochemistry (Central European Journal of Chemistry, 2009-)
- K. Polgár
- Hungarian Advisor of the International Organization for Crystal Growth
  - Member of the International Advisory Committee of the 17th Intern. Conference on Crystal Growth and Epitaxy (ICCGE-17)
- L. Rosta
- International Scientific Advisory Council of BNC (Budapest Neutron Centre)
  - European Spallation Source, Steering Committee
- F. Siklér
- Hungarian delegate to European Committee for Future Accelerators (ECFA)
  - Member of CMS Publication Committee, Heavy Ions editorial board
- J. Sólyom
- Chairman of the Physics Section of the Hungarian Academy of Sciences
- S. Szalai
- Member of Hungarian Space Research Council
  - Member of ARTEMIS-H steering
  - Member of Rosetta Lander steering
- K. Szegő
- Member of Committee on Astronomy and Space Physics of MTA
  - Member of IAA
  - Guest Editor of Space Science Reviews
- E. Szilágyi
- International Committee of the Conference series of Ion Beam Analysis, member
- Z. Szőkefalvi-Nagy
- Member of the Editorial Board, International Journal of PIXE
  - Honorary Member of the International Advisory Board, PIXE
  - Member of the Committee of International Relations of MTA
- K. Tompa
- Member of the Natural Science Committee of the Hungarian Scholarship Board (2011-2013)
  - Member of PhD Council of ELTE (2008-2012)
- L.K. Varga
- Member of the International Organising Committee (2005-), International Conference on Soft Magnetic Materials (SMM)
  - Member of Advisory Committee (2004-), Czech and

## Membership

### Slovak Conference on Magnetism (CSMAG)

- P. Ván
- Member of the Scientific Advisory Board of Joint European Congress in Thermodynamics (Brescia, Italy 2013)
  - Executive chairman of the Organizing Committee of 6th Finno-Ugric International Conference of Mechanics with Special Symposia (Ráckeve, 2013)
  - Editor of The European Physics Journal A: Hadrons and Nuclei Topical Issue on Relativistic Hydro- and Thermodynamics in Nuclear Physics
- G. Veres
- Consultative Committee EURATOM - Fusion
  - EFDA Steering Committee – deputy chair
- S. Zoletnik
- European Expert in the EU-Korea fusion collaboration committee;
  - International Tokamak Physics Activities (ITPA) "Diagnostics Topical Group" EU representative
  - EURATOM Science and Technology Advisory Committee (STAC), deputy chair
  - MAST Programme Advisory Committee, Culham, UK
  - International Board of Advisors of the Institute of Plasma Physics, Prague
  - Governing Board of Fusion for Energy, Barcelona, Spain
  - EURATOM Scientific and Technical Committee (STC)
  - Editorial Board of Plasma Physics and Controlled Fusion, IOP

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**CONFERENCES**

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***ALICE DAQ upgrade meeting. MTA Wigner RCP, March 6-7, 2012. Organizers: Hungarian ALICE group.***

Number of participants 15-20 (CERN delegates and Hungarian ALICE group).

***CETS 6<sup>th</sup> Central European Training School on Neutron Scattering.***

The school was held in Budapest, Hungary, from 14th May to 18th May 2012 and organized by the Neutron Spectroscopy Department at the Budapest Neutron Centre (BNC) with support of the associate laboratories of our research centre.

The main scope of this course was to provide insight into neutron scattering techniques and their application for studies on structure and dynamics of condensed matter. After attending the lectures the students participated in practical works in groups (powder diffractometer, small-angle neutron scattering instrument, polarized neutron reflectometer, three-axis spectrometer, time-of-flight (TOF) spectrometer, prompt-gamma activation analysis were used). The course consisted of 5 days lectures and experimental works. A lecture by Ferenc Mezei (BNC/ESS) opened the school, giving an overview on the possibilities of neutron scattering techniques in condensed matter. Further lectures were given by renowned scientist from various European institutions. Besides the neutron training aspect the school also provided a forum for some specific topics. George Grüner (UCLA), a renowned expert in nanotechnologies and successful businessman in this field, gave a lecture “Business of Academic Research” that opened a vivid discussion on the opportunities of making business with table-top science or at large scale facilities. CETS was also an opportunity to include in the programme a half-day series of presentations on cultural heritage in order to promote the EU FP7 CHARISMA project activities.

***International School on Quantum and Nano Computing Systems and Applications QANSAS-2012, Agra, India, November 29-December 2, 2012.***

Number of participants 80-120. Member of Steering Committee: L. Diósi.

***RMC-5 — 5<sup>th</sup> International Reverse Monte Carlo Conference (“The first 24 years of Reverse Monte Carlo Modelling”), Budapest, Hungary, September 20-22, 2012.***

The conference was preceded by tutorial sessions (18-19 September). Out of the 50+ participants, more than 40 conferees arrived from abroad (from the USA to Japan).

***Professional Training, Mianyang, China, June 18 - July 20, 2012***

The Neutron Spectroscopy Department in cooperation with MIRROTRON Co. organized a training course in Neutron Research and Instrumentation with the specific purpose of training in Three-Axis Spectroscopy (TAS) for a group of scientists and engineers of the Institute of Nuclear Physics and Chemistry, Mianyang, China. The training consisted of education in neutron scattering with specific orientation on neutron inelastic scattering, including lectures given by leading scientists of the Budapest Neutron Centre (BNC) and renowned European experts invited by BNC as well as hands-on training using BNC neutron facilities. The training has included the following items: Introduction to neutron techniques and instruments at BNC, training in MC simulation for spectrometer components, training in neutron

## Conferences

spectrometer function utilizations, assistance in performing real experiments at BNC TAS instruments, training in data treatment.

***Sixth International Workshop Spacetime-Matter-Quantum Mechanics DICE2012, Castello Pasquini Castiglioncello, Tuscany, Italy, September 17-21, 2012.***

Number of participants 120. Co-organizer: L. Diósi.

***YouResAstro2012, 6th Workshop for Young Astronomers and Astrophysicists. MTA Wigner RCP, Budapest, Hungary, September 3-6, 2012.***

Number of participants 68. Homepage: <http://astro.elte.hu/YouResAstro2012/>. The conference gave a great opportunity for young postdoc researchers and PhD students working in astronomy, astrophysics and related topics to present their results. Each session was introduced by a review talk presented by internationally recognized experts of the given topic. Main organizer: G.G. Barnaföldi.

***Zimányi Winter School on Relativistic Heavy Ion Physics, Wigner RCP and ELTE), Budapest, Hungary, December 3-7, 2012***

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**SEMINARS**


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**Weekly meetings of the Budapest and Debrecen Compact Muon Solenoid (CMS) groups:**

<http://www.grid.kfki.hu/twiki/bin/view/CMS/WeeklyBudapestDebrecenMeetings>

**Talks for the annual Zimányi School**

<http://zimanyischool.kfki.hu/12/>

**RMI Seminars**

- 16-01-2012 K. Krajczár, A CMS nehézion-eredményeinek áttekintése (Reviewing the heavy Ion results of CMS, in Hungarian)
- 30-01-2012 K. Márton, Kisimpulzusú részecskedetektor az NA61/SHINE kísérlethez (Low pulse particle detector for the NA61/SHINE experiment, in Hungarian)
- 09-03-2012 P. Ván, Egy könyv, ami nem létezik (Imre Fényes, Foundations of Thermodynamics, Academic Publishers, Budapest, 1952). (A book that does not exist, in Hungarian).
- 23-03-2012 I. Marshall, Poisson reduction on the space of polygons
- 06-04-2012 P. Ván, Nemegyensúlyi termomechanika (Nonequilibrium thermomechanics, in Hungarian)
- 13-04-2012 M. Jackson, Effective field theory of inflation”
- 20-04-2012 G.G. Barnaföldi, Nukleáris effektusok tesztje a CERN LHC tervezett 4.4 ATeV p+Pb ütközéseiben (Testing nuclear effects in the proposed 4.4ATeV pPb collisions of the LHC, in Hungarian)
- 04-05-2012 P. Kovács, Fizikai részecskék  $q\bar{q}$  állapotokkal történő megfeleltetése a kiterjesztett lineáris-sigma modellben (Assignment of physical particles to  $q\bar{q}$  states in the extended linear  $\sigma$ -model, in Hungarian)
- 14-05-2012 F. Siklér, Új kiértékelési módszerek és alkalmazásuk az erős kölcsönhatás vizsgálatában (New evaluation methods, and their application in the study of strong interactions, in Hungarian)
- 15-05-2012 T.S. Biró, Non-extensive thermodynamics and superstatistics, NA61 Collaboration Meeting, Budapest
- 01-06-2012 G. Székely, Faster than light particles
- 08-06-2012 G. Domokos, Kavicsformák evolúciója térben és időben (Pebble shape evolution in space and time, in Hungarian)
- 09-07-2012 G.G. Barnaföldi, GPU-alapú AliRoot szimulációk (GPU based AliRoot Simulations, GPU day, in Hungarian)
- 20-07-2012 R.J. Glauber (Harvard University, Nobel Laureate in Physics, 2005), Quantum mechanics of light: interference, entanglement and ghost imaging
- 07-09-2012 C. Tsallis, Non-extensive thermostatics

## Seminars

### *SZFI Seminars*

- 10-01-2012 D. Horváth, Ultragyors neutrínók (Ultrafast neutrinos, in Hungarian)
- 17-01-2012 P. Hartmann, Komplex viszkozitás 2D-ben (Complex viscosity in 2D, in Hungarian)
- 24-01-2012 L. Péter, Elektrokémiai fémleválasztás: Egy út a nanostruktúrák felé (Electrochemical metal deposition: A road to nanostructures, in Hungarian)
- 31-01-2012 I. Horváth (National University of Public Service, Budapest), Kozmológiai kutatásokért adták a 2011 évi fizikai Nobel-díjat (2011 Nobel Prize was awarded for cosmological research, in Hungarian)
- 07-02-2012 A. Jánossy (Department of Experimental Physics, BME),  $Gd_3N@C_{80}$ : a jövő MRI kontrasztanyaga? ( $Gd_3N@C_{80}$ : future's contrast material? In Hungarian)
- 14-02-2012 P.D. Ispánovity (ELTE TTK, Anyagfizikai Tanszék), Diszlokációrendszerek és a szubmikronos plaszticitás statisztikus tulajdonságai (Statistical properties of dislocation systems and the submicron plasticity, in Hungarian)
- 21-02-2012 J. Sólyom, Normális, szimmetriasértő és szimmetriát nem sértő, mégsem normális elektronrendszerek szilárd testekben. Paradigmaváltás a szilárdtest-fizikában (Normal, symmetry-breaking and non-symmetry breaking, yet not normal electronic systems in solids, in Hungarian)
- 28-02-2012 L. Gránásy, Homogén és heterogén kristály nukleáció atomisztikus fázismező elmélete (Atomistic phase field theory of homegeneous and heterogeneous crystal nucleation, in Hungarian)
- 06-03-2012 Penc Karlo, Rendeződés  $SU(3)$  és  $SU(4)$  Heisenberg modellekben (Ordering in  $SU(3)$  and  $SU(4)$  Heisenberg models, in Hungarian)
- 13-03-2012 M. Kling (Max-Planck-Institut für Quantenoptik, Germany), Generation of high-energy electrons and photons via nanoplasmonic field enhancement
- 20-03-2012 I. Kézsmárki (Budapest University of Technology and Economics), Új magneto-optikai módszerek a maláriakutatás és maláriadiagnózis területén (New magneto-optical methods in the fields of malaria research and diagnostics, in Hungarian)
- 03-04-2012 A. Pályi (Dept. of Material Science, ELTE), Elektronállapotok koherens kontrollja szén nanocsövekben (Coherent control of electronic states in carbon nanotubes, in Hungarian)
- 10-04-2012 S. Varró, Max Planck elfelejtett öröksége II (Max Planck's forgotten heritage II, in Hungarian)
- 08-05-2012 P. Dombi, Hosszú rezonátoros Ti,zafír oszcillátorok fejlesztése és felhasználása az alap- és alkalmazott kutatásban (Development and application of long resonator Ti:Sapphire oscillators in basic and applied research, in Hungarian)
- 25-05-2012 F. Alberto Grünbaum (University of California, Berkeley, USA), Spectral methods for discrete time quantum walks: limit laws and recurrence
- 01-06-2012 Barry Sanders (University of Calgary Canada), Coin quantum walks in ion traps and in superconducting circuit quantum electrodynamics

Annual Report 2012

- 13-06-2012 N. Babcsán (Institute for Logistics and Production Engineering (BAY-LOGI)), Fémolvadék kolloidok és vizsgáló technikái (Metal melt colloids and their investigation technics, in Hungarian)
- 14-06-2012 L. Almásy, Szerves sók vizes és nemvizes oldatainak szerkezetvizsgálata kisszögű neutronsórással (Structural investigations of aqueous and non-aqueous solutions of organic salts by small angle neutron scattering, in Hungarian)
- 21-06-2012 K. Berkesi (Pannon University), Adszorpciós folyamatok radioelektrokémiai vizsgálata (Radioelectrochemical studies of adsorption processes, in Hungarian)
- 12-07-2012 F. Tian (KTH Stockholm, Sweden), First principle calculations on high entropy alloys
- 20-07-2012 R.J. Glauber (Harvard University, USA), Quantum Mechanics of Light, Interference, entanglement and ghost imaging
- 30-08-2012 T. Tonegawa (Department of Physics, Kobe University, Japan), Ground-State Phase Diagram of an Anisotropic S=2 Antiferromagnetic Quantum Spin Chain, Existence of the Intermediate-D Phase
- 11-09-2012 K.A. Suresh (Centre for Soft Matter Research, Bangalore, India), Electrical conductivity of Langmuir–Blodgett films of some novel discotic mesogenic molecules
- 13-09-2012 S. Amarie (Neaspec Com., Garching, Germany), Chemical mapping on the nanoscale by Fourier-transform infrared spectroscopy
- 18-09-2012 S. Varró, Digitális véletlen és fekete sugárzás (Digital randomness and black radiation, in Hungarian)
- 20-09-2012 V. Zólyomi, Megvalósítani a lehetetlent, Kétdimenziós szilíciumtól az óriási hiperfinom kölcsönhatást mutató szén nanocsövekig (To realize the unreal, from two-dimensional silicon to carbon nanotubes showing giant hyperfine interaction, in Hungarian)
- 25-09-2012 Á. Gali, Electro-luminescence of single nitrogen-vacancy defect in diamond, theory
- 16-10-2012 H. Alloul (Laboratoire de Physique des Solides, Orsay), NMR investigation of the pressure induced Mott transition to superconductivity in the  $\text{Cs}_3\text{C}_{60}$  isomeric compounds
- 30-10-2012 Z. Donkó, Franck-Hertz kísérlet: 100 éve és ma (The Franck-Hertz experiment: 100 years ago and today, in Hungarian)
- 06-11-2012 K. Tompa, Hidrogén 'csontváz' és mozgékonyaság proteinekben (Hydrogen 'skeleton' and mobility in proteins, in Hungarian)
- 13-11-2012 P. Domokos, Munkára fogott kvantummechanika, a 2012. évi fizikai Nobel-díj (Quantum mechanics set to work, in Hungarian)