AGH University of Science and Technology
Faculty of Physics and Applied Computer Science

Annual Report 2010

Akademia Górniczo-Hutnicza
im. Stanisława Staszica w Krakowie
Wydział Fizyki i Informatyki Stosowanej

Raport Roczny 2010
Faculty of Physics and Applied Computer Science
Wydział Fizyki i Informatyki Stosowanej AGH

DEAN
prof. dr hab. inż. Wojciech Łużny

DEPUTY DEAN FOR GENERAL AFFAIRS
prof. dr hab. inż. Marek Przybylski (until 2010-10-31)
prof. dr hab. Janusz Wolny (since 2010-11-01)

DEPUTY DEAN FOR EDUCATION
dr hab. Andrzej Lenda, prof. AGH

DEPUTY DEAN FOR STUDENT AFFAIRS
dr inż. Krzysztof Malarz

ADMINISTRATIVE DIRECTOR
dr inż. Janusz Chmist

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The Faculty of Physics and Applied Computer Science (FPACS) is one of the fifteen Faculties of the AGH University of Science and Technology in Cracow. The origins of the Faculty are dated back to 1919, when the Academy of Mining was founded, within which the Chair of Physics was erected. It has undergone several organizational transformations until in 1991 the AGH Senate has decided to form the Faculty of Physics and Nuclear Techniques. In 2004 the name was changed to Faculty of Physics and Applied Computer Science, accordingly to the changes in the fields of scientific and educational activity.

Scientific activity of the Faculty comprises both basic and applied research in solid state physics, nuclear and elementary particles physics, medical physics and physics of the environment.

There are six departments within the Faculty:

1. Department of Solid State Physics (Katedra Fizyki Ciała Stałego)
2. Department of Medical Physics and Biophysics (Katedra Fizyki Medycznej i Biofizyki)
3. Department of Condensed Matter Physics (Katedra Fizyki Materii Skondensowanej)
4. Department of Applied Informatics and Computational Physics (Katedra Informatyki Stosowanej i Fizyki Komputerowej)
5. Department of Particle Interaction and Detection Techniques (Katedra Oddziaływań i Detekcji Cząstek)
6. Department of Applied Nuclear Physics (Katedra Zastosowań Fizyki Jądrowej)

All together 176 persons are employed including 121 scientists and 55 technical and administrative staff. There are 40 full professors and 81 assistant professors or post-docs.

Faculty offers several degree programs leading to B.Sc., M.Sc. and Ph.D. degrees. The undergraduate studies consist of seven-semester bachelor programs in three distinct areas: technical physics, medical physics and applied computer science. They are followed by three-semester graduate programs, leading to the M.Sc. degree in the various specializations.

Area: Medical Physics; specializations: Dosimetry and Electronics in Medicine, Imaging and Biometrics,
Area: **Technical Physics**; specializations:
- Computer Physics,
- Solid State Physics,
- Nuclear Physics,
- Environmental Physics,

Area: **Applied Computer Science**; specialization:
- Computer Techniques in Science and Technology.

Faculty members teach both general physics courses and selected branches of physics for students of twelve Faculties of the AGH-UST. The teaching covers both reading lectures as well as organizing tutorials (physics problems classes) and laboratory work. Faculty’s teaching assignments for students of other faculties include both undergraduate and graduate levels. Some of lectures are offered in English.

Faculty organizes complementary courses for the 1st year students of the University in physics (parallel to complementary courses in mathematics, organized by the Faculty of Applied Mathematics). The aim of the courses is to fill possible gaps in the high-school education that discourage young candidates from electing technical- and science-oriented areas of study and – for the candidates who undertook such studies – increase the efficiency of the training.

Faculty hosts three four-year programs of Ph.D. Studies in Physics. The first of them are the regular Ph.D. studies in the fields related to the research interests of Faculty members, i.e. technical nuclear physics, condensed matter physics, high energy physics, nuclear electronics, environmental physics.

The second Ph.D. program started on the 1st October 2009 co-organized with Cracow’s Institute of Nuclear Physics and Institute of Catalysis and Surface Chemistry (both Institutes are units of the Polish Academy of Science – PAS). The program under the name “**Interdisciplinary Ph.D. Studies (ISD): New Materials for Modern Technologies and Future Energetics**” is financed by the EU Structural Funds (Program: Kapitał Ludzki). The ISD goal is training high-class specialists, with the Ph.D. degree, in fields recognized as strategically important in EU and presented under the general terms: Info, Bio, Nano and Techno. The program of the Ph.D. studies covers a wide variety of physical, chemical and technological topics in materials science and modern energetics.

Finally, the third Ph.D. program run in co-operation with Institute of Catalysis and Surface Chemistry of PAS and selected research institutes of 10 European countries is a common **International PhD program in Nanoscience**. The project is financed by European Union Innovative Economy Program acting via Foundation for Polish Science. It had been selected for financial support as one of three projects in the first call for the International PhD Studies Programs and started in September 2008. Research is scheduled for 4 or 5 years, of which 6 to 24 months the students will spend abroad, mostly in Western European institutes that belong to the consortium.

Faculty offers also a three semester Post-diploma (part-time) Study for Teachers. The studies are intended for primary and secondary school teachers, who want to gain additional qualifications giving them right to teach: physics, mathematics, chemistry, computer science, natural sciences and technical education.
Physicists – Doctors Honoris Causa of AGH University of Science and Technology

PROF. MARIAN MIĘSOWICZ 1979
PROF. ANDRZEJ OLEŚ 1995
PROF. MICHAŁ HELLER 1996
PROF. ANDRZEJ Z. HRYNKIEWICZ 1999
PROF. MANUEL RICARDO IBARRA 2008
PROF. JURGEN M. HÖNIG 2010

Physicist – Honorary Consul of AGH University of Science and Technology

PROF. ROLF-DIETER HEUER (GENERAL DIRECTOR OF CERN) 2009

Physicist – AGH-UST Honorary Professor

PROF. JERZY NIEWODNICAŃSKI 2009

Long-term visitors


GWYNNE JAMES MORGAN, UNIVERSITY OF LEEDS, GB, VISITING PROFESSOR 3.04.2010 – 27.05.2010

AJITH ABRAHAM, NCNU TRONDHEIM, NORWAY, VISITING PROFESSOR 30.09.2010 – 18.11.2010

RIVETTI ANGELO, ITALY, INTERNATIONAL COLLABORATION 24.07.2010 – 23.09.2010
Departments, Groups and Leaders, Achievements in 2010
Katedry, Zespoły i ich kierownicy, Najważniejsze osiągnięcia w 2010 r.

Department of Solid State Physics
Katedra Fizyki Ciała Stałego

STAFF

HEAD

prof. dr hab. Kapusta Czesław, full professor

MAGNETIC BULK- AND NANOMATERIALS GROUP
ZESPÓŁ MATERIAŁÓW MAGNETYCZNYCH LITYCH I NANOMATERIAŁÓW

prof. dr hab. Kapusta Czesław, full professor
dr Japa Ewa, assistant professor
dr Przewoźnik Janusz, assistant professor
dr inż. Sikora Marcin, assistant professor
dr Żukowski Jan, assistant professor
dr inż. Rybicki Damian, teaching assistant
mgr inż. Lemański Andrzej, teaching assistant
mgr inż. Pilipowicz Aleksander
Syrek Jolanta
mgr inż. Musiał Waclaw
inż. Kazała Tadeusz
Bąkowski Mariusz

MAGNETIC, ELECTRICAL AND STRUCTURAL RESEARCH GROUP
ZESPÓŁ BADAŃ MAGNETYCZNYCH, ELEKTRYCZNYCH I STRUKTURALNYCH

dr hab. Paja Antoni, associate professor
dr Gondek Łukasz, assistant professor
dr Joanna Czub, research assistant
dr inż. Niewolski Janusz, teaching assistant

SUPERCONDUCTING AND MAGNETIC MATERIALS GROUP
ZESPÓŁ MATERIAŁÓW NADPRZEWODZĄCYCH I MAGNETYCZNYCH

prof. dr hab. Kołodziejczyk Andrzej, full professor
dr hab. inż. Kołodowski Andrzej, associate professor
dr hab. inż. Tarnawski Zbigniew, associate professor
dr inż. Chmista Janusz, assistant professor
dr inż. Tokarz Waldemar, assistant professor
dr Woch Wiesław, assistant professor
mgr Zalecki Ryszard
PROFILE

Scientific activity of the Department concentrates on the studies of structural, magnetic and electronic properties and phenomena in the nano- and sub-nanometric thin films and multilayers for magnetic and catalytic applications, in the rare earth-3d element intermetallics and their interstitial solutions of hydrogen, carbon and nitrogen, in superconductors, including the HTc ones, in magnetic oxides, including the colossal and low field magnetoresistive ones, in nanoparticle magnetic materials for MRI contrast and magnetic hyperthermia as well as in disordered metallic materials.

The research staff of the Department extensively uses synchrotron beamlines as well as neutron and muon facilities at the laboratories abroad.

Działalność naukowa Katedry koncentruje się na badaniach własności i zjawisk strukturalnych, magnetycznych i elektronowych w nano- i sub-nanometrowych cienkich warstwach i wielowarstwach do zastosowań magnetycznych i katalitycznych, w związkach międzymetalicznych ziem rzadkich z pierwiastkami 3d i ich rozworów międzywęzłowych wodoru, węgla i azotu, w nadrzędowikach, w tym wysokotemperaturowych, w tlenkach magnetycznych, w tym wykazujących kolosalny i niskopolowy magnetooopór oraz w magnetycie, w materiałach nanokształtkowych na środki kontrastowe do MRI i do hipertermii magnetycznej oraz w nieuporządkowanych materiałach metalicznych.

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ACHIEVEMENTS

Revealing of the magnetization structure in epitaxial Fe films on W(110) in the vicinity of an in plane spin reorientation transition using the nuclear resonant scattering of synchrotron radiation.
Development of the method of neutron imaging of hydrogen storage systems.
Development of new synchrotron method for the study of magnetic bulk materials and buried layers; RIXS-XMCD
Determination of manganese valence in La$_{0.67}$(Ca,Pb)$_{0.33}$(Mn$_{1-x}$Fe$_x$)$_3$O$_7$ colossal magnetoresistive oxides from XANES and X-ray photoemission spectroscopies.
Revealing of the same lattice dynamics at the first and the second order Verwey transitions in magnetite.

ACTIVITY

ACTIVITY IN SCIENTIFIC BOARDS, ACADEMIES, SCIENTIFIC SOCIETIES, COMMITTEES ETC.

A. PAJA

- Member of the Interdisciplinary Committee for Supporting International Scientific Cooperation at the Ministry of Science and Higher Education.
- President of the General Control Committee of the Polish Physical Society

Ł. GONDEK, J. CZUB

- Member of the Małopolska Regional Committee of the Physics Competition

CZ. KAPUSTA

- Member of the Condensed Matter Physics Board of the European Physical Society.
- Członek Małopolskiego Okręgowego Komitetu Olimpiady Fizycznej
- Członek Komitetu Fizyki Fazy Skondensowanej Europejskiego Towarzystwa Fizycznego.
Department of Medical Physics and Biophysics
Katedra Fizyki Medycznej i Biofizyki

STAFF

HEAD

prof. dr hab. inż. Lankosz Marek, full professor

BIOMEDICAL AND ENVIRONMENTAL RESEARCH GROUP
ZESPÓŁ BADAN BIOMEDYCZNYCH I ŚRODOWISKOWYCH

prof. dr hab. inż. Lankosz Marek, full professor
dr hab. inż. Węgrzynek Dariusz, associate professor
dr inż. Chwiej Joanna, assistant professor
dr inż. Dudała Joanna, assistant professor
dr inż. Furman Leszek, assistant professor
dr inż. Samek Lucyna, assistant professor
dr inż. Stęgowski Zdzisław, assistant professor
dr inż. Szczerbowska-Boruchowska Magdalena, assistant professor
mgr Ostachowicz Beata, teaching assistant
inż. Wierzbicki Adam
gmgr Ostrowski Antoni
Tomasik Ryszard

MOLECULAR BIOPHYSICS AND BIOENERGETICS GROUP
ZESPÓŁ BIOFIZYKI MOLEKULARNEJ I BIOENERGETYKI

dr hab. Burda Kvetoslava, associate professor
dr Fiedor Joanna, assistant professor
dr Orzechowska Aleksandra, teaching assistant

BIOMEDICAL IMAGING AND MODELING GROUP
ZESPÓŁ OBRAZOWANIA I MODELOWANIA

prof. dr hab. Figiel Henryk, full professor
dr inż. Jung Aleksandra, assistant professor
dr inż. Matusiak Katarzyna, assistant professor
dr Matuszak Zenon, assistant professor
dr Turek Krzysztof, assistant professor

MOESSBAUER SPECTROSCOPY GROUP
ZESPÓŁ SPEKTROSKOPII MOSSBAUEROWSKIEJ

prof. dr hab. Dubiel Stanisław, full professor
dr inż. Cieśliak Jakub, assistant professor
PROFILE

The Department of Medical Physics and Biophysics consists of four research groups. The research activities of Biomedical Imaging and Modeling Group cover the development of Magnetic Resonance Imaging technique, optical imaging, modeling of physiological processes and nuclear medicine diagnostic imaging. The research at Biomedical and Environmental Research Group relates mainly to the investigation of the role of biomodulators in the biochemical mechanism of the pathogenesis and progress of cancers, neurodegeneration and epilepsy. Molecular Biophysics and Bioenergetics Group research is focused on: photosynthetic electron transport and oxygen evolution, organization and physical/chemical properties of native and model dye-protein-lipid systems, topography, elasticity and adhesion of normal and pathological cells as well as chemical properties of functionalized carbon nanotubes. The research interest of Mossbauer Spectroscopy Group includes bio-farmaceutical-medical physics. The main object of the research conducted in the Laboratory of Mössbauer Spectroscopy concerns investigation of various physical properties of technologically important alloys and compounds. Additional interest includes use of the Mössbauer Spectroscopy in the investigation of Fe-containing samples of organic or/and pharmaceutical origin or application (like ferritin, anitane mic medicaments etc).

BIOMEDICAL AND ENVIRONMENTAL RESEARCH GROUP

The research at the Biomedical and Environmental Research Group relates to the development and application of nuclear analytical methods and examination of dynamic systems. The main topics of interest are biomedical research, environmental science, and protection of cultural heritage. Of particular importance is the investigation of the role of biomodulators in the biochemical mechanisms of the pathogenesis and progress of brain gliomas, neurodegeneration, and epilepsy. The elemental and molecular chemical micro imaging is performed with the use of the techniques based on synchrotron radiation, i.e. synchrotron radiation X-ray fluorescence (SRXRF), X-ray absorption near edge structure (XANES) spectroscopy, extended X-ray absorption fine structure (EXAFS) spectroscopy and Fourier transform infrared micro spectroscopy (FTIR).

Another research topics of interest are development and applications of methods based on X-ray microbeams for chemical analysis of elements in heterogeneous samples and utilization of coherent synchrotron beams in studies of living organisms. A research is conducted on utilization of coherent synchrotron beam for investigating of the morphology/physiology of insect-vectors transmitting diseases.

Projects badawcze realizowane w Zespole Badań Biomedycznych i Środowiskowych dotyczą opracowania i zastosowania jądrowy metod pomiarowych oraz badania systemów dynamicznych. Główne kierunki zainteresowań obejmują badania biomedyczne, środowiskowe jak również ochronę dziedzictwa kulturowego. Szczególnie ważne jest wyjaśnienie roli biomodulatorów w procesach biochemicznych wzrostu nowotworów, neurodegeneracji i epilepsji. Do obrazowania rozkładu pierwiastków i biomolekuł w tkankach na poziomie komórkowym stosowane są techniki oparte na promieniowaniu synchrotronowym tzn. synchrotronowa rentgenowska analiza fluorescencyjna (SRXRF), absorpcja promieniowania X w pobliżu progu absorpcji (XANES), spektroskopia wykorzystująca strukturę subtelną blisko progu absorpcji (EXAFS) oraz mikro-spektroskoja promieniowania podczerwonego z zastosowaniem transformacji Fouriera (FTIR). Innym obszarem działalności jest opracowanie i zastosowanie metod opartych na mikro-wiązce promieniowania X do badania rozkładu pierwiastków w prób kach silnie niejednorodnych i wykorzystanie koherentnego promieniowania synchrotronowego w badaniach żywych organizmów. Prace te dotyczą badań morfologicznych i fiziologicznych insektów przenoszących choroby.
The investigations in environmental science are connected with the influence of air pollution on cultural heritage and on urban and rural environments. Statistical methods are used for identification of possible sources of air pollutants emission. The scope of research is also application of computational fluid dynamics (CFD) methods for prediction of related physical phenomena and evolution of dynamic system. The CFD results are validated by radiotracer experiments. These methods have been applied to characterize flow in jet mixers and in hydrocyclone classifiers.

The laboratory is equipped with state-of-art facilities including X-ray fluorescence and infrared confocal microscopes, multifunctional X-ray fluorescence spectrometer for localized and bulk elemental ultra trace analysis.

MOLECULAR BIOPHYSICS AND BIOENERGETICS GROUP

Our research is focused on:
- electron transport in photosystem II and bacterial reaction centers;
- role of non-hem iron on the acceptor side activity of type II photosystems;
- oxygen evolution in photosynthesis;
- structure, organization and physical/chemical properties of native and model dye-protein-lipid systems;
- protective and structural functions of carotenoids in native and model photosynthetic complexes;
- physical properties - topography, elasticity, adhesion forces - of normal and pathological cells and their organelles, and determination of the influence of selected stimuli on these properties in both cell types;
- mechanical properties of biopolymers and their influence on cell vital functions such as migration, proliferation and adhesion;
- influence of ionizing radiation and metal ions on membrane stability of human erythrocytes;
- physical and chemical characterization of carbon nanotubes;

Applied experimental methods: absorption and fluorescence spectroscopy, fluorescence with double modulation, thermoluminescence, fast polarography, atomic force microscopy (AFM), Mössbauer spectroscopy.

Badania zespołu dotyczą:
- transportu elektronów w fotosystemie II i bakteryjnych centrach reakcji;
- wpływu żelaza niehemowego na aktywność strony akceptorowej fotosystemów typu II;
- wydzielania tlenu w procesie fotosyntezy;
- struktury, organizacji i własności fizyko-chemicznych natywnych i modelowych układów barwnikowo-białkowo-lipidowych;
- funkcji strukturalnych i ochronnego działania karotenoidów w natywnych i modelowych kompleksach fotosyntetycznych;
- badania wpływu wybranych czynników na własności fizyczne – topografię, elastyczność i siły adhezji - niezmienionych i patologicznych komórek;
- analizy wpływu własności mechanicznych biopolimerów na funkcje życiowe komórek, m.in. migrację, polifierację i adhezję;
- wpływu promieniowania jonizującego i jonów metali na stabilność błon erytrocytów;
- charakterystyki fizycznych i chemicznych własności nanorurek węglowych;

Stosowane metody badawcze: spektroskopia absorpcyjna i fluorescencyjna, fluorescencja o podwójnej modulacji, termoluminescencja, szybka polarografia, mikroskopia sił atomowych (AFM), spektroskopia mőssbauerowska.
BIOMEDICAL IMAGING AND MODELING GROUP

The scientific subjects of the group consist of:
- nuclear magnetic resonance imaging,
- optical imaging,
- modeling of physiological processes,
- estimation of radiation doses in clinical diagnostics and therapy.

Research concerning MRI is related to the low field systems based on permanent magnets. The main interest is focused on development of new r.f. coils specially designed for such low field imaging and on investigations concerning programs leading to improvement of the image quality.

The other research interest of the group encompasses problems related to cancer radio- and phototherapy of melanomas and free radical processes in biology. These include both experimental and theoretical investigations. The group develops mathematical modeling of selected physiological processes. It focused especially on application of compartment modeling for extracorporeal liver support therapy. The scientific activity of the group concerns also nuclear medicine diagnostic imaging and QA (Quality Assurance) procedures and in this field designing of phantoms for static and dynamic studies was successfully developed.

MOESSBAUER SPECTROSCOPY GROUP

Our current research interests include two areas: (1) solid state physics and (2) bio-farmaceutico-medical physics. Our current activities of the former are concentrated on experimental and theoretical investigation of various physical properties of the sigma-phase in binary alloy systems (e.g. Fe-Cr, Fe-V, Co-Cr) as well as dynamical properties of poly- and nanocrystalline bcc Fe-Cr alloys, using different experimental (e.g. Mößbauer Spectroscopy, Nuclear Magnetic Resonance, Neutron Diffraction, Magnetometry) and theoretical (e.g. Korringa-Kohn-Rostoker Green’s function) methods. Regarding the latter issue, we are interested in forms and properties of iron present in samples of an organic origin (e.g. ferritin) as well as those having application in medicine (e.g. antianemic medicaments).

Zakres aktualnych badań naukowych dotyczy dwóch dziedzin: (1) fizyki ciała stałego oraz (2) fizyki biomedyczno-farmaceutycznej. W zakresie (1) prowadzone są doświadczalne i teoretyczne badania różnych własności fizycznych fazy sigma w stopach dwuskładnikowych (np. Fe-Cr, Fe-V, Co-Cr) a także własności dynamicznych polikrystalicznych i nanokrystalicznych stopów Fe—Cr przy zastosowaniu różnych technik eksperymentalnych (np. Spektroskopia efektu Mößbauer, jądrowy rezonans magnetyczny, dyfrakcja neutronów, magnetometria) i teoretycznych (np. metoda funkcji Greena w przybliżeniu KKR). W zakresie (2), badane są formy i własności żelaza w próbkach pochodzenia organicznego (np. ferrytyna) oraz w próbkach farmaceutycznych (np. leki przeciwko anemii).
ACHIEVEMENTS

BIOMEDICAL ENVIRONMENTAL RESEARCH GROUP

- Development of the Monte Carlo model for confocal 3D X-ray fluorescence microspectroscopy
- Development of a complex software for controlling the confocal 3D XRF setup
- Experimental evidence that the RTD may be used to assess accuracy of numerical CFD results
- Construction of the model assisting differentiation and/or classification (diagnosis) of brain tumors based on their elemental content.
- Conformational changes of proteins in the direction of beta type structure and increase in the saturation level of phospholipids observed in animals treated with pilocarpine suggest that protein aggregation and oxidative stress may play a significant role in the pathogenesis of neurodegenerative changes occurring in epileptic brain.
- Organization of the Atomic Spectrometry Updates X-Ray Fluorescence Spectrometry Topic Group Meeting, 4-6 June 2010, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Kraków, Poland.
- Participation in Intercomparison Excercise for ambient mass concentration measurement of Atmospheric Particulate Matter in Greece.

MOLECULAR BIOPHYSICS AND BIOENERGETICS GROUP

- We show that low and high spin ferrous states of the non-heme iron occur in native bacterial reaction centers of type II and their dynamical properties are regulated by the fluctuations of their surrounding protein matrix.
- Our studies on different oxidation/purification methods of multiwall carbon nanotubes (MWCNT) give experimental evidence that functionalization may additionally modify chemical and physical properties of MWCNT due to their Fe contaminations.
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BIOMEDICAL IMAGING AND MODELING GROUP

- Application of the thermoluminescent dosimetry for radiation dose estimation in radiiodine therapy.
- Design and set up of a new phantom for gamma-beta fields measurements.
- Analysis of an influence of different time schedules on extracorporeal liver support therapy efficiency.
- Evaluation of the application of the radiation protection of the personnel in the nuclear medicine hot laboratory.
- Construction of surface and low temperature r.f. coils for low field Magnetic Resonance Imaging system.
- Development of numerical programs based on Adaptive Weight Smoothing Algorithm and Wavelet Transform for the noise reduction (improvement of SNR) in Magnetic Resonance Imaging.
- Monte Carlo modeling of the light transport in the pigmented tissues.

MOESSBAUER SPECTROSCOPY GROUP

- Theoretical determination of the electronic and magnetic structures of the sigma-phase Fe-Cr and Fe-V alloys.
- Measurement of the kinetics of the sigma-to-alpha phase transformation for Fe-Cr alloys and demonstration that the nucleation mechanism responsible for the transformation changes in the near-critical temperature.
- Experimental evidence that the dynamics of isolated $^{57}$Fe atoms embedded into a chromium lattice is anomalous viz. (1) the $^{57}$Fe atoms are very weakly coupled to the lattice, and (2) their vibrations are harmonic below ~145 K and highly nonharmonic above ~145 K.

ACTIVITY

M. LANKOSZ

- Member of X-Ray Spectrometry Advisory Board (since 2008)
- Member of Scientific Council of the Institute of Nuclear Chemistry and Technology (since 2002)
- Chairman of the Organizing Committee of the International Conference on Development and Applications of Nuclear Technologies NUTECH 2011 (since 2008)
- Member Committee of Nuclear Technology at the National Atomic Energy Agency (since 2009)
- Member of Editorial Board of „Nukleonika“ (since 2010)

- Członek Komitetu Doradczego czasopisma X-Ray Spectrometry (od 2008)
- Członek Rady Naukowej Instytutu Chemii i Techniki Jądrowej (od 2002)
- Przewodniczący Komitetu Organizacyjnego Międzynarodowej Konferencji Rozwój i Zastosowania Technologii Jądrowych - NUTECH 2011 (od 2008)
- Członek Komitetu Technologie Jądrowe przy Państwowej Agencji Atomistyki
- Członek Komitetu Redakcyjnego czasopisma “Nukleonika” (od 2010)
Z. STĘGOWSKI
- Member Committee of Nuclear Technology at the National Atomic Energy Agency (since 2009)
- Member of Editorial Board – Nucleonic Bulletin
- Członek Komisji Technik Jądrowych przy Radzie ds Atomistyki PAA
- Członek Komitetu Redakcyjnego Biuletynu Nukleonickiego

D. WĘGRZYNEK
- Secretary of the Organizing Committee of the International Conference on Development and Applications of Nuclear Technologies NUTECH 2011 (since 2008)
- Sekretarz Komitetu Organizacyjnego Międzynarodowej Konferencji Development and Applications of Nuclear Technologies NUTECH 2011

K. BURDA
- A member of Scientific Council at Multidisciplinary School of Engineering in Biomedicine, AGH University of Science and Technology (since 2009)
- Head of the BIONAN consortium (since 2008)
- Członek Rady Programowej Międzywydziałowej Szkoły Inżynierii Biomedycznej AGH – Akademii Górniczo-Hutniczej (od 2009)
- Kierownik konsorcjum BIONAN (od 2008)

H. FIGIEL
- Member of the Main Board of the Polish Physical Society
- Chairman of the board of BIOMAR Consortium
- Member of the Programme Board of the Inter-Faculty School of Biomedical Engineering
- Member of International Steering Committee of the International Symposia on Metal Hydrogen Systems
- Member of the Scientific Committee of the Second Polish Forum - Fuel Cells and Hydrogen Technology
- Secretary of the Krakow Branch of the Societas Humboldtiana Polonorum
- Chairman of the Audit Committee of the Polish Hydrogen and Fuel Cell Association
- Chairman of the Audit Committee of the Polish Neutron Association
- Członek Zarządu Głównego Polskiego Towarzystwa Fizycznego
- Przewodniczący Rady Konsorcjum BIOMAR
- Członek Rady Programowej Międzywydziałowej Szkoły Inżynierii Biomedycznej AGH
- Członek Międzynarodowego Komitetu Sterującego Międzynarodowych Sympozjów na temat Układów Metal-Wodór
- Członek Komitetu Naukowego II Polskiego Forum Ogniwa Paliwowe i Technologie Wodorowe
- Sekretarz Oddziału Krakowskiego Societas Humboldtiana Polonorum,
- Przewodniczący Komisji Rewizyjnej Polskiego Towarzystwa Wodoru i Ogniw Paliwowych
- Przewodniczący Komisji Rewizyjnej Polskiego Towarzystwa Neutronowego

A. JUNG
- Vice Chairman of the Krakow Branch of the Polish Society of Medical Physics
- Coordinator for Medical Physics field in the project "Now physics. New forms of education closer to employers"
- Zastępca Przewodniczącego Oddziału Krakowskiego Polskiego Towarzystwa Fizyki Medycznej

Z. MATUSZAK
- President of Cracow Branch of the Polish Biophysical Society
- Prezes Krakowskiego Oddziału Polskiego Towarzystwa Biofizycznego
S. M. DUBIEL

- Member of the Senate Commission for Discipline of Students
- Fellow of the Institute of Physics, London (since 2002)
- Member of the Mössbauer Century Club, USA (since 2005)
- Member of the Research Board of Advisors of The American Biographical Institute (since 2005)
- Vice-president of the Krakow Branch of the Polish Physical Society (since 2009)
- Panel Member for Fellows at the Institute of Physics (IOP), London
- Panel's Chair for Fellows at IOP
- Chairman of session at 4th Seeheim Conference on Magnetism, SCM2010, Frankfurt a/Main, 17 March-1 April, 2010
- Reviewer for Intermetallics
- Member of the Editorial Board for Applied Sciences

POST-GRADUATED FELLOWS

- Mr. Christian Priesley Kofi DAGADU
  Department of Nuclear Engineering & Material Science
  National Nuclear Research Institute, Ghana Atomic Energy Commission
  P.O. Box Lg 80, Legon, Accra, Ghana.
  Fellowship from IAEA Vienna

- Członek Senackiej Komisji ds. Dyscyplinarnych Studentów
- Członek Instytutu Fizyki w Londynie w randze Fellow
- Członek Mössbauer Century Club, USA
- Członek Komitetu Doradczego Amerykańskiego Instytutu Biograficznego (ABI)
- Zastępca Przewodniczącego Krakowskiego Oddziału PTF
- Członek Komisji ds. Fellows w Instytucie Fizyki w Londynie (IOP)
- Przewodniczący Komisji ds. Fellows w Instytucie Fizyki w Londynie (IOP)
- Przewodniczący sesji podczas 4th Seeheim Conference on Magnetism, SCM2010, Frankfurt a/Main, 17 March-1 April, 2010
- Recenzent czasopisma Intermetallics
- Członek Komitetu Redakcyjnego czasopisma Applied Sciences
Department of Condensed Matter Physics
Katedra Fizyki Materii Skondensowanej

STAFF

HEAD

prof. dr hab. inż. Krzysztof Wierzbanowski, full professor
prof. dr hab. Oleś Andrzej prof. zw. emerytowany dr h.c. AGH
prof. dr hab. Kaprzyk Stanisław, full professor
prof. dr hab. Łużny Wojciech, full professor
prof. dr hab. Wolny Janusz, full professor
prof. dr hab. Sikora Wiesława, associate professor
prof. dr hab. inż. Zięba Andrzej, associate professor
dr hab. inż. Tobola Janusz, associate professor
dr hab. inż. Baczmański Andrzej, associate professor
dr hab. inż. Tarasiuk Jacek, associate professor
dr hab. inż. Bernasik Andrzej, associate professor
dr inż. Armataś Paweł, assistant professor
dr inż. Haberko Jakub, assistant professor
dr inż. Kulka Jan, assistant professor
dr Nizioł Jacek, assistant professor
dr Pytlik Lucjan, assistant professor
dr inż. Wiendlocha Bartłomiej, assistant professor
dr inż. Wroński Sebastian, assistant professor
mgr inż. Wawszczak Roman, teaching assistant

Władysław Błaszczyk
Ryszard Skotnicki

PROFILE

Scientific activities of the Department are mainly focused on the following topics:
- Properties and symmetry analysis of selected phases of ordered structures
- Studies of aperiodic structures
- Deformation, recrystallisation and stress in polycrystalline materials
- Electron structure of the solid state
- Polymer research
- Theory of measurement uncertainty

Działalność naukowa Katedry dotyczy następujących zagadnień:
- Własności i analiza symetryczna wybranych faz struktur uporządkowanych
- Badanie struktur aperiodycznych
- Odkształcenia, rekryrstalizacja oraz naprężenia wewnętrzne w materiałach polikrystalicznych
- Struktura elektronowa ciał stałych
- Teoria niepewności pomiarów
ACHIEVEMENTS

- Structure refinement of decagonal Al-Ni-Co, superstructure type I
- Determination of misorientation characteristics in deformed and recrystallized zirconium using new analysis method
- Symmetry analysis in examination of complex socio-technical systems (optimisation of evacuation models from big objects)
- It was demonstrated theoretically that a small change in magnetic moment in MnAs compound results in appearance of the phonon soft mode, responsible for magneto-structural transition, and in consequence, for the observed giant magneto-caloric effect.
- Experimental and theoretical demonstration of a unique role of Fe electronic states in adjustment of thermoelectric properties in Mo3-xFxSb7 alloy with complex Zintl structure.
- Observation of dendritic structures that grow spontaneously when thin films are spin cast from polymer blends of polyaniline.
- Wyznaczenie dekagonalnej struktury Al-Ni-Co, superstruktura typu I.
- Wyznaczenie charakterystyk dezorientacji w odkształconym i rekrytalizowanym cyrkonie przy użyciu nowej metody analizy
- Uwzględnienie roli symetrii w badaniach zachowania się złożonych układów socjo – technicznych (zastosowane w optymalizacji modeli ewakuacji z dużych obiektów)
- Wykazano teoretycznie, że niewielka zmiana momentu magnetycznego w kryształze MnAs prowadzi do powstania miękkiego drgania fononowego odpowiedzialnego za przejście magnetostrukturalne i w konsekwencji za obserwowany potężny efekt magnetokaloryczny
- Badania eksperymentalne i teoretyczne unikalnej roli elektronowych stanów Fe w regulacji własności termoelektrycznych stopu Mo3-xFxSb7 o złożonej strukturze Zintl
- Obserwacja spontanicznie tworzących się struktur dendrytycznych w czasie rozlewania cienkich warstw mieszanin polimerów zawierających polianilinę

ACTIVITY

A. BACZMAŃSKI

- Member of Scientific Committee of International Conferences: European Conference on Residual Stresses (ECRS) and Size-Strain Conference
- Członek Komitetów Naukowych Międzynarodowych Konferencji: European Conference on Residual Stresses (ECRS) oraz Size-Strain

J. TARASIUK

- Member of Rectors’s jury for: Lecture Notes in Internet
- Członek jury JMK Rektora Notatki w Internecie

W. SIKORA

- Member of Committee of Crystallography, Polish Academy of Science
- Członek Komitetu Krystalografii Polskiej Akademii Nauk
K. WIERZBANOWSKI

- Member of Board of review: Archives of Metallurgy and Materials (PAN)
- Reviewer of Physical Review Letters & Physical Review B
- Dean’s representative for Assurance of Quality of Teaching
- Member of International Scientific Committees of Conferences on Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation (MECA SENS)

J. TOBOŁA

- Reviewer of Physical Review Letters & Physical Review B
- Member of International Scientific Committees of ECT Conferences by European Thermo-Electrical Society and of CIMTEC Forum on New Materials

J. WOLNY

- Member of Committee of Crystallography, Polish Academy of Science

A. ZIĘBA

- Polish Physical Society: member of Main Board, member of Commission of Rewards and Distinctions
- Member of Section of Foundations of Metrology of Committee of Metrology and Measurement Equipment, Polish Academy of Sciences

W. ŁUŻNY

- Dean of Faculty
- Member of International Scientific Committee of VIII Int. Conference on X-Ray Investigations of Polymer Structure XIPS 2010

- Członek komitetu recenzentów czasopisma Archiwum Metallurgii and Materials (PAN)
- Pełnomocnik Dziekana ds. Jakości Kształcenia
- Członek międzynarodowych komitetów naukowych organizujących konferencje: Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation (MECA SENS))

- Stały recenzen APS czasopism Physical Review Letters & Physical Review B.
- Członek międzynarodowych komitetów naukowych organizujących konferencje: ECT Europejskiego Towarzystwa Termoelektrycznego oraz CIMTEC Forum on New Materials

- Członek Komitetu Krystalografii Polskiej Akademii Nauk

- Polskie Towarzystwo Fizyczne: członek Zarządu Głównego, członek Komisji Nagród i Wyróżnień
- Członek Sekcji Podstaw Metrologii Komitetu Metrologii i Aparatury Pomiarowej, Polska Akademia Nauk

- Dziekan wydziału
- Członek International Scientific Committee of VIII Int. Conference on X-Ray Investigations of Polymer Structure XIPS 2010
Department of Applied Informatics and Computational Physics
Katedra Informatyki Stosowanej i Fizyki Komputerowej

STAFF

HEAD

prof. dr hab. Kułakowski Krzysztof, full professor

COMPLEX SYSTEMS GROUP

ZESPÓŁ UKŁADÓW ZŁOŻONYCH

prof. dr hab. Kulakowski Krzysztof
prof. dr hab. Maksymowicz Andrzej, full professor
prof. dr hab. Spalek Józef, full professor
prof. dr hab. inż. Kąkol Zbigniew, full professor
dr hab. inż. Saeed Khalid, associate professor
dr hab. Lenda Andrzej, associate professor
dr inż. Dydejczyk Antoni, assistant professor
dr inż. Gawroński Przemysław, assistant professor
dr inż. Groniec Piotr, assistant professor
dr inż. Krawczyk Małgorzata, assistant professor
dr inż. Malarz Krzysztof, assistant professor
dr inż. Wołoszyń Małgorzata, assistant professor
mgr inż. Panasiuk Piotr, teaching assistant
mgr inż. Szczepański Adam, teaching assistant
dr inż. Kawecka-Magiera Barbara, senior lecturer
dr inż. Malinowski Janusz, senior lecturer
dr inż. Krupińska Grażyna, senior lecturer
mgr inż. Wolak Tomasz

THEORY OF NANOSTRUCTURES AND NANODEVICES GROUP

ZESPÓŁ TEORII NANOSTRUKTUR I NANOURZĄDZEŃ

prof. dr hab. Stanisław Bednarek, full professor
prof. dr hab. Janusz Adamowski, full professor
dr hab. inż. Bartłomiej Szafran, associate professor
dr inż. Tomasz Chwiej, assistant professor
dr inż. Bartłomiej Spisak, assistant professor
PROFILE

COMPLEX SYSTEMS GROUP

Research is conducted in a few threads; below the topics are mentioned which are concentrated in the Complex Systems Group. One of them is connected with the collaboration with the Departamento Física de Materiales at the Universidad del País Vasco, Spain. This research deals with modeling the stray field of amorphous microscopic wires of complex domain structure, including simulations of the process of remagnetization of these wires due to their bistability. Another research deals with modeling sociological processes in general frames of game theory. Since 2009, the subject is conducted in frames of 7FP EU on applications of complexity theory to socio-technical systems. Our contribution is based, among other things, on simulations of crowd dynamics within the social force model. Our new direction of research is biometrics. This research area deals with the applications of computer science, in particular the pattern recognition, to the methods of human identification and verification.

THEORY OF NANOSTRUCTURES AND NANODEVICES GROUP

- theory of electronic properties of quantum dots
- computer simulations of qubits and logic gates in nanodevices
- theory of electron quantum transport in quantum wells and nanowires
- computer simulations of the stability of metallic clusters
- modeling spin-orbit coupling effects in quantum dots
- teoria elektronicznych własności kropek kwantowych
- symulacje komputerowe kubitów i bramek logicznych w nanoprzyrządach
- teoria kwantowego transportu elektronów w studniach i drutach kwantowych
- symulacje komputerowe stabilności klastrów metalicznych
- modelowanie oddziaływania spin-orbita w kropkach kwantowych

ACHEIEVEMENTS

COMPLEX SYSTEMS GROUP

- Description of remagnetization of bistable wires in the presence of circular field
- Introduction of of social processes to simulations of crowd dynamics
- New method of compression of phase space in discrete systems
- Theory of line graphs of complex networks
- Description of avalanches in complex networks with antiferromagnetic interaction of spins at the network nodes
- Opis przemagnesowania bistabilnych drutów w obecności pola kolowego
- Wprowadzenie procesów społecznych do symulacji dynamiki tłumu
- Nowa metoda kompresji przestrzeni stanów w układach dyskretnych
- Teoria grafów krawędziowych na sieciach złożonych
- Opis lawin w sieciach złożonych z antyferromagnetycznym oddziaływaniem spinów w węzłach sieci
THEORY OF NANOSTRUCTURES AND NANODEVICES GROUP

- designing and simulation the work of the nanodevice to spin accumulation and spin read-out without magnetic field.
- computer simulations of the electron transport through the nanowire with the embedded quantum dot.
- calculation the current-voltage characteristics of the triple barrier resonant tunneling diode.
- explanation of the role of classical Lorentz force in quantum transport through semiconductor quantum wires.
- simulation of anisotropic spin exchange in spin-orbit coupled double quantum dots.
- opracowanie i symulacja działania nanourządzeń do akumulacji i odczycu spinu elektronu bez użycia pola magnetycznego.
- symulacje komputerowe transportu elektronowego przez nanodrut z kropką kwantową utworzoną pomiędzy dwoma obszarami barier.
- wyznaczenie charakterystyk prądowo-napięciowych asymetrycznej diody tunelowej z trójkątną barierą.
- wyjaśnienie roli klasycznej siły Lorentza w transporcie przez półprzewodnikowe pierścienie kwantowe.
- symulacje anizotropowej wymiany spinów w podwójnych kropkach kwantowych ze sprzężeniem spin-orbita.

ACTIVITY

S. BEDNAREK

- member of Editorial Advisory Board, The Open Nanomedicine Journal
- referee of scientific journals: Physical Review Letters, Physical Review B etc.
- członek Redakcyjnego Komitetu doradczego czasopisma The Open Nanomedicine Journal

J. ADAMOWSKI

- director of Interdisciplinary PhD Study
- member of the Programme Committee of the Laboratory for Physical Fundamentals of Information Processing
- member of the Physics Committee of the Polish Academy of Sciences
- kierownik Interdyscyplinarnych Studiów Doktoranckich
- członek Rady Programowej Laboratorium Fizycznych Podstaw Przetwarzania Informacji
- członek Komitetu Fizyki PAN (2008-2010)

B. SZAFRAN

- coordinator of Krakow Interdisciplinary PhD Programme in Nanoscience and Advanced Nanostructures,
- editor in Central European Journal of Physics
- koordynator programu Krakow Interdisciplinary PhD Programme in Nanoscience and Advanced Nanostructures finansowanego za pośrednictwem Fundacji na rzecz Nauki Polskiej z funduszy strukturalnych
- edytor w Central European Journal of Physics
- recenzent we wszystkich znanych czasopismach z zakresu fizyki ciała stałego oraz w Physical Review Letters oraz w Nanotechnology
Z. KĄKOL
- Vice Rector for Education
- Member of Jury of the Małopolska Grant Foundation „Sapere Auo”
- Member of Board of the Zielinscy Foundation of Educational Help for Young People
- Member of Jury of the Prize of Prof. Takiński
- President of the Board of the Foundation of Students and Alumni AGH ACADEMICA

K. KUŁAKOWSKI
- Coordinator of session Soft Magnetic Materials at the Joint European Magnetic Symposia, August 23-28, 2010, Cracow, Poland
- Member of the Scientific Committee, 5th Polish Symposium of Econo- and Sociophysics, November 25-27, 2010, Warsaw, Poland

K. MALARZ
- Managing Editor, Central European Journal of Physics (since 2006)
- Member of the Scientific Council of Polish Conferences on Computer Games Engineering (since 2005)
- Deputy dean of the Faculty of Physics and Applied Computer Sciences, AGH-UST (since 2005)
- Member of the Audtorial Commission for Section of Physics in Economy and Social Sciences, Polish Physical Society (since 2009)

K. SAEED
- Editor-in-Chief of International Journal on Computer Information Systems and Industrial Management Applications (since 2008), Publishers: MIR Labs, USA
- Conference General Chair, ICBAKE 2009 – International Multi-Conference on Biometrics and Kansel Engineering, June 25-28, Cieszyn, Poland
- Conference General Chair, CISIM 2010, October 8-10, Cracow, Poland
- IEEE Computer Society Senior Member (Member since 1994); 2011-2013 nominated for IEEE CS DVP Distinguished Visitor Program

J. SPALEK
- Member of the Science Council, Ministry of Science and Higher Education for the period 2008-11
Department of Particle Interaction and Detection Techniques
Katedra Oddziaływań i Detekcji Cząstek

STAFF

HEAD

prof. dr hab. Kisielewska Danuta, full professor

ELEMENTARY PARTICLES PHYSICS GROUP
ZESPÓŁ FIZYKI CZĄSTEK ELEMENTARNYCH

prof. dr hab. Kisielewska Danuta, full professor
prof. dr hab. Muryn Bogdan, full professor
dr inż. Przybycień Mariusz, associate professor
dr inż. Adamczyk Leszek, assistant professor
dr inż. Bold Tomasz, assistant professor
dr inż. Grabowska-Bold Iwona, assistant professor
dr inż. Obląkowska-Mucha Agnieszka, assistant professor
dr inż. Szumlak Tomasz, assistant professor
dr Szuba Janusz, teaching assistant
dr inż. Ciba Krzysztof

NUCLEAR ELECTRONICS AND RADIATION DETECTION GROUP
ZESPÓŁ ELEKTRONIKI JĄDROWEJ I DETEKCOJI PROMIENIOWANIA

prof. dr hab. inż. Dąbrowski Władysław, full professor
dr hab. inż. Idzik Marek, assistant professor
prof. dr hab. Jeleń Kazimierz, full professor
dr inż. Flutowski Tomasz, assistant professor
dr inż. Hottowy Paweł, assistant professor
dr inż. Kowański Tadeusz, assistant professor
dr inż. Mindur Bartosz, assistant professor
dr inż. Skoczeń Andrzej, assistant professor
dr inż. Wiącek Piotr, assistant professor
mgr Aguilar Jonathan, research assistant
mgr Ambalathankandy Prasoon, research assistant
mgr Imran Ahmed Mohammed, research assistant
mgr Koperny Stefan, teaching assistant
mgr inż. Dwużnik Michał, research assistant
mgr inż. Prochal Bogusław
inż. Terlecki Przemysław
Filipek Wiesław
Jędrzejowski Franciszek
Pieron Jacek
Tora Tadeusz
PROFILE

The scientific activity of Department cover three areas of research:
- basic research of elementary constituents of the matter and their interactions in high energy collisions
- design and construction of detectors and readout electronics for high energy physics experiments,
- development of detectors and readout electronics for neuroscience experiments and medical imaging.

The high energy experiments are long term projects and because of high cost of large accelerators and detection facilities they are performed by large international collaborations. Our participation in experiments is as complete as possible and covers all phases of the projects: preparations of the research programs, design and construction of the experimental apparatus, data analyses as well as maintaining and upgrading detector systems.

Currently we participate in analysis of data from three experiments, which have finished data taking:
- ZEUS e+e- at HERA (DESY),
- DELPHI e+e- at LEP (CERN),
- OPAL e+e- at LEP (CERN).

Over last decade have contributed to design and construction of two new experiments:
- ATLAS pp and Pb-Pb at LHC (CERN),
- LHCb pp at LHC (CERN),
and in 2010 we started running these two experiments and we participated in data analysis.

A special attention is paid to processes leading to a New Physics, particularly to Higgs and supersymmetric particles discoveries in ATLAS experiment. Study of the CP symmetry breaking in LHCb experiment could explain matter – antimatter asymmetry as well as search for rare decays of the beauty B mesons can also be a link to New Physics.

In parallel, we carry out R&D programs aiming at development of the detector concepts and new detector technologies for an upgrade of the ATLAS experiment and for a future experiment at the International Linear Collider.

The activity in the area of detectors and front-end electronics focuses on development of readout systems for position sensitive detectors employing Application Specific Integrated Circuits. We carry out development of readout ASICs for the following detector technologies:
- tracking detectors for high energy physics experiments based on silicon microstrip detectors,
- detectors for X-ray imaging based on silicon microstrip detectors,
- detectors for charge particles and X-ray imaging based on Gas Electron Multipliers (GEM).

Tematyka naukowa Katedry obejmuje trzy kierunki badań:
- badania podstawowe elementarnych składników materii i ich oddziaływania metodą zderzeń wysokoenergetycznych wiązek,
- rozwój detektorów i aparatury elektronicznej dla eksperymentów fizyki wysokoenergetycznych,
- projektowanie i budowę detektorów i aparatury elektronicznej dla eksperymentów neurobiologicznych oraz dla obrazowania medycznego.

Eksperymenty wysokoenergetyczne są projektami długofalowymi, a budowa akceleratorów i aparatury detekcyjnej wymaga dużych nakładów finansowych prace z dziedziny fizyki cząstek elementarnych mogą być prowadzone tylko w ramach dużych międzynarodowych zespołów. Nasz udział w eksperymentach obejmuje wszystkie ich fazy od przygotowania programu fizycznego poprzez projektowanie i budowę elementów aparatury detekcyjnej, jej obsługa i modernizację, po analizie danych.

Zespół pracowników Katedry uczestniczy w trzech eksperymentach, które zakończyły już zbieranie danych, ale analiza materiału doświadczalnego trwa nadal:
- ZEUS na akceleratorze e+p HERA w ośrodku DESY
- DELPHI na akceleratorze e+e-, LEP w CERN-ie
- OPAL na akceleratorze e+e-, LEP w CERN-ie

W ostatnim dziesięcioleciu uczestniczyliśmy w projektowaniu i budowie aparatury dla dwu nowych eksperymentów na akceleratorze LHC w CERN-ie:
- ATLAS – p+p i Pb-Pb
- LHCb – p+p

a od 2010 roku po uruchomieniu akceleratora LHC uczestniczymy w procesie zbierania i analizy danych. Specjalną uwagę zwraca się na bezpośrednie odkrycie obiektów związanych z tzw. Nową Fizyką. Poszukiwanie cząstki Higgsa oraz cząstek supersymetrycznych jest priorytetowym zadaniem eksperymentu ATLAS. Z kolei badanie stopnia łamania symetrii CP oraz rzadkich rozpadów w eksperymentie LHCb może również prowadzić do odkrycia Nowej Fizyki i być może wyjaśniać głębokiej asymetrii pomiędzy materią a antymaterią.

Równolegle prowadzone są prace projektowe w celu zastosowania nowych technologii detektorowych dla przyszłej modernizacji detekta ATLAS oraz przygotowania aparatury detekcyjnej dla eksperymentu na akceleratorze liniowym ILC.

Działalność w dziedzinie detektorów i systemów elektroniki odczytu koncentruje się na rozwoju systemów odczytu detektorów pozycji-czułych z wykorzystaniem techniki specjalizowanych układów scalonych.
I parallel, investigation of radiation effects in semiconductor devices and circuits is carried out, which are of primary importance in the front-end electronics for readout of silicon strip detectors in the high energy physics experiments. In the area of neuroscience we develop systems for imaging of neural activity in live neural tissues, including retina and cortex. A common aim of various research projects carried out in collaboration with neuro-scientists is to develop two ways communication between live neurons and electronic circuits.

ACHIEVEMENTS

- Participation in a QCD analysis of ZEUS diffractive data (published in Nuclear Physics),
- Participation in combined measurements of ZEUS and H1 experiments and QCD analysis of the inclusive $e^+p$ scattering cross section which determines a new set of parton distributions functions (published in Journal of High Energy Physics),
- Participation in the first direct observation of a phenomenon known as “jet quenching” made by ATLAS collaboration, which may be a sign of strong interactions between jets and a hot dense medium (quark-gluon plasma) formed by the colliding ions Pb-Pb. (published in Physical Review Letters),
- Work on the Electron Structure Function in DELPHI experiment,
- Searches for New Physics in rare B semileptonic decays in the LHCb experiment,
- Preparation of the software for the calibration and data analysis for VELO detector in LHCb experiment,
- Reconstruction of functional connectivity in retina at the resolution of photoreceptors (published in Nature),
- Development of position sensitive X-ray detector for diffraction instrumentation (published in Nuclear Instruments and Methods A),
- Udział w analizie procesów dyfrakcyjnych obserwowanych w eksperyencie ZEUS, opisywanych przez QCD (praca opublikowana w Nuclear Physics),
- Udział w pomiarach inkluzywnych przekrojów czynnych w rozpraszaniu $e^+p$ przy użyciu połączonych danych z eksperymentów ZEUS i H1 na akceleratorze HERA i wyznaczenie w analizie QCD nowych rozkładów gęstości partonów (praca opublikowana Journal of High Energy Physics),
- Udział w pierwszej bezpośredniej obserwacji dokonanej przez kolarację ATLAS zjawiska zwanej „jet quenching”, które jest sygnaturą powstania plazmy kwarkowo-gluonowej w zderzeniach jonów Pb-Pb (praca opublikowana w Physical Review Letters),
- Praca nad wyznaczeniem Funkcji Struktury Elektronu w głęboko nieelastycznych oddziaływaniach w eksperyencie DELPHI,
- Poszukiwanie procesów związanych z tzw. Nową Fizyką poprzez badanie rzadkich półleptonowych rozpadów mezongów $B$ w eksperyencie LHCb,
- Opracowanie oprogramowania służącego do kalibracji i analizy danych detektora wierzchołka VELO w eksperyencie LHCb,

• Rekonstrukcja połączeń funkcjonalnych w siatkówce z rozdzielczością odpowiadającą indywidualnym fotoreceptorom (praca opublikowana w Nature)

• Opracowanie detektoru promieniowania X do zastosowań w dyfraktometrii (praca opublikowana w Nuclear Instruments and Methods A)

• Opracowanie scalonego wielokanałowego przetwornika analogowo-cyfrowego (praca opublikowana w Journal of Instrumentation)

ACTIVITY

K. JELEŃ

• Head of AGH Centre of Energy Studies (from 2009)
• Member of Scientific Council of the Henryk Niewodniczański Institute of Nuclear Physics
• Polish Academy of Sciences (2008-2011)
• Member of Scientific Council of the Institute of Atomic Energy POLATOM (2008-2011)
• Chairmen of Scientific Council of Małopolska & Podkarpackie Clean Energy Cluster (from 2009)
• Member of Council for Atomic Energy Matters of National Atomic Energy Agency (2009-2012)
• Member of Monitoring Committee EURATOM Fission – National Contact Point.
• Member of the Council of the National Centre for Research and Development (2010-2012)

D. KISIELEWSKA

• Member of the Physics Committee of III Department of Polish Academy of Sciences (2007-2010)
• Member of Scientific Council of The Henryk Niewodniczański Institute of Nuclear Physics
• Polish Academy of Sciences (2008-2011)
• Member of Scientific Council of The Andrzej Sołtan Institute for Nuclear Studies (2008-2011)
• Member of Central Committee of the Scientific Degrees (2007-2010)
• Member of Collaboration Board of the ATLAS Collaboration at CERN

• Member of the Physics Committee of III Department of Polish Academy of Sciences (2007-2010)
• Member of Scientific Council of The Henryk Niewodniczański Institute of Nuclear Physics
• Polish Academy of Sciences (2008-2011)
• Member of Scientific Council of The Andrzej Sołtan Institute for Nuclear Studies (2008-2011)
• Member of Central Committee of the Scientific Degrees (2007-2010)
• Member of Collaboration Board of the ATLAS Collaboration at CERN
W. DĄBROWSKI

- Member of the Consortium Council of the National Centre for Hadron Radiotherapy.
- Member of the editorial board of the Journal of Instrumentation.
- Member of the editorial board of the Nukleonika journal

M. PRZYBYCIEŃ

- Member of the Organizing Committee of the Workshop of Timing Detectors (Electronics, Medical and Particle Physics Applications) November 29 – December 1 2010, Krakow, Poland.

B. MURYN

- Member of Collaboration Board of the LHCb experiment at CERN.

T. SZUMLAK

- Honorary Fellowship position with School of Physics and Astronomy - University of Glasgow.
- The LHCb VELO Software and Calibration Project leader.

M. IDZIK

- Technical Coordinator of FCAL (International Collaboration for Forward Detectors in future Linear Collider ILC/CLIC).

Członek Rady Zarządzającej Narodowego Centrum Radioterapii Hadronowej
Członek komitetu redakcyjnego czasopisma Journal of Instrumentation
Członek komitetu redakcyjnego czasopisma Nukleonika

Członek Komitetu Organizacyjnego „Workshop of Timing Detectors (Electronics, Medical and Particle Physics Applications)” 29.11.2010 - 1.12. 2010, Krakow

Członek Komitetu Fizyki Wysokich Energii Państwowej Rady Atomistyki (2008-2011)
Członek Komitetu Współpracy Eksperymentu LHCb w CERN-ie.

Honorowy członek kolegium Szkoły Fizyki i Astronomii Uniwersytetu w Glasgow
Koordynator grup oprogramowania i kalibracji detektora VELO w eksperyencie LHCb

Koordynator techniczny międzynarodowej współpracy FCAL (Forward Detectors in Future Linear Colliders ILC/CLIC)
Department of Applied Nuclear Physics
Katedra Zastosowań Fizyki Jądrowej

STAFF

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ZESPÓŁ FIZYKI MATERIAŁÓW FUNKCJONALNYCH

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ZESPÓŁ FIZYKI ŚRODOWISKA

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dr inż. Nęcki Jarosław, assistant professor
dr inż. Nguyen Dinh Chau, assistant professor
dr inż. Przybyłowicz Wojciech, assistant professor
dr inż. Rosieł Janusz, assistant professor
dr inż. Wachniew Przemysław, assistant professor
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Pach Franciszek
Wróblewski Ryszard

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ZESPÓŁ METOD JĄDROWYCH

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dr Bolewski Andrzej, assistant professor
dr inż. Ciechanowski Marek, assistant professor
dr Czapiński Wilhelm, assistant professor
dr inż. Petryka Leszek, assistant professor
dr hab. inż. Markowicz Andrzej, associate professor
Department Applied Nuclear Physics (DANP) is composed of three groups: (i) Environmental Physics Group, (ii) Nuclear Methods Group, and (iii) Functional Materials Group. Research activities of DANP cover selected topics of nuclear physics and its applications in areas such as environmental sciences, material sciences as well as industrial applications of nuclear methodologies. Moreover, DANP is responsible for two specializations being thought in the framework of the Technical Physics discipline offered by the Faculty at B.Sc. and M.Sc. level.

Major instrumentation available at DANP:
- an arc melting system with contact-less ignition for synthesis of materials,
- a system for production of monocrystals using Czochralski method,
- a system to measure magnetoelectric effect of materials,
- electrolytic enrichment system for low-level tritium assay in natural waters,
- analytical systems for determination of trace gases in the atmosphere,
- analytical systems for determination of stable isotope ratios of light elements (H, C, O, N) in environmental materials,
- liquid scintillation spectrometers for measurements of low-level activities of selected radionuclides (3H, 14C, 90Sr, 210Pb, 222Rn, isotopes of uranium, thorium and radium) in environmental materials,
- low-level gamma spectrometry for measurements of low-level activities of selected radionuclides in environmental materials,
- Analytical set-up for measuring neutron parameters of materials.

Katedra Zastosowań Fizyki Jądrowej składa się z trzech zespołów badawczych: (i) Zespołu Fizyki Środowiska, (ii) Zespołu Metod Jądrowych oraz (iii) Zespołu Fizyki Materiałów Funkcjonalnych. Badania naukowe prowadzone w Katedrze obejmują wybrane zagadnienia fizyki jądrowej w kontekście jej zastosowań takich jak nauki o środowisku, nauki o materiałach, a także przemysłowe aplikacje metod jądrowych. Katedra i jej zespół sprawuje opiekę merytoryczną nad dwoma specjalnościami nauczycielskimi na studiach drugiego stopnia Wydziału, a poprzedzonymi analogicznymi kierunkami dyplomowania na studiach pierwszego stopnia.

Ważniejsza aparatura naukowa będąca w posiadaniu Katedry:
- układ do syntezy materiałów w łuku elektrycznym;
- aparatura do otrzymywania monokryształów metodą Czochralskiego;
- aparatura do pomiaru efektu magnetoelektrycznego w materiałach;
- aparatura do elektrolitycznego wzbogacania prób wody w tryt;
- systemy analityczne do pomiaru gazów śladowych w atmosferze;
- systemy analityczne do pomiaru stosunków izotopowych pierwiastków lekkich (H, C, O, N) w różnych matrycach;
- system do pomiaru aktywności naturalnych i sztucznych nuklidów gamma-promieniotwórczych w próbkach stałych i ciekłych z wykorzystaniem spektrometrii gamma;
- spektrometria ciekło-scintylacyjne do pomiarów niskich aktywności izotopów promieniotwórczych (3H, 14C, 90Sr, 210Pb, 222Rn, izotopy uranu, toru i radu);
- stanowisko pomiarowe do pomiarów parametrów neutronowych materiałów.
ACHIEVEMENTS

- publication of a monograph entitled “Natural radioactivity of selected mineral waters in the Polish Carpathians;
- publication of a novel isotope method of palaeotemperature reconstructions based on oxygen isotope analyses of selected compounds of lake sediments;
- determination of the influence of 3d-electrons on the crystal structure, electrical and magnetic properties as well as hyperfine interactions observed in Terfenol-D type intermetallic compounds with Mn/Fe, Fe/Co, Fe/Ni or Co/Ni substitutions in the transition metal sublattice;
- set-up completion of the magnetoelectric effect measuring system;
- Preparation technology development and magnetoelectric effect measurements of PVDF/Tb0.27-Dy0.73-\((Y_{x+y}Fe)^2\) composites;
- publikacja monografii zatytułowanej “Promieniowoczość naturalna wybranych wód mineralnych Karpat Polskich”;
- opublikowanie oryginalnej metody określania palaeotemperatur na podstawie pomiaru składu izotopowego tlenu w wybranych składnikach osadów jeziornych;
- określenie wpływu elektronów 3d na strukturę krystaliczną, właściwości elektryczne, magnetyczne oraz oddziaływania nadsubtelne w związках międzymetalicznych typu Terfenol-D z podstawieniami Mn/Fe, Fe/Co, Fe/Ni i Co/Ni w podsieci metalu przejściowego;
- Ukończenie zestawienia oraz uruchomienie aparatury do pomiarów efektu magne-toelektrycznego;
- Opracowanie technologii otrzymywania oraz pomiary efektu magnetoelktrycznego w kompozycjach PVDF/Tb0.27\( \times \)Dy0.73\( \times \)Y\(_{x+y}\)Fe\(_2\).

ACTIVITY

K. RÓŻAŃSKI

- Member of the Council for Atomic Energy Matters of the National Atomic Energy Agency
- Member of the Polish National Committee, International Geosphere and Biosphere Programme of the International Council for Science
- Member of the Editorial Board of the journal “Isotopes in Environmental and Health Studies (since 2000)
- Vice-chairman of the Society of Research on Environmental Changes “GEOSPHERE”

A. KREFT

- Member of the Council for Atomic Energy Matters of the National Atomic Energy Agency
- Chairman of the Commission on Nuclear Techniques of the Council for Atomic Energy Matters
- Member of the Coordinator team of the Clean Energy Cluster
- Członek Rady d/s Atomistyki przy Państwowej Agencji Atomistyki
- Członek Polskiego Komitetu “Global Change” Międzynarodowego Programu Badań Geosfery i Biosfery, Międzynarodowego Komitetu Nauki
- Członek komitetu redakcyjnego czasopisma “Isotopes in Environmental and Health Studies (od 2000 roku)
- Vice-prezes Towarzystwa Badania Przemian Środowiska “GEOSFERA”

J. PSZCZOŁA

- Member of the Interfaculty Commission of Technical Sciences of the Polish Academy of Arts and Sciences
- Członek Rady d/s Atomistyki przy Państwowej Agencji Atomistyki
- Przewodniczący Komisji Techniki Jądrowej Rady d/s Atomistyki przy Państwowej Agencji Atomistyki
- Członek zespołu koordynującego Klaster Czystej Energii
- Członek Komisji Nauk Technicznych przy Polskiej Akademii Umiejętności
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<td>Brożek Marcin</td>
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<td>Ociejewa Magdalena</td>
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<td>Pajor Anna</td>
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<td>Ambalathankandy Prasoon</td>
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Selected results

Non-collinear magnetization structure at the thickness driven spin re-orientation transition in epitaxial Fe films on W(110)

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The bcc iron is known as an archetypal collinear ferromagnet. The deviations from this fundamental magnetic structure are expected for the ultrathin Fe films as a consequence of symmetry breaking at surfaces or interfaces as well as a magnetoelastic effects originating from the misfits between Fe film and the substrate. Recently, we showed that at certain conditions collinear ferromagnetism becomes less favorable then a spin spiral-like, vertically inhomogeneous magnetization state [1]. This happens at the spin reorientation transition (SRT) in Fe films grown on W(110). SRT in the case of Fe/W(110), consists in the switching of spontaneous magnetization during the film growth from the [1 T 0] to the [001] in-plane direction as the iron film approaches the critical thickness, d_c. Our thickness-induced SRT was monitored in-situ using grazing incidence nuclear resonant scattering (NRS) of synchrotron radiation [2]. The numerical analysis of the NRS data indicated that, a non-collinear magnetization structure is formed in the vicinity of the critical thickness, with a strong surface magnetization pinning along the [1 T 0] direction. With increasing thickness, the transition is initiated at the bottom atomic layers, neighboring with the tungsten substrate, and finally is completed at the surface layer. The measurements were done at the Nuclear Resonance beamline ID18 [3] at the ESRF. ⁵⁷Fe was evaporated on a freshly cleaned W(110). During the preparation, a set of the NRS time spectra was collected in thickness steps corresponding to a fraction of the Fe monolayer. The deposition of Fe was not interrupted from the beginning up to the completion of the SRT process, and the spectra were accumulated on-line during the film growth. The fitted time spectra are shown in Figure 1 for the selected Fe film thicknesses. A regular beat structure that is exemplified in Fig.1a reflects, according to the theoretical fits, the uniform magnetization state along the [1 T 0] direction, with the hyperfine magnetic field close to bulk Fe (B_H = 32.9 T). Such a state persists up to the thickness of about d = 51 Å. Similarly, the spectra for the coverages above 56 Å (see Fig.1f) can be easily fitted assuming a homogeneous magnetization but now parallel to the [001] direction. It is clear that the SRT process is not abrupt but extends over a relatively large thickness range of δ ~ 6 Å, corresponding to 3 ML. The most unique and also challenging to fit were the time spectra accumulated during the progress of SRT (Fig.1b-e). The two most commonly considered ways of the magnetization transition from [1 T 0] to [001]: (i) coherent rotation and (ii) coexistence of [001] and [1 T 0] magnetized domains, assuming a homogeneous magnetization depth profile across the Fe(110) films, produced distinctly different spectra, however, neither of them could satisfactorily fit the experimental data in the transition. The successful fits (Fig.1) could be obtained when the distribution of the magnetization directions was modeled by dividing the film with nominal thickness d into five equivalent sub-layers. For each sub-layer, an in-plane orientation of the hyperfine magnetic field (sublayer magnetization M_n) was defined by the angle φ_n with respect to the [1 T 0] in-plane direction. The orientation of the sub-layer magnetizations M_{1-5}, as derived from the analysis of the NRS data, is shown schematically in Fig.2 for the successive Fe thicknesses. The onset of the transition was noticed for the thickness of 51.6 Å. SRT from [1 T 0] to [001] is initiated at the deepest layers (neighboring the tungsten substrate), which switch first, while the magnetization of the remaining sub-layers forms a fan-like structure. With increasing thickness, the mag-
netization of the subsequent sub-layers rotates, and finally the transition is completed by the top-most surface layers. Our studies clearly show that non-collinear, exotic magnetic phase of epitaxial Fe films is stabilized at the vicinity of a critical SRT thickness. Such a magnetic structure resembles a planar domain wall with its center propagating towards the surface as the thickness increases.

![FIG.1 The time spectra accumulated during continuous Fe evaporation, labeled with the corresponding Fe thicknesses](image)

![FIG.2 The magnetization structure during the thickness-induced SRT for the Fe/W(110) system, as derived from the NRS measurements using a five sublayer model. The sublayer magnetization vectors are labeled as $\vec{M}_{1-5}$.](image)

REFERENCES

Magnetic axis switching phenomenon in magnetite: NMR Studies

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Magnetite is certainly one of the most fascinating materials ever found. The phenomenon strictly related to the Verwey transition is the switching of magnetic easy axis (axis switching, AS). Since the structure changes at $T_V$, each of high temperature cubic $h100$ directions may become the low temperature monoclinic c axis, doubled in comparison to the cubic lattice constant. As a result, the material breaks into several structural domains unless some external anisotropic factor, e.g. uniaxial stress, or a magnetic field $B > 0.2$ T is applied along particular $<h00>$ direction while cooling through the transition; this direction will then become both the unique c axis and also the magnetic easy axis. If now magnetite sample is magnetized along another direction of $<h00>$ type at temperatures lower than $T_V$, a reorientation of magnetic moments, i.e. easy axis switching, may take place and this direction becomes a new easy axis. We have recently proved that also crystallographic c axis is forced to this particular direction. This means the manipulation of structure is possible by the magnetic field and one would expect that also the charge ordering will follow. To prove it, the NMR measurements were undertaken [1], taking into account that these measurements can easily see all different iron positions, i.e. are the most sensitive probe to observe lattice distortion, charge and orbital order in magnetite below $T_V$.

The sample was the sphere of stoichiometric magnetite oriented with [001] axis vertical, parallel to the RF coil axis. External magnetic field, up to 1T, could be set horizontally and the sample could be rotated to allow all the directions in [001] zone to be examined. Only tetrahedral lines were checked what amounts to A iron nucleus being a probe for its nearest neighbors (B atoms) arrangement.

We have first field cooled the sample to 20K, which sets the c axis in the field direction (say [100]), establishing some atomic arrangement. Then the field of 0.3T was applied along [100] and the corresponding NMR signal for all A lines is shown on Fig. 1a. The field was then rotated such that it points in other cubic direction (Fig. 1b); since the field was small enough not to force AS, the NMR pattern reflects the different hyperfine field but with the same atomic arrangement as before. Axis switching was subsequently forced (with the field B=1.3T) after heating the sample to $T=80K$ just below $T_V$ and the sample was measured again in $B=0.3T$ and at $T=20K$, revealing the NMR pattern (Fig. 1c) almost identical to the original one. It thus looks as if all octahedral surroundings of the A atom we observe are, in relation to the field B direction, the same as before.

Finally, when the magnetic field axis was reverted to its initial direction and the whole procedure was repeated, the pattern almost came back to the one found before (Fig 1d-f). Cooling the sample in 1.3 T through the Verwey transition down to 57 K (the field was along [100] axis) and applying 0.5T field along [010] direction enabled the observation of axis switching dynamics (only lines $A_3-A_7$ were measured in order to obtain reasonable signal/noise ratio). It is apparent (see Fig. 2) that the electronic system evolved from that on Fig. 1b (the external field was slightly higher) to the one on Fig. 1c within approximately 20 hours.

The final conclusions of our studies is that not only lattice distortion, but also orbital and charge orders, were changed simultaneously after the application of external magnetic field.

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**Fig. 1.** Selected tetrahedral sites spectra revealing axis switching. Figures 1a, 1c and 1e correspond to external magnetic field (0.3T, T=20K) set along the easy axis (however c and d show the pattern after axis
switching) while in 13b, 13d and 13f the external field is perpendicular to the easy axis. Between b and c, and d and e, the sample was heated up to 80K and the field of 1.3T was applied to switch the easy axis. Scheme on right side describes the steps of the experiment.

Fig. 2. Axis switching dynamics observed by NMR (T=57K, B=0.5T)

REFERENCE:
Xanes study of poly(3,4-ethylenedioxytiophene) modified by iron hexacyanoferrate

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Hybrid materials consisting of electroactive polymers and redox inorganic compounds such as hexacyanometallates attract attention due to their potential use in electrocatalysis, energy conversion and storage devices as well as sensors or electrochemical capacitors. Thin films of such materials are capable of accumulating charge efficiently and exhibit high discharging current density. Iron hexacyanoferrate (Fe(CN)$_6$) is the most popular metal hexacyanometalate used as a dopant for modified electrodes with electroactive polymers.

Thin films of the materials were synthesized with electropolimerisation and the samples were characterised with ex-situ XPS and Raman spectroscopies as well as with AFM. The preparation procedure and the results of characterisation are described in [1]. Synthesis of organic–inorganic composite materials may cause direct interaction between both compounds, which can modify its properties. In order to determine local electronic and structural properties of the Fe sites which work an X-ray Absorption Near Edge Spectroscopy (XANES) study at the Fe K edge has been undertaken.

XANES spectra were collected at the ID26 beamline of the European Synchrotron Radiation Facility in Grenoble, France, using the undulator fundamental monochromated by a pair of Si(311) crystals. The Fe K fluorescence yield signal was acquired using a Si photodiode placed at 90° in horizontal scattering geometry in order to minimize the elastic contribution, while the sample surface was typically at 45° with respect to the direction of the incoming beam. All the measurements were performed at ambient conditions.

The theoretical modelling of XANES spectra was performed using FDMNES programme [2]. The calculations were performed on small clusters, up to the second next neighbours, using molecule mode calculations and dipole only contribution to the absorption spectra.

XANES provides the information about the valence state and coordination of the probed element in the material, which are reflected in the shape and energy of the absorption edge. The presence of different atoms in the coordination space of the probed element causes that the spectrum obtained is a sum of spectra of all surroundings of the probed element present in the sample. Thus, in the case of the Fe K-edge spectrum it is a sum of Fe(CN)$_6^{2-}$ and Fe(NC)$_6^{2-}$ for low- and high spin iron centre, respectively, and of FeS$_6$ if present, as XPS and Raman results suggest. Figure 1 shows XANES spectra of the materials studied. One can see that the shape of the spectrum for pEDOT/Fe(CN) and pEDOT/FeCN reveal common features.

Fig. 1. XANES spectra of the pEDOT/Fe(CN), pEDOT/FeCN films and Fe foil.

The shape of absorption edge - small pre-edge peak and distinct ‘white line’ - resembles that observed for materials with the iron atoms being coordinated by six ligands. It suggests the octahedral structure for the iron central atom. The edge energy at about 7123 eV, which indicates that both Fe$^{2+}$ and Fe$^{3+}$ ions are present in the studied materials. However, the spectral shapes for pEDOT/FeCN and pEDOT/Fe(CN) are not identical. The former spectrum is dominated by Fe-C bonds coming from hexacyanoferrate ions present in the material and acting as counterions for the positively charged polymer matrix as expected. The edge shape of the latter spectrum suggests a mixed neighbourhood of the central iron atom. This mixed neighbourhood is related to the presence of Fe-C and Fe-N.
bonding for low- and high spin iron centres. Thus, one can conclude that the Prussian Blue structure is present in the pEDOT/Fehcf material.

![Graph a) FeS₆](image)

![Graph b) FeS₄(CN)₂, FeS₃(CN)₃](image)

![Graph c) Fe(CN)₆, Fe(NC)₆](image)

Figure 2a-c) shows a theoretical simulation of the Fe K-edge XANES spectra for the FeS₆, FeS₄(CN)₂, FeS₃(CN)₃, Fe(CN)₆, and Fe(NC)₆ coordinations of the iron centre. The theoretical XANES spectrum obtained for FeS₆ (Fig. 2a) is more similar to pEDOT/Fehcf than to pEDOT/FeCN (Fig. 1). It may be caused by the fact that the curve of pEDOT/FeCN is dominated by the iron – cyanide coordination and the interaction Fe-S is very likely to be not visible. Nevertheless, one can see the similarity between pEDOT/Fehcf (Fig. 1) and FeS₆ (Fig. 2a) curves. The maximum of the peak at higher energies is flat in both cases. Thus, it is possible that there is some interaction between atoms within the polymer film. This interaction is very likely to originate from the Fe-S connection between iron atom from Prussian Blue and sulphur atom from the polymer chain.

It is difficult to conclude whether there is a mixed environment like FeS(CN) in the pEDOT/Fehcf film (see Fig. 2b). The energy for both mixed environments is the same which is in disagreement with experimental data (Fig. 1).

The theoretical spectra of Fe(CN)₆ and Fe(NC)₆ are similar to the experimental results. It suggests that the iron centre in the octahedral coordination is surrounded by six cyanide ligands. Thus, it also confirms that there are hexacyanoferrate species in pEDOT/FeCN and pEDOT/Fehcf materials. In the pEDOT/FeCN film iron atoms are bonded to carbon atoms of the cyanide groups whereas in the case of pEDOT/Fehcf, one may see, that iron is coordinated by both carbon and nitrogen atoms from cyanide group. Such a situation is typical for Prussian Blue compounds.

Summarising, formation of Prussian Blue type structure inside the polymer and the presence of iron (II) and iron (III) in the hybrid material has been confirmed. The XANES results show that the central metal atom is symmetrically coordinated by six ligands. This confirms the octahedral molecular geometry of the iron environments in the pEDOT/FeCN and pEDOT/Fehcf films.

Changes observed in the XANES spectra of pEDOT/Fe(CN)₆³⁻/⁴⁻ and pEDOT/Fehcf indicate that the formation of Fe-S proceeded during preparation of the hybrid material from the polymer with counter-ions. If some Fe(II)/Fe(III) species were not trapped by hexacyanoferrate(ferrite) counter-ions, iron might be chemically attracted to sulphur atoms from polymer without other ligands.

REFERENCES


Magnetic, magnetotransport and electronic properties of the La$_{0.67}$Ca$_{0.33}$Pb$_{0.33}$Mn$_{1-x}$Fe$_x$O$_3$ compounds

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A study of magnetic, electronic and electrical transport properties of Fe-doped colossal magnetoresistive manganese perovskites La$_{0.67}$Pb$_{0.33}$(Mn$_{1-x}$Fe$_x$)O$_3$ ($x = 0, 0.01, 0.03, 0.06, 0.10, 0.15$) and La$_{0.67}$Ca$_{0.33}$(Mn$_{1-x}$Fe$_x$)O$_3$ is presented. Polycrystalline compounds were prepared by the sol-gel low-temperature method [1].

The dc magnetization measured in the fields 50 Oe and 1 kOe and hysteresis loops up to 89 kOe were measured from 4 K up to 400 K.

**Figure 1.** Magnetisation as a function of applied magnetic field up to 89 kOe at 4 K for the (La$_{0.67}$Pb$_{0.33}$)(Mn$_{1-x}$Fe$_x$)O$_3$ compounds. The inset shows the saturation magnetisation values (filled circles) and the theoretical values (straight line).

Four-probe magnetoresistance measurements have been performed in the same temperature range at the applied magnetic fields up to 80 kOe.

**Figure 2.** Temperature dependences of the zero-field resistivity $\rho$ for (La$_{0.67}$Pb$_{0.33}$)(Mn$_{1-x}$Fe$_x$)O$_3$ compounds. Vertical arrows indicate the corresponding macroscopic Curie temperatures $T_C$.

**Figure 3.** Temperature dependences of the magnetoresistance $MR$ at different applied magnetic fields: (a) $H_f=0$ Oe, $H_{H}=10$ kOe, (b) $H_f=0$ Oe, $H_{H}=80$ kOe and (c) $H_f=10$ kOe, $H_{H}=80$ kOe for (La$_{0.67}$Pb$_{0.33}$)(Mn$_{1-x}$Fe$_x$)O$_3$ compounds with $x=0$, $0.01$, $0.03$, $0.06$ and $0.1$. 
Iron doping up to $x = 0.1$ does not change the crystal structure of parent compound and leads to very small expansion of the unit cell volume ($\pm 0.3\%$) but it suppresses locally the double exchange interaction. This causes a reduction of the saturation magnetic moment, an increase of the resistivity, as well as a decrease of the Curie ($T_C$) and metal-insulator ($T_{MI}$) transition temperatures.

Figure 4. The relationship between the iron composition, $x$, and the Curie temperature ($T_C$), the Curie-Weiss temperature ($\theta_{CW}$), the metal-insulator transition temperature ($T_{MI}$) for $(La_{0.67}Pb_{0.33})(Mn_{1-x}Fe_x)O_3$ compounds with $x = 0.00, 0.01, 0.03, 0.06$ and 0.1. Solid lines denote fitted straight lines. The dashed line is a guide for eye.

The $x=0.1$ compound exhibits the largest magnetoresistance effect of about 300% around its $T_{MI}$ temperature in the applied field of 80 kOe. The resistivity above $T_C$ for the compounds follows the thermally activated behaviour with the activation energy of about 0.12 eV.

Significantly larger values of the paramagnetic Curie-Weiss temperature $\theta_{CW}$ than the corresponding $T_C$ at larger $x$ are presumably related to increased microscopic inhomogeneity of the samples.

The temperature and magnetic field dependences of magnetoresistance of these polycrystalline compounds with small grain sizes are governed by the magnitudes of $T_{MI}$ and $T_C$ temperatures and their mutual relation. The increasing Fe content reduces the magnetization and increases the magnetoresistance. It is more effective in reinforcing “extrinsic” magnetoresistance than in affecting the “intrinsic” magnetoresistance. In all the compounds studied the “extrinsic” part of the electrical resistance plays a dominant role.

The $(La_{0.67}Ca_{0.33})(Mn_{1-x}Fe_x)O_3$ and $La_{0.67}Pb_{0.33}(Mn_{1-x}Fe_x)O_3 (x = 0, 0.01, 0.03, 0.06, 0.10, 0.15)$ samples were also studied with high resolution Mn K-edge XANES. The spectra of the samples and the reference oxides have been acquired in total K fluorescence yield using undulator fundamental monochromatized by a pair of Si (311) single crystals at the XAS-XES ID26 beamline of the ESRF, Grenoble. The spectra of all the samples reveal similar shape with a small, but significant gradual shift of the edge energy (Fig.1), which is attributed to Mn charge disproportion upon Fe substitution. A shift towards higher energy can be interpreted within the model of preferential Fe $3d^6$ configuration and gradual decrease of the average Mn $3d$ occupation upon substitution.

The shift by $\pm 0.25$ eV from $x = 0.0$ to $x = 0.15$ agrees well with the expected average valence change from Mn$^{3.33+}$ to Mn$^{3.45+}$, assuming linear relationship between edge position and Mn oxidation [3].

Photomission measurements were carried out by use of the angle resolved X-ray and ultraviolet XPS/ARUPS Omicron photoemission spectrometer. The XP spectra were measured for $x = 0, 0.08$ and 0.10 with the Al-K$_\alpha$ X-ray source with energy resolution about 1 eV at 300 K. Special attention was focused to the analysis of the Mn $2p$ core-level lines and the multiplet splitting (MS) of the lines was taken into account. It arises when, upon ejection of core electron, the angular momenta of the partially filled core shell can couple with the angular momenta of open atomic valence shell to form several multiplets of different energies [4]. The MS is expected to be observed if the specimen possesses unpaired electrons in its outer valence shells, e.g. for the ground-state configuration $2p^33d^2$ for Mn$^{3+}$ and $2p^33d^1$ for Mn$^{4+}$ ions. To analyse the MS of the Mn $2p$ core-level line we have adopted the results of the MS calculations for Mn$^{3+}$ and Mn$^{4+}$ ions presented in [4,5] in order to fit the Mn $2p_{3/2}$ spectra. The selected spectra and the fittings are shown in Fig.2.
Figure 2. The Mn $2p_{3/2}$ spectra and the fitting of four multiplet for each Mn$^{3+}$ $2p_{3/2}$ and Mn$^{4+}$ $2p_{3/2}$ ions according to the analysis in [4,5], as well as with the Pb 4$p_{3/2}$ line overlapping the Mn $2p_{3/2}$ lines. The XPS Peak program was used [6].

As the result of the fit the areas under the Mn$^{3+}$ and Mn$^{4+}$ lines were obtained and the ratio of Mn$^{3+}$/Mn$^{4+} = 1.9 \pm 0.2$ for La$_{0.67}$Ca$_{0.33}$(Mn$_{1-x}$Fe$_x$)O$_3$ ($x$=0.08) and 1.6 $\pm$ 0.2 for La$_{0.67}$Pb$_{0.33}$(Mn$_{1-x}$Fe$_x$)O$_3$ ($x$=0.10) were obtained. The ratios are in fair agreement with the expected values and with assumption that for $x$=0 the ratio is equal to 2.0.

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http://www.phy.cuhk.edu.hk/~surface/XPSPEAK
Neutron imaging of hydrogen storage systems.

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The possible applications of hydrogen as an energy carrier have caused intensive development of wide range of hydrogen-related applications. Today’s applications require efficient hydrogen storage systems of high safety level. As high-pressure hydrogen storage systems can be hardly accepted in transport applications (eg. cars) or even totally unsuitable for mobile electronic ones (eg. notebooks, robots) there is a need for developing low-pressure hydrogen storage systems of similar properties. Up to now, the metal-hydride (MH) based storage vessels are believed to be very promising in the future. However, there are significant drawbacks of the MH storage systems to be overcome. Namely, the weight ratio of stored hydrogen is about 2% of the total mass of the container. On the other hand, optimization of internal structure of the MH container should provide enhancement of heat dissipation from the active material as well as easy hydrogen access to whole volume of the material.

Neutron imaging techniques (radiography and tomography) are the only ones that give an insight into phenomena happening inside of MH storage container under its operation. The hydrogen is an excellent neutron attenuator while the common metals are quite transparent to neutrons. As the difference is of two orders of magnitude, a very strong contrast between hydrided and unhydrided active material can be expected. This special feature may be used for tracking of the hydrogenation kinetics during loading/unloading of MH storage container.

Fig. 1 Radiographic images of the investigated MH storage container.

In figure 1 a radiography image of aluminum MH storage tank filled with LaNi₅ alloy is presented. As one can see, interior structure of the tank and active material distribution is clearly visible. In figure 2 a reconstruction of hydrogen distribution in the investigated container is presented.
Hydrogen is not absorbed in the whole volume of the active material. Apparently, elevated concentration is visible at the interfaces. The upper surface of the powder, that is visible at depths between 0-3 mm, is almost completely saturated by hydrogen. When proceeding down, to bulk of the powder, the hydrogen concentration is lowered to the level of about 0.4 %wt. The high concentration of hydrogen is visible along the vessel’s walls, as well. This supports claims about crucially importance of heat transfer within the absorbing bed as well as between the bed and the walls.

It was shown, that neutron imaging techniques are a very good tool for in-situ studying of the hydrogen storage system. Neutron imaging is the only technique that gives a first-hand insight into phenomena happening inside storage vessel. It seems that a complementary investigation by means of radio- and tomography may be crucial for further development of efficient hydrogen storage. Especially, it allows optimization of the internal structure of such devices, by testing some details of its construction.
“Fingerprinting” of brain tumors based on the synchrotron radiation X-ray fluorescence and multiple discriminant analysis

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In recent years literature studies indicate an essential role of minor and trace elements in a number of pathological processes. Selected elements may contribute, directly or indirectly, on the carcinogenic process [1]. The elemental abnormalities, including these related to Zn, Cu, Fe, K, Rb, Mn, Se, Ca, in various forms of cancer were reported over the past decade [2-4]. However, the exact role of these and many other elements in carcinogenesis remains unknown. Molecular oncology is in need of the application of structural methods which are capable of monitoring biochemical processes and interactions within the neoplastic tissues. The recent development of microprobe beamlines of third generation synchrotron sources enables spatially resolved XRF (X-ray fluorescence) at cellular and subcellular levels.

A sort of “elemental fingerprinting” of brain tumors could provide a very useful tool assisting the process of diagnosing of tumors in difficult or disputable cases. In the present work it was verified if the multiple discriminant analysis of elements commonly found in brain tumor tissues can be used to differentiate neoplastic samples according to their histopathological classifications.

The samples designed to elemental micro-imaging were taken intraoperatively from brain tumors of different types i.e.: glioblastoma multiforme, gemistocytic astrocytoma, oligodendrogloma, anaplastic oligodendrogloma, ganglioglioma, fibrillary astrocytoma, atypical transitional meningioma. The investigation included also brain tissue apparently without malignant infiltration. In each case the samples were cryosectioned at 20 μm and freeze-dried.

The synchrotron radiation based XRF (SR-XRF) measurements were performed at the bending magnet beamline L at HASYLAB/DESY. The primary photon energy was set to 17 keV. The beam was focused to a size of 15 μm in diameter.

Multiple discriminant analysis (MDA) was applied to grouping and classification of brain tissue samples based on their elemental content. The SR-XRF technique revealed that the elements such as P, S, Cl, K, Ca, Fe, Cu, Zn, Br and Rb are present in all analyzed neoplastic tissues. The masses per unit area of elements from the representative region of each sample were used for further statistical analysis.

MDA allowed finding that S, Cl, Cu, Fe, K, Br and Zn are the elements of the highest importance for the general discrimination of tumor type. It seems justifiable to suppose that the abnormal reactions related with these elements are a source of the unique elemental fingerprint of different types of brain tumors. It is worth to mention that the possible role of these elements in oncogenetic processes has been previously reported [2-4].

Examining of the group discrimination was performed based on simple scatter plot between two discrimination variables (see Fig. 1). Eight clearly separated classes corresponding to the histopathological diagnosis of brain tumors and control sample were obtained.

The utility of the calculated canonical roots was examined via their ability to correct classification. The mean percent of correct prediction estimated according to the a posteriori probabilities procedure was 99.93%. Additionally, the leave-one-out method was used to evaluate the classification efficiency. The prediction ability of 95% was achieved. It suggests that the created elemental fingerprinting may be a very useful tool assisting the process of histopathological diagnosis of tumors especially in difficult or disputable cases. The MDA based on elemental composition of tissue may be a potentially valuable method assisting differentiation and/or classification (diagnosis) of brain tumors.
ACKNOWLEDGMENTS
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Figure 1. The scatterplot of observations in the space of discriminant variables for different types of brain tumors and control group (GM glioblastoma multiforme, AG – gemistocytic astrocytoma, C – control, OA – anaplastic oligodendroglioma, O – oligodendroglioma, G – ganglioglioma, M – meningioma, AF - fibrillary astrocytoma).
A. Non-heme iron in photosynthetic bacterial reaction centers of type II.
B. Analysis of iron compounds in functionalized multiwall carbon nanotubes.

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A. Non-heme iron (NHFe) is a conservative component of type II photosynthetic reaction centers (RC) of unknown function. NHFe is localized between the two ubiquinones (QA and QB) sites on the acceptor side of RCs. The temperature dependence of electron transfer (ET) steps and the role of NHFe in photosynthetic charge separation are among the most challenging issues. Intriguingly, QA in RCs from various organisms remains fully active at cryogenic temperatures whereas ET from reduced QA to QB slows down at temperatures below 200±20 K. It is not clear whether NHFe plays any structural role in stabilization of the QA and QB binding sites and/or it is actively involved in the primary ET. These problems prompted us to investigate in detail the properties of NHFe in RCs from two different species of purple photosynthetic bacteria, *Rh. sphaeroides* and *Rs. rubrum*. In order to compare the valence and spin states as well as dynamic properties of NHFe in these two RCs and to monitor the collective motions in the NHFe-binding sites we have applied highly selective techniques, i.e. Mössbauer spectroscopy and the nuclear inelastic absorption of synchrotron radiation (NIS), respectively.

![Mössbauer spectra of reaction centers from *Rh. sphaeroides* (A) and *Rs. rubrum* (B), measured at T=83 K. Density of vibrational states ρ(E) in the reaction centers from *Rh. sphaeroides* and *Rs. rubrum*, measured at 60 K, are shown in (C). Figures adapted from [1].](image-url)
Our results show that in the chromatophores as well as in RCs isolated from *Rs. rubrum* NHFe exists mainly in the low spin (LS) state whereas in those from *Rb. sphaeroides* an almost equal contribution of its HS (high spin) and LS state is observed (Fig. 1A and B). The temperature dependent Mössbauer measurements show that the two spin states of ferrous NHFe are characterized by different Debye temperatures (~165 K and ~207 K for the HS and LS state, respectively). Furthermore, NIS measurements of the collective motions in the *Rb. sphaeroides* reaction center show that the density of vibrational states, originating from non-heme iron, has well-separated modes between lower (4–17 meV) and higher (17–25 meV) energies while in the one from *Rs. rubrum* its distribution is more uniform with only little contribution of low energy (< 6 meV) vibrations (Fig. 1C). It is the first experimental evidence that the fluctuations of the protein matrix in type II reaction center are correlated to the NHFe spin state. We propose a simple mechanism in which the spin state NHFe directly determines the strength of coupling between the two quinone acceptors, Q$_A$ and Q$_B$.

B. Carbon nanotubes are the nanocylindrical forms of pure sp2 carbon which can be imagined as the plane of graphene rolled into different kinds of cylinders (Fig. 2A). The unique carbon nanotubes structures result in numerous superior physical and chemical properties. Synthesis, even using the same method, leads to production of a mixture of various types of carbon nanotubes exhibiting different features. We studied iron compounds included in non-functionalized (as prepared) and functionalized multiwall carbon nanotubes (MWCNTs) using Mössbauer spectroscopy (Fig.2B). In the as prepared MWCNTs the Fe$_3$C carbide has the main contribution but its content decreases by about 20 % and 40 % in carboxylated carbon nanotubes (MWCNTs-COOH) and ammonium salt of carboxylated carbon nanotubes (MWCNTs-COONH$_4$), respectively. A small amount of α-Fe and Fe$_x$C$_y$ iron forms are always observed in all studied carbon nanotubes. In MWCNTs-COOH, additionally, ferrihydrates and/or Fe$_x$C$_y$ with oxygen in the second coordination sphere of iron are present (at the level of about 17%). In MWCNTs-COONH$_4$ their content increase by a factor of 3. The experimental data shows that purification and functionalization of as prepared MWCNTs result in removal of about 90% of iron contaminations. All these results are important to optimize the as prepared MWCNTs purification process and to find a new way to produce different Fe phases inside MWCNTs.

Fig. 2. (A) TEM image of MWCNTs-COOH. The arrows indicate localization of iron clusters. (B) Example Mössbauer spectrum of MWCNTs-COONH$_4$ measured at 80 K. Figures adapted from [2].

REFERENCES


Application of the adaptive Weight Smoothing Algorithm and The Wavelet Transform for the Noise Reduction in MRI

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INTRODUCTION
Finding the best way of the SNR improvement in MRI is a key problem of the image quality correction. The Adaptive Weight Smoothing algorithm [1] and the wavelet transformation method were examined to test their application to improve the MRI images. Both methods were implemented in the MATLAB environment.

ALGORITHMS DESCRIPTION
Adaptive Weight Smoothing requires two input parameters: $\lambda$ (power of image smoothing in each iteration step) and $h_{max}$ which describes the maximum pixel surrounding. In each iteration step for every pixel, intensities of surrounding pixels are modified by the sets of weights. In each next iteration step $h$ value is increased. The set of weights depends on the difference in the intensities of pixels in previous steps controlled by the parameter $\lambda$. In the next step the images are merged. It is based on weighted summation of three images: $\alpha$ – input image with the high noise level $\beta$ – image processed with the low $\lambda$ value and $\gamma$ – image processed with the high $\lambda$ value. In result the image with improved quality is expected.

In wavelet transform a set of two functions is needed: the wavelet function (responsible for high pass filtration and keeping the signal details) and the scaling function (responsible for low pass filtration). To apply the wavelet transformation the numerical method called the Discrete Wavelet Transform (DWT) is used. Signal is processed in the series of filters. It is decomposed into two subsignals representing low and high frequencies. Subsignal (subimage) which contains low frequencies represents the input signal’s approximation. Subsignal which contains high frequencies represents image details. Only subsignal with high frequencies is sampled again for new approximation. In each sampling step the detail coefficients are expressed by the Wavelet Transform coefficients, and the approximation coefficients are expressed by scaling function coefficients. A method of calculating the scaling function coefficients and the wavelet function coefficients in case of the two-dimensional signals is called Mallat’s algorithm. This method decomposes an input image into four component subimages – representing the image’s approximation, vertical, horizontal, and diagonal edges. This method allows for an implementation of the multi-level resolution.

RESULTS
Application of the AWS algorithm
Based on the AWS algorithm the program dedicated to the MRI application was written. The Figure 1 illustrates the AWS algorithm functioning. In the beginning for an image choosen for the noise removing, the $\lambda$ and $h_{max}$ parameter values are defined. After the 1st iteration the image is smoothed and the noise is partly reduced. In subsequent iterations smoothing and noise reduction effects are stronger. Basing only on the visual evaluation it is advisable to terminate the algorithm after the 3rd or the 4th iteration. Finding the best, but not to high $\lambda$ value is needed to prevent too strong image smoothing.

Application of the DWT algorithm
After image loading to Matlab wavelet Toolbox it is possible to choose denoising parameters. For the selected wavelet function the iterations are proceeded (as described above). When the denoising effect is satisfactory, image is reconstructed by using the Inverse Discrete Wavelet Transform (IDWT). In the case of MRI, the best effects are achieved using the biorthogonal wavelets.

The SNR and the CNR
The Signal to Noise Ratio (SNR) is defined as:

$$SNR = \frac{\mu}{\sigma}$$

where:
- $\mu$ – the mean signal
- $\sigma$ – the noise standard deviation (the background standard deviation)

The Contrast to Noise Ratio (CNR) describing the signal difference between two structures (for example two tissues) is used to describe images according to the equation:

$$CNR = \frac{C}{\sigma} = \frac{S_A - S_B}{\sigma}$$

C means contrast, $S_A$ and $S_B$ are signal intensities for structures $A$ and $B$, $\sigma$ is a standard deviation of the background. The input image has the highest SNR, and noised image – the lowest. For the AWS algorithm in each noise reducing iteration SNR and CNR increase. In each successive iteration the image is brighter and more smoothed. The same SNR and CNR analysis was applied in case of the DWT to...
choose the best wavelet family for the MRI applications. The images with the highest SNR value were received after using biorthogonal 4.4 wavelet type (SNR=6.446,CNR=1).

**Detection of edges**
A simple edge detection algorithm was used. After its application for the noiseless image, all the anatomical edges were sharpened. Using the same method for noised image shows a big number of the false edges. The image is unreadable and diagnostically useless. After the AWS filtration all the redundant edges were removed but the edges became diffused (significant disadvantage). The DWT method detected all the needed edges, but also some of the false ones. The degree of redundant edges detection depends on wavelets family.

**SUMMARY AND CONCLUSIONS**
The application of the AWS method needs high time consumption because the weights are calculated for each pixel within the surrounding. The DWT algorithm allows shortening calculation time. However it does not remove all the false edges and requires bigger number of the input parameters. The AWS algorithm gives good visual effects (merging images). It keeps the edges, and the brightness of the average image slightly increases. The AWS algorithm can be applied to improve MRI images in the case of medium noise and low SNR. Application of the DWT increases image brightness and makes it more homogenous.

The presented results prove that the further application of the AWS and DWT methods to improve MRI images can be useful.

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Physical properties of the sigma-phase Fe-Cr and Fe-V alloys

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Fe-Cr and Fe-V alloy systems play important roles both in science and industry. The former stems from their treatment as model alloys, while the latter is caused by the fact that these alloys constitute basic ingredients in a steel making industry. Fe-Cr alloys are especially technologically significant as they are used in the production of a variety of stainless steels (SS) that thanks to their properties, like excellent high-temperature corrosion resistance, have been used as the most important structural materials in many strategic branches of industry e. g. power plants, oil refineries. Some properties of SS, like precipitation of a \( \sigma \)-phase, are inherited from the parent alloy. The \( \sigma \)-phase has a tetragonal structure (type D\(^{14}4h\), P4\(_2\)/mm) with 30 atoms distributed over five different sites – see Fig. 1. Its physical properties are, in general, quite different than those of the \( \alpha \)-phase of similar composition, from which the \( \sigma \)-phase precipitates. Some properties, like the magnetic ones, are even dramatically different [1], other properties, like the Debye temperature, seem to be very similar [2]. The latter is rather unexpected as the hardness of \( \alpha \) in the Fe-Cr system is by a factor of \( \sim 3 \) larger than that of \( \alpha \). A very complex crystallographic structure and a lack of stoichiometry make, on one hand, an interpretation of experimental results difficult and non-unique task, and on the other hand, it causes that theoretical calculations are tedious. Nevertheless, the latter can be very useful and helpful in a proper interpretation of experimental data [3].

Fig. 1 The unit cell of the \( \alpha \)-phase. Additionally, all five lattice sites A, B, C, D, E are shown with their nearest-neighbour (NN) shells.

Here we report both experimental and theoretical results obtained for the \( \alpha \)-phase in Fe-Cr and Fe-V alloy systems. Concerning the latter, using the Mössbauer spectroscopy, we have measured a series of spectra in a temperature range of 80–300 K on samples with vanadium content between 34.4 and 59 at%. From a temperature dependence of the centre shift and applying the Debye model, the Debye temperature, \( \Theta_D \), was determined [4]. Its compositional dependence is illustrated in Fig. 2, showing an interesting non-monotonous character.
Fig. 2 Debye temperature, $\Theta_D$, versus vanadium content, $x$, and the lattice constant, $a$, for $\sigma$-FeV alloys (circles) [4]. For comparison, the data obtained for the $\sigma$-FeCr alloys are added (triangles) [2].

The theoretical studies based on the charge- and spin-self-consistent Korringa-Kohn-Rostoker (KKR) method combined with a coherent potential approximation (CPA) one, were used to study the electronic structure of the $\sigma$-phase of paramagnetic Fe-V alloys [5] as well as magnetic properties of the $\sigma$-FeCr alloys [6]. Concerning the former, Fe-site charge-densities were calculated for each of the five sublattices as a function of Fe atoms situated in the NN-shell revealing a linear correlation. Based on these results, the average isomer shift was calculated and found to be in an excellent accord with the measured one. Finally, electric field gradients were determined theoretically for each lattice site. The calculated results were successfully used to analyze measured spectra.

For the $\sigma$-FeCr alloys, a magnetic structure was calculated. In particular, it was shown that the magnetic moments of Fe/Cr atoms occupying all five sites are proportional to the number of NN-Fe atoms, and the average magnetic moment per Fe atom is linearly correlated with the average NN-distance – see Fig. 3.

Fig. 3 Magnetic moments for five sublattices versus the number of NN-Fe atoms for (a) Fe and (c) Cr atoms. The correlation between the average Fe-moment and the average NN-shell distance is shown in (c) [6].

REFERENCES
Lattice rotation in plastic deformation models

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The deformation modeling of polycrystalline material plays an important role in material science [1]. The predicted deformation textures depend very strongly on the definition of crystal rotation. The rotation based on classical mechanics is commonly used. The other approach [2] is based on the condition of the preservation of some directions and/or planes of the sample with respect to the applied forces, i.e., to the laboratory reference frame.

Mechanisms of plastic deformation
Plastic deformation undergoes by non-reversible mechanisms such as crystallographic slip or (and) mechanical twinning. In slip and twinning processes, two parts of a crystal (or grain) are sheared one with respect to another. The crystallographic slip is schematically presented in Fig. 1. Neighbouring blocs of crystal are relatively displaced. This movement (i.e. slip) occurs on a slip plane \( n \): \((hkl)\) and along a slip direction \( m \): \([uvw]\). Due to crystal symmetries a family of equivalent slip systems \(<uvw>(hkl)\) exists.

Fig. 1. Displacement of the material during slip; \( m \) and \( n \) are slip direction and plane.

Mechanical twinning consists of shearing movements of consecutive atomic planes, which leads to the formation of a crystal region with the crystal lattice being a mirror image of the original crystal (matrix) – Fig. 2. In f.c.c. or b.c.c. metals deformed in room temperature slip is dominating mechanism [1].

Basic variables in deformation models
The basic equation in the deformation model defines the relation between macroscopic variables of the sample \((\Sigma_i, E_{ij})\) and local ones \((\sigma_{ij}, \epsilon_{ij})\) for a polycrystalline grain – Fig. 3.

Fig. 3. Applied external load \( \Sigma_{ij} \) creates a local stress \( \sigma_{ij} \) in a grain. Deformation of the sample is \( E_{ij} \) and that of a grain is \( \epsilon_{ij} \).

In our model [3,4] the following relation between a grain and the sample variables is used:

\[
\sigma_{ij} = \Sigma_{ij} + L(E^p_{ij} - E^m_{ij})
\]

It is convenient to define the slip system orientation factor: \( R_l = m \cdot n \), where \( m \) and \( n \) are unit vectors of slip direction and slip plane, respectively. If a grain is sheared of \( \Delta \gamma \) on a slip system, a grain deformation described by the displacement tensor \( \epsilon_{ij} \) is:

\[
\Delta \epsilon^p_{ij} = R_l \Delta \gamma
\]

In general, slip occurs on several slip systems (numbered by “s”) simultaneously, hence:

\[
\Delta \epsilon^p_{ij} = \sum_s R_s^i \Delta \gamma^s
\]

Plastic deformation tensor, is the symmetric part of \( \epsilon_{ij} \):

\[
\Delta \epsilon^m_{ij} = \frac{1}{2} \sum_s (R_s^i + R_s^j) \Delta \gamma^s
\]

The deformation of the sample is calculated as the average deformation of all grains.
Two definitions of lattice rotation

Due to the definition given by classical mechanics, the plastic rotation of a body (of a grain) is equal to the asymmetric part of $\Delta \mathbf{C}^{pl}$:

$$\Delta \alpha^{pl}_{ij} = \frac{1}{2} \sum_s (R^s_{ij} - R^s_{ji}) \Delta \gamma^s$$

$\Delta \alpha^{pl}_{ij}$ is a rigid body grain rotation produced by slip.

If there was not interaction between a grain and the matrix – crystal lattice orientation would not change (see Fig.4 a,b). However, some constraints are imposed on a grain by a neighbouring material and the deformation device. As a consequence, a compensating rotation $\Delta \alpha^{latt}_{ij}$ occurs and it changes the grain lattice orientation: $\Delta \alpha^{latt}_{ij} = - \Delta \alpha^{pl}_{ij}$

Therefore, in classical approach:

$$\Delta \alpha^{latt (class)}_{ij} = \frac{1}{2} \sum_s (R^s_{ij} - R^s_{ji}) \Delta \gamma^s$$

Crystal rotation can be also defined by the condition of preservation of some sample directions/planes with respect to the applied forces [5]. For example, in the tensile test of a single crystal presented in Fig.4, the direction defined by a tensile force (i.e., $x_3$) has to be preserved in the laboratory reference frame (it means that a string of material being initially parallel to the tensile direction has to preserve this orientation). Similarly, if one considers the rolling deformation (with $x_3$ as rolling direction and $x_5$ as normal direction), the orientations of rolling plane and direction have to be preserved in the laboratory reference frame. This leads to the following lattice rotation:

$$\Delta \alpha^{latt}_{21} = - \Delta \epsilon_{21} = - \sum_s R^s_{21} \Delta \gamma^s$$
$$\Delta \alpha^{latt}_{31} = - \Delta \epsilon_{31} = - \sum_s R^s_{31} \Delta \gamma^s$$
$$\Delta \alpha^{latt}_{32} = - \Delta \epsilon_{32} = - \sum_s R^s_{32} \Delta \gamma^s$$

Example of application

Rolling texture of polycrystalline $\alpha$-brass was predicted with two types of lattice rotations, i.e., based on the classical definition (DEF1 – Eq.6) and on the preservation condition (DEF2 – Eq.7). Taking grain-matrix interaction level L=100 MPa and <110>{111} slip systems, DEF2 leads to a texture close to the measured brass rolling texture, while DEF1 gives a wrong prediction – Fig.5.

Fig. 5. Predicted rolling textures using two definitions of rotations (L=100 MPa and <110>{111} slip systems were used) and predicted $\alpha$-brass texture

The presented results show that the lattice definition based on the preservation conditions should be taken into account in plastic deformation models. In many cases it gives better texture predictions, closer to experimental results.

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Properties of DNA complexes with new cationic surfactants

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Bio-derived materials possess uncommon properties that are virtually impossible to be mimicked in industrial organic or inorganic materials. Furthermore biomaterials are a renewable resource, often obtained from post-production wastes. Their nature provides inherent biodegradability. Among all available natural polymers, a range of outstanding properties are characteristics of the DNA (deoxyribonucleic acid). DNA is a long, thin, organic polymer, the rare macromolecule that represents the atomic scale in one dimension (the width equal to 2.37 nm) and the human scale in another (a molecule of DNA can be many centimetres long). A single DNA strand can be viewed as a polymer built of elementary bricks referred to as nucleotides. The nucleotides pair with each other in a complementary fashion. DNA multiplies through a natural process, running in living cells, known as DNA replication. The replication provides mono-dispersed molecular mass of a bulk DNA sample – a feature impossible to achieve for any of industrial polymers. Nowadays, technology enables DNA synthesis under a tailored composition at affordable prices. Even a single DNA strand can be artificially replicated using so-called PCR technique. It allows amplifying the initial amount of DNA millions of times in a few hours with exponentially rising yield. All this features make DNA extremely well defined material. The DNA double helix may be imagined as a tunnel of \( \pi-\pi^* \) stacking nucleic base pairs system available for charge migration. The relatively weak \( \pi-\pi^* \) electron conjugation renders material with a large optical transparency window. However, regarding the electrical charge transport there is still discussed whether the DNA belongs to the class of insulators, semiconductors, conductors or even superconductors of the transport in DNA molecules.

The extracted DNA is soluble exclusively in water and is very sensitive to hydration [1] what may substantially influence the final device performance. Fabrication of complex composed of a cationic surfactant and DNA results in material insoluble in water but retaining properties of the pristine DNA. Films of best quality were those fabricated form DNA complex with cetyltrimethylammonium (CTMA). Therefore the most extensive research has been devoted to DNA–CTMA for the last decade. Now, this complex is considered as a flagship of DNA derived materials for application in photonics [2] and molecular electronics [3]. Among “practical” solvents, DNA–CTMA is soluble only in some alcohols. That is why it is reasonable to pursue the quest for new cationic surfactants which would extend the range of possible solvents for resulting DNA complexes.

The most exploited form of DNA complexes in organic electronics are thin films. Up to date there has not been reported any report describing the kinetics of their formation. In frame of our work we applied X-ray diffraction to attack this problem. In addition we proposed two candidates competitive to CTMA regarding the solubility. Complexes of DNA with benzalkonium chloride (BA), didecyldimethylammonium chloride (DDCA) in addition to all solvents suitable for DNA–DDCA, were also soluble in a range of ketones and notably in chloroform. The surfactant molecule attaches its cationic head to negatively charged phosphate groups of DNA strand. In the case of CTMA aliphatic queue is supposed to stretch out. This queue hampers solubility in water and enhances in other solvents. Following such reasoning BA and DDCA surrounding DNA helix and possessing twice as much queues as CTMA does, would improve even better the solubility of DNA in less polar solvents.

DNA sodium salt, extracted from salmon milt and roe, was purchased from CIST (Chitose Institute of Science and Technology, Japan). Complexes were manufactured by ion exchange reaction. The diffraction data were collected in grazing incidence geometry. Experimental procedure was as follows. A microscope slide, was covered with a DNA or DNA complex solution and horizontally placed in the apparatus. A plastic hood was put over it to prevent too rapid drying. Film of pure DNA was amorphous. The others featured broad peaks. The intensities were dependent on a range of factors hard to control. In order to compare the results backgrounds were subtracted and signals normalized as in Fig. One can see there a shift of peaks maxima related to the surfactants nature. Peaks maxima in terms of distance between diffraction planes read as 32.5Å (DNA–CTMA), 29.8Å (DNA–BA) and 30.3Å (DNA–DDCA). The difference between DNA–BA and DNA–DDCA is in range of experimental uncertainty, but the value calculated for DNA–CTMA is clearly larger by 2Å. This fact may be attributed to longer CTMA alkyl queue (16 carbon atoms in contrast to 11 and 8). The creation of organized structure was a temporally dynamic process like it is illustrated in Fig. for DNA–CTMA complex structure. A similar behaviour was observed in the case of the two others DNA-surfactant complexes. Quantitative discussion of this phenomenon would be very risky unless the samples are prepared exactly in the same form and geometry and statistically convincing amount of data collected. Therefore the further analysis is only qualitative. As shown in mentioned above Fig. the whole transition process between amorphous and structured phases...
takes place between only two successive scans, recorded in 26 and 28 minutes. This suggests existence of a critical concentration of DNA-CTMA inducing spontaneous macromolecules organization. The transition must have been relatively rapid because the whole drying lasted for 60 minutes until the diffraction pattern evolution stopped (taking the same as registered 4 hours later). The visible shift of the peak maximum before final drying may account for initially adopted liquid crystalline – like structure by DNA-CTMA complex macromolecules. They align being still surrounded by the solvent molecules. Upon successive solvent removing they approach each to the other until the final state is reached.

The proposed here model is supported by dielectric and ellipsometric studies performed on such films and will be published elsewhere [4].

Fig. 1 DNA-CTMA. Drying process monitored on-line by X-ray diffraction. Region without structural features were skipped in the picture.

Fig. 2 Diffraction peaks after background subtraction and normalization.

REFERENCES
Spin accumulation and spin read-out without magnetic field.

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Many extensive efforts have been made recently to fabricate a nanodevice that performs quantum logical operations on the electron spin. In all nanodevices constructed for this purpose, manipulation of electron spins required an external magnetic field, which induces a continuous precession of spins of all the confined electrons. Recently, we proposed a couple of devices rotating the electron spins without the external magnetic field [1, 2]. We introduced an idea and simulated the operation of nanodevices that perform the single-qubit Haddamard, negation and phase change quantum gate operations.

In this work we propose and simulate operation of two nanodevices. One of them can be used to extract from the electron gas single electrons of a well defined spin state or to spin accumulation, i.e. storage of electrons of opposite spin orientations in two separate regions of the nanodevice. The second device serves for the spin read out. It performs a projective measurement which for a positive answer leaves the spin in the identified state. The spin read out has the “interaction free measurement” character since the electron whose state could be perturbed implies a negative answer to the question asked. The nanodevices work without the external magnetic field. Its operation is controlled by low DC voltages applied to gates.

The proposed device is based on a planar heterostructure similar to the one previously used in Ref. [1]. Nanostructure contains a quantum well 10 nm wide sandwiched between two barriers each of 10 nm width. The quantum well is separated from the substrate by a 50 nm thick undoped layer. On top of the upper blocking layer the metal electrodes are deposited. Electron confined in the quantum well forms a charge “cloud” distribution that induces an appearance of positive charge on the lower surface of the metal electrodes. The electric field stemming from the positive induced charge possesses an in-plane components directed to the center of the electron charge distribution. The wave function of the electron that is formed in this way becomes a stable packet that can move within the quantum well with a constant shape. When the self focusing effect is strong enough (the quantum well is close to the electrodes and the dielectric constant is not too large) the scattering properties of the wave packet become classical, i.e. the electron backscatters or transfers through a potential defect with a 0 or 100% probability. We perform a simulation of operation of nanodevices by iterative solving of the time-dependent Schrödinger equation for the single electron. In every time step electric field is calculated by numerical solving of the Poisson equation. Thanks to this, changes in the confinement potential, as a result of gates voltage changing, and the electron density movement in the quantum dot are taken into account.

![Fig. 1.](image)

FIG. 1. The system of electrodes in the nanodevice that filters out the electrons with spin that is not parallel to the z axis.

The trajectory of an electron that is put in motion within a quantum well, in which the Rashba spin-orbit coupling is present, depends on the direction of its spin. Only the electron whose spin is parallel or antiparallel to the z axis moves along a straight line that is parallel to the x axis. The Rashba coupling induces rotation of the electron spin moving along the x axis around the z axis, hence for both considered spin orientations they remain unchanged as the electron moves. However, when the electron wave function contains a contribution of any other spin component the electron trajectory is no longer a straight line. This effect can be used to filter out the electrons with spins that are not parallel to the z axis. This operation can be performed using the nanodevice presented in Fig. 1. The electron is initially confined under electrode e1 in the lowest energy state for a given spin orientation. Then, the voltage on electrodes e1 and e2 is lowered by 0.1 mV. The electron is ejected under electrode e3 and acquires a velocity parallel to the x axis. The width of e3 electrode and the distance to the lateral electrodes e4 and e5 is adjusted in a way that the center of the packet is localized under electrode e3 and the tails of the packet reach the lateral e4 and e5 electrodes. On electrodes e4 and e5 we put a voltage 0.1 mV higher than the one applied to the to e3.
FIG. 4: (a) Nanodevice for the spin accumulation. The system of electrodes (grey color) and electron trajectories of spin up (down) marked in red (blue). The trajectory is defined by mean positions of the electron packet. (b) Average spin and position of the electron following the trajectories depicted in (a).

Hence the straight motion is only weakly stabilized and any deviation of the electron direction leads to its extraction to one of the lateral electrodes. In consequence only electrons with spin parallel or antiparallel to the z axis cross the entire length of the electrode and follow the trajectory depicted in (a). Even a small admixture of the spin that is neither parallel nor antiparallel to the z axis leads to the electron escape to the area below the lateral electrodes. We use the idea of the spin filter of Fig. 1 for a larger nanodevice dedicated to spin accumulation [see Fig. 2(a)]. The spin filter is placed at the lower left corner of the plot. The electrons with spins parallel or antiparallel to the z axis pass through this filter and get to the area below the large electrode. The electron trajectory turns by 90 degrees upon reflection on a 45 degree cut of the electrode for x = 1300 nm. After the electrons trajectory is changed, the spin-up and spin-down electrons follow different trajectories: the spin-up electron is deflected to the left and the spin-down electron to the right [blue curve in Fig. 2(a)]. Figure 2(b) shows the time dependence of the mean values of the electron positions x(t) =< x >, z(t) =< z > and the mean value of the z component of the spin s_z(t) =< s_z >. The black solid curve shows z(t) which is the same for both initial spin orientations. The red (blue) curve shows x(t) for the spin oriented initially “up” (“down”). The x(t) curves overlap only at the first part of the trajectory when the electron moves ideally parallel to the z axis. The mean values of the spin s_z(t) are given in Fig. 2(b) by dashed red (blue) lines for the initial spin up (down) orientation. The electron spin undergoes precession when it follows a curved trajectory. Thus one needs to allow the electron to cross a distance equal to SO length (for the applied material parameters λ_SO = 1750 nm) after which the initial electron spin orientation is restored and the trajectory becomes parallel to the z axis again [see Figs. 4(a) and 4(b)]. Then, the electron is reflected for the second time from a properly cut top edge of the electrode. It starts to move parallel to the x axis and the spin precession is terminated. The electrons with spin oriented initially up get under electrode e8 (e7). The electrons can be stored therein, or taken away to other locations within the nanodevice.

FIG. 3: (a) Nanodevice for the spin read out and trajectories of electrons with spins initially oriented up (red curve) and down (blue curve). (b) Same as Fig. 4(a) only for the spin-up electron following the red trajectory in the spin read out device of (a).

Figure 3 contains a schematic drawing of a nanodevice which is supposed to read the electron spin after completion of a quantum computation.

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The line graphs are clustered and assortative [1,2]. They share these topological features with some social networks [3]. We argue that this similarity reveals the cliquish character of the social networks. In the model proposed here [4], a social network is the line graph of an initial network of families, communities, interest groups, school classes and small companies. These groups play the role of nodes, and individuals are represented by links between these nodes. The picture is supported by the data on the LiveJournal network of about 8 × 10^6 people. In particular, sharp maxima of the observed data of the degree dependence of the clustering coefficient C(k) are associated with cliques in the social network.

From a given graph G of N nodes and L links, a line graph G’ can be constructed as follows. A node of G’ is assigned to each link of G. Two nodes of G’ are linked if and only if the respective links in G shared a node. In this way, the number N’ of nodes in G’ is equal to the number L of links in G. The number L’ of links in G’ depends on the degree distribution P(k) in G. We have shown numerically in [1], that for three kinds of networks (Erdős-Renyi networks, the growing exponential networks and the growing scale-free networks) the degree distribution of G’ is close to the degree distribution of G. Basically, a node of degree k is converted to a clique (fully connected graph) of k nodes and k(k − 1)/2 links. Further, a link in G joining nodes of degrees k1 and k2 is converted into a node in G’ of degree k1 + k2 − 2 which belongs to two cliques, one of k1 nodes and another of k2 nodes.

LiveJournal is a remarkably popular platform for personal blog management, populated with over 8 million blogs and over 1 million of communities. LiveJournal was among the first of such platforms available online and it still remains one of the most active and popular. Its users manage personal blogs where they share their daily experiences, political views or discuss news events. Users can also comment on posts of other users. Unlike more dynamic systems like Facebook and Twitter that gained their popularity rather recently, LiveJournal is not based on personal messages or applications. Typical LiveJournal post may contain a significant amount of text with embedded images or video and may be followed by discussion that in times exceed thousands of comments.

The LiveJournal system encourages users to bookmark and monitor particular blogs. This feature is exercised by virtually all users and results in a network of references between these blogs. The vast majority of blogs regularly read by a person are typically stored in the form of bookmarks as part of his profile. This degree of penetration of this behavior is driven by two main reasons. First, its convenience: it is impractical to periodically search for a particular blog and check whether it has new posts. The system automatically notifies users of the updates to the bookmarked blogs. Second, to protect their privacy, many users limit visibility of their posts to the users listed in their list of friends. Overall, the personal nature of these blogs and the intimate relationship between their authors give this network a powerful social aspect. In fact, we conducted a large number of case studies analyzing the threads of comments to verify that authors of many of the connected blogs actually know each other in person. It is therefore legitimate to refer to the network of blog bookmarks as social network.

Suppose that a new medium of communication - LiveJournal - appears in a given social network of friends, acquaintances etc. We deduce from what was told above that the network can be described as a line graph L(G) constructed on a scale-free graph. It seems obvious that not all links of the social network L(G) are established in the frames of LiveJournal. In particular, the links of LiveJournal are directed, while those of the social network modelled as L(G) are undirected (or bidirectional). On the other hand, some links of LiveJournal do not exist in L(G). Having this in mind, we propose a qualitative reconstruction of the structure of LiveJournal from L(G). This reconstruction should fulfill two conditions: (i) the directionality of links, and (ii) the limitation of the number of outgoing links, which appears in the data of LiveJournal.

The reconstruction is made as follows: first, an uncorrelated scale-free network is constructed in the growing process, by the preferential attaching new nodes to old ones, each with M=5 links. The initial size of the scale-free network is 10000, then the size of the line graph is $N_S=50000$. This selection of N and M does not influence qualitatively the results. The line graph represents the structure of a social network, still undirected. Now we have to design a directed graph of contacts according to LiveJournal. We apply the rule: older blogs are observed by new blogs attached to them. According to the construction of the line graph, this condition can be kept only approximately, as the order of nodes of the initial scale-free graph does not
determines the order of nodes. At the last stage of the reconstruction, we check nodes of the network one by one; if the degree k of out-going links of a node exceeds some prescribed value k_m, we remove randomly selected links till the degree is equal to k_m.

As noted above, LiveJournal consists of about $8 \times 10^6$ nodes, and a network of this size can hardly be worked out computationally. Then our reconstruction remains qualitative, and in particular the value k_m of maximal possible number of out-going links is to be chosen arbitrarily. Still our numerical results indicate, that indeed some characteristics of LiveJournal can be reproduced by modeling it as a line graph constructed on an uncorrelated scale-free network. For the reconstructed graph, the degree distribution agrees with the power law $k^{-\gamma}$ only in some range of degree k. The maximum of $P(k)$ at low degree, is characteristic for all line graphs [1]. However, both in LiveJournal and the reconstructed network, the shape of $P(k)$ is the same for in- and out-links. The difference between these curves is that the number of out-links is limited from above, at $k_m=2500$ for LiveJournal and at $k_m=100$ in the reconstructed network. The ratio of these numbers reveals the deficiency of our computational resources. In our case, the limitation of the out-degree produces an artificial point at $k=k_m$.

The rule "older is observed" is introduced to our reconstruction as the condition that the link between i and j is deleted if i<j, but our results are found to be the same if the condition is i>j. This rule produces the qualitative accordance of the plots on assortativity for LiveJournal with those of the reconstructed network. Finally, we note that the degree-dependent clustering coefficient C for the reconstructed network displays a noised character. This is in some correspondence to the LiveJournal data. The values of the clustering coefficient C in LiveJournal for nodes of degree larger than one are: 0.22 for in-degrees, 0.27 for out-degrees. The term "in-degrees" means here that the links are included between neighbours of a node, with links from the neighbours to the node. The same coefficients are respectively 0.32 and 0.34 for the reconstructed network.

Aside from suggesting a natural mechanism for the social network construction, a direct application of this result appears, if we are interested in a simulation of the process of spread of information, as alerts or gossips, in a community. For a large network, the direct simulation of the state of each particular node can be burdensome and memory consuming. Instead, we can consider a hypothesis that within the cliques, the information is shared almost immediately, when compared with the time of its transmission between the cliques. Such mechanism has been suggested by a number of social science researchers. In fact, it is implied by the Granovetter’s groundbreaking "strength of the weak ties". If this is the case, it is possible to simulate the process on a much smaller network, where nodes represent cliques.

REFERENCES
First observation of jet quenching with ATLAS at the LHC

ATLAS Collaboration

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ATLAS observes striking imbalance of jet energies in heavy ion collisions

Highly asymmetric dijet event

The ATLAS experiment has made the first observation of an unexpectedly large imbalance of energy in pairs of jets created in lead-ion collisions at the LHC [1]. This striking effect, which is not seen in proton–proton collisions, may be a sign of strong interactions between jets and a hot, dense medium (quark-gluon plasma) formed by the colliding ions. Concentrated jets of particles are formed in the head-on (central) collisions of lead ions at the LHC. The jets materialize from the hadronization of quarks and gluons scattered from the protons and neutrons in the colliding ions. If a quark-gluon plasma is formed in the collisions of the high-energy ions, then as the jets materialize they will traverse this hot, dense medium. In so doing they should lose energy to the medium through multiple interactions, in a process called jet quenching.

The jets are most often produced in pairs (dijets) travelling in opposite directions with equal transverse energies, but if the jets travel different distances before escaping the medium, then their energies will no longer be equal. Experiments at the Relativistic Heavy Ion Collider at Brookhaven observed signs of this effect in single-particle distributions; however, the result from ATLAS represents the first direct observation of energy loss by jets, and the first in which the effect is visible on an event-by-event basis (figure 1). The excellent angular coverage, segmentation and energy resolution of its calorimeters make ATLAS well suited for measuring jets. For this analysis, the collaboration looked at a sample of 1693 events with at least one jet having transverse energy greater than 100 GeV. Then they quantified the asymmetry in energy in the dijet system by the ratio of the difference of the leading and sub-leading jet energies to the sum of their energies. In studying this dijet asymmetry they found that it varies as a function of the centrality of the colliding nuclei, as figure 2 shows, where the fraction of events with a given asymmetry is plotted versus the measured asymmetry for four different ranges of centrality with the most central events in the plot on the right and the least central on the left.

Dijet asymmetry distributions

The plots show the dijet energy asymmetry for lead-ion collisions at 2.76 TeV per nucleon pair in the centre-of-mass system and for 7 TeV proton–proton collisions together with the prediction from a Monte Carlo simulation that does not include interactions between the jets and the medium. The non-zero asymmetry shows up for higher centrality values: its distribution broadens and the mean shifts to higher values. To confirm the effect, the collaboration performed numerous studies to verify that events with the large asymmetry are not produced by energy fluctuations, background, or detector effects.

The observation of the centrality-dependent dijet asymmetry by ATLAS has a natural interpretation in terms of QCD energy loss and may point to a strong energy loss by the jets in the quark-gluon plasma. The ATLAS collaboration consists of more than 3000 physicists and engineers from 174 universities and laboratories in 38 countries.

Cracow group (INP PAS and FPACS AGH-UST) has participated in ATLAS since its very beginning. We contributed to design and construction of the Inner Detector (SCT - semiconductor tracker, TRT - transition radiation tracker) and ATLAS trigger system (for p-p and heavy ions collisions). These two activities played an important role in observing the jet quenching phenomenon in Pb-Pb collisions in ATLAS.
A team from the AGH-UST had a significant contribution in preparation of a dedicated trigger menu which has been developed for heavy-ion Pb-Pb running in Nov-Dec 2010.

A trigger menu is a set of triggers which are designed to select data for physics and performance studies. Each physics trigger defines selection criteria for events to be accepted for storage. In 2010 the LHC collided lead ions for the first time, therefore it was a commissioning period also for the ATLAS trigger. Ions were grouped in bunches (1 bunch in the very first run up to 129 ones towards the end of the running period) which resulted in output rates ranging from few Hz to 500 Hz of detector readouts being written to tape. The trigger menu was designed to rely primarily on Level-1 which is a hardware trigger in ATLAS. Level-1 was constructed in a way to trigger on the presence of deposits in interactions indicating devices with Minimum Bias Trigger Scintillators (MBTS) and Zero Degree Calorimeters (ZDC) among them. A big chunk of data has been collected in that way. This relatively unbiased sample was successfully used to make the first observation of the energy asymmetry in dijet events. Also a dedicated so called minimum bias trigger was designed to look at signals in the Inner Detector and choose collision events based on a number of hits there. This trigger was further used for offline performance studies. A majority of Level-1 triggers was based on information which was read out from the calorimeters and muon spectrometer defining Regions-of-Interest (RoI) for the High Level Trigger (HLT). A small fraction of HLT-based triggers was also part of the heavy-ion trigger menu. Those triggers were designed to select events enhanced in jets, muons, photons and electrons. However, they were running in monitoring mode in 2010. This means a trigger decision was based on the Level-1 trigger only but at the same time information from the HLT triggers was accessible for future performance studies.

In the course of the 2010 run it turned out an interaction rate given by the MBTS and ZDC detectors is too high to be accepted for storage. Therefore, new HLT based triggers had to be introduced to the menu and further used to clean up events from beam backgrounds and in consequence to decrease an output interaction rate for physics analyzes.

REFERENCES

Prompt $K^0_s$ production in pp collisions at $\sqrt{s} = 0.9$ TeV  [1]

LHCb Collaboration

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First data collected at LHCb experiment in 2009 serve a verification of all the sub-detectors involved and their appropriate calibration, tests of conformity with previously obtained by other experiments results and search for new processes including those leading to a New Physics. A typical channel of that type is the $K^0_s$ (strange meson) inclusive production. Strangeness production in p-p collision provide sensitive test of soft hadronic interactions since such a production is suppressed in non-perturbative (soft) regime of the Quantum Chromodynamics (QCD) being part of the Standard Model. The hadronic production of $K^0_s$ has been recently analyzed at the Tevatron (CDF experiment, [2]) showing disagreement between data and the predictions resulting from hadronization models. The collected by LHCb detector data sample corresponds to an integrated luminosity of $6.8 \pm 1.0 \mu b^{-1}$. The two-dimensional differential cross section $d^2\sigma/dp_Td\eta$ has been measured, partly in a phase-space region that was not available for previous experiments. A new method of integrated luminosity determination based on vertex detector VELO has been used. A $K^0_s$ is defined to be prompt if it originates directly from pp primary vertex or if it is decay product of strongly decaying resonances. The measurement was performed in a rapidity interval, $2.5 < \eta < 4.0$, a region not yet explored by any of the experiments in past and is complementary to the coverage of remaining LHC experiments. All possible, model dependent, predictions agree reasonably well with obtained by LHCb cross-section although there is a tendency to overestimate the MC predictions for highest $p_T$ values. The comparison of the LHCb cross-section with those obtained by other experiments is shown in Fig.1.

The red points representing new LHCb data overlap with the data obtained by other experiments leaving alone points belonging to latest CDF data [2] and are found to be in reasonable agreement with generator expectations. Obtained result does not confirm a deviation from existing hadronization models expressed in terms of MC generated data. The ability of LHCb detector to provide very sensitive measurements is apparent.

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A sophisticated neural recording system has been developed to investigate in detail the retina functionality, in particular the connectivity in the neural circuitry that transfer signals from individual photoreceptors to the retinal ganglion cells, which in turn send visual signals from the eye to the brain. The concept of the experiment is illustrated in Fig. 1.

Fig. 1. Illustration of the experimental principle how to stimulate optically retina’s photoreceptors (top layer of the retinal tissue) and record electrical signals from the ganglion cells (bottom layer of the retinal tissue) using an array of microelectrodes. Image by Zina Deretsky, NSF.

A computer generated images are projected through an optical system onto living retinal tissue placed on an array of electrodes facing the retina’s ganglion cells. The photoreceptors detect the visual stimulus, convert it into electrical signals, and then send it through a complex network of interconnected neurons for further processing. At the bottom of retinal tissue there is a layer of about 20 distinct types of retinal ganglion cells, which are responsible for sending encoded information in the form of series of electrical spikes to the brain via the optical nerve. In the experiment those signals generated by the ganglion cells are recorded by a high density microelectrode arrays with spatial resolution comparable with sizes of individual ganglion cells.

The purpose of the present study was to investigate entire input-to-output connectivity and this way to understand signal processing performed by complex neuronal circuits in the retina at single-cell resolution. Visual stimulation of high spatial resolution and a high spatial resolution recording system were used to identify the path, type and strength of the functional input of each cone to each ganglion cell. These data allow us to more deeply understand neuronal computations in the visual system and ultimately may help us construct better retinal implants."

For the present study a high-density 519-electrode array with 30 µm electrode spacing and a recording system based on Application Specific Integrated Circuits developed for this purpose have been used. The high-density electrode arrays were developed by the Particle Physics Experiment Group at the University of...
Glasgow and the multichannel integrated circuits to read out the electrical signals have been developed by the Nuclear Electronics and Radiation Detection Group in the Faculty of Physics and Applied Computer Science at the AGH University in Krakow. The new technology opens the way to a wide range of possible biomedical applications, including the development of better methods for retinal prosthesis. So far, the investigations have focused on retinal processing, but the developed technique can be applied to further studies, how the complex neuronal circuitry of the retina develops, and how the brain process the data received from the retina.

REFERENCES

Determination of the isotopic composition of boron in boric acid by means of the thermal neutron absorption technique

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Boron and its compounds are extensively used in nuclear industry as strong thermal neutron absorbers. In particular, boric acid \((\text{H}_3\text{BO}_3)\) is added to the primary circuit coolant of pressurized water reactors (PWR) to control the chain reaction. Owing to the use of the neutron-absorbing coolant instead of neutron-absorbing control rods, the irregularities in the power density distribution and fuel consumption within the reactor core can be avoided. Uncontrolled changes of the neutron absorber content would lead to operational problems, so the continuous monitoring of its concentration in the reactor coolant is of great significance. Natural boron is a mixture of \(^{10}\text{B}\) and \(^{11}\text{B}\) isotopes with abundances of about 20 % and 80 %, respectively. Thermal neutron absorption cross sections of \(^{10}\text{B}\) and \(^{11}\text{B}\) are 3839 \(\text{b}\) and 0.0055 \(\text{b}\), respectively. In this connection, the actual factor affecting the reactor performance is the concentration of \(^{11}\text{B}\) isotope in the coolant. It is known that the isotopic composition of natural boron varies significantly depending on the origin of the raw material. The content of \(^{10}\text{B}\) in boric acid is frequently not known even at the moment of purchasing (Shul et al., 2007). Therefore, chemical methods are not adequate for determining the concentration of \(^{11}\text{B}\) in the reactor coolant. This resulted in motivation for the development of measurement systems sensitive specifically to \(^{10}\text{B}\) isotope. Techniques based on the thermal neutron absorption, i.e. on the same physical principle that is applied to the reactor control, appeared to be especially suitable for this purpose. Different versions of such devices designed for continuous on-line or by-line monitoring the concentration of \(^{10}\text{B}\) in the reactor coolant have been developed and perfected since the beginning of the PWR technology [1, 4, 5, 6, 7, 8]. All instruments of this type require calibration. For the sake of metrological traceability of the measurement system, any calibration procedure should finally refer to a certified boric acid isotopic reference material like those available from National Institute of Standards (USA) or Institute of Reference Materials and Measurements (Belgium). However, because of high cost, the isotopic reference materials are seldom if ever used directly for preparation of calibration solutions. Usually some secondary standard of boric acid is used for this purpose. In any case, the concentrations of \(^{10}\text{B}\) in calibration solutions of boric acid must be known.

The aim of this work was to improve the thermal neutron absorption technique developed earlier [2, 3] and to apply it to determining the concentration of \(^{10}\text{B}\) in water solution of boric acid. A good deal of attention was given to optimizing the measurement set up and procedure in order to reduce an uncertainty of assays. Monte Carlo modeling proved to be useful for optimizing the measurement system. In particular, computer simulations revealed that the sample container in the shape of double-walled tube with external tube made of polyethylene and internal one made of polytetrafluoroethylene (teflon) offered a distinct advantage over the sample container wholly made of polyethylene. With the use of the improved sample container the concentration of \(^{10}\text{B}\) can be measured within a considerably wider limits, at least up to 750 ppm. The measurement procedure has been optimized both in respect of selecting the concentration of \(^{10}\text{B}\) in the calibration standard and partition of the total time allotted to determining the ratio of two counting rates.

With the use of 1370-cm\(^3\) sample, \(^{252}\text{Cf}\) neutron source emitting about 2 \(\times 10^6\) neutrons/s and assuming 30-minute total counting time, the relative uncertainty (2 \(\sigma\)) of 0.3 % can be attained for determining the concentration of \(^{10}\text{B}\) in water solution of boric acid in the range 200 - 750 ppm. The relative uncertainty steadily increases with decreasing concentration of \(^{10}\text{B}\), however it is still below 1 % at 20 ppm.

Through the measurement of the concentration of \(^{10}\text{B}\) in water solution of boric acid \((\text{C})\) the concentration of \(^{10}\text{B}\) in this boric acid \(\left(\text{C}_{\text{BA}}\right)\) can be easily determined. Namely,

\[
\text{C}_{\text{BA}} = \frac{\text{C}}{\text{C}_{\text{A}}}
\]

where \(\text{C}_{\text{A}}\) is the concentration (mass fraction) of boric acid in its water solution.

If boric acid diluted in water is of stoichiometric purity, the measurement of \(^{10}\text{B}\) concentration in this solution \((\text{C})\) will form basis for determining the isotopic composition of boron in this boric acid. The following relationship between an abundance (atom amount fraction) of \(^{10}\text{B}\) \((\text{A}_{\text{B10}})\) and its concentration in water solution of boric acid can be derived:

\[
\text{A}_{\text{B10}} = \frac{\text{C}[\text{M}_{\text{B11}} + 3(\text{M}_{\text{H}} + \text{M}_{\text{O}})]}{\text{C}_{\text{A}}\text{M}_{\text{B10}} + \text{C}(\text{M}_{\text{B11}} - \text{M}_{\text{B10}})}
\]

where \(\text{M}_{\text{B10}}\) and \(\text{M}_{\text{B11}}\) are molar masses of two isotopes of boron whereas \(\text{M}_{\text{H}}\) and \(\text{M}_{\text{O}}\) are molar masses of hydrogen and oxygen, respectively.

If the actual goal of the measurement is determining the isotopic composition of boron, the conc-
centration of $^{10}$B in the specially prepared water solution of boric acid should be properly chosen. Provided that $200 \text{ ppm} < C < 750 \text{ ppm}$, all three quantities, $C$, $C_{BA}$, and $A_{B10}$, can be determined with the relative uncertainties of 0.3 % (understood as $2 \delta$).

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Hyperfine interactions and electronic band structure in Tb$_{0.27}$Dy$_{0.73}$(Fe$_{1-x}$Co$_x$)$_2$ intermetallics

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The RM$_2$-type ferrimagnetic intermetallics consisting of heavy rare earth (R) and transition metal (M) are widely studied for both their fundamental interest and for their practical applications. The Terfenol-D (Tb$_{0.27}$Dy$_{0.73}$Fe$_2$) based compounds with various substitutions in the rare earth or transition metal sublattices are intensively tested as strongly magnetostrictive constituents of composites or laminates with piezoceramics in order to obtain materials with a giant magnetoelectric effect [1,2].

The ferrimagnetism of these intermetallic compounds results from the coexistence of rare earth 4f5d electron magnetism and transition metal 3d electron magnetism [3-8]. The substitution of Fe with another transition metal in RFe$_2$ type compounds changes the number $n$ of 3d electrons in the M-sublattice, ipso facto strongly influences the 3d-band magnetism and hyperfine interactions [3-8]. Therefore, it was revealing to study systematically by Mössbauer effect the influence of the rising 3d electron population on the resulting mainly from the 3d-band properties magnetism of the M-sublattice and especially on the hyperfine interactions in Terfenol-D type compounds with Fe/Co substitution. Moreover, it was interesting to perform the electronic band structure calculations using the FLAPW method, and finally to make a comparison of experimentally obtained quantities with theoretically calculated properties of the tested Tb$_{0.27}$Dy$_{0.73}$(Fe$_{1-x}$Co$_x$)$_2$ intermetallic series.

The polycrystalline materials Tb$_{0.27}$Dy$_{0.73}$(Fe$_{1-x}$Co$_x$)$_2$ ($x=0,0.1,...,0.9$ and $1.0$) are characteristic of a pure cubic, Fd3m, MgCu$_2$-type (C15) crystal structure [5,8]. The $^{57}$Fe Mössbauer effect measurements were performed at 4.2K using a standard transmission technique with a $^{57}$Co in Pd source [3-8]. The exemplary Mössbauer effect spectrum of the Tb$_{0.27}$Dy$_{0.73}$(Fe$_{0.5}$Co$_{0.5}$)$_2$ compound is presented in Fig.1a. Spectra for the whole series are characteristic of the [100] easy axis of magnetization and were fitted considering the random distribution of the Fe/Co atoms in the transition metal sublattice. The random distribution of the Fe and Co atoms introduces different neighbourhoods of the probed iron atom. A particular Fe/Co neighbourhood shows locally its own subspectrum contributing to the resulting measured
Mössbauer effect pattern, and therefore determines its proper hyperfine interaction parameters. The probability of particular neighbourhoods and thus the amplitude of particular subspectra is calculated using Bernoulli distribution formula. The hyperfine interaction parameters weighted by the subspectra amplitudes i.e. an isomer shift, a magnetic hyperfine field and a quadrupole interaction parameter were obtained both for the local area and for the sample as bulk. The isomer shift and the quadrupole interaction parameter are almost constant throughout the tested series [5, 8]. The weighted average magnetic hyperfine field $\mu_0 H_{hf}$ vs. Co content $x$ or an average number $n$ of 3d electrons resembles a Slater-Pauling-type dependence (Fig.2a). The average number of 3d electrons is calculated using expression $n=6(1-x)+7x$ considering the stoichiometry of the series. Moreover, local analysis of the magnetic hyperfine fields revealed that local neighbourhoods of the tested iron atom also create local-type dependences similar to a Slater-Pauling curve [5, 8]. Initially weak ferromagnetic type behaviour of the $M$-sublattice is present. In this case two 3d subbands with opposite spin are not filled up [9]. The magnetic hyperfine field grows with $x$ or $n$ across the investigated series and the maximum value of the field is reached at $x=0.3$ (Fig.2a). At this composition the filling up of the majority 3d subband by 3d electrons is terminated. Further Co-substitution introduces a strong ferromagnetic type behaviour of the $M$-sublattice [9]. The filling-up of the minority 3d subband continues and the observed field decreases gradually with $x$ or $n$.

The electronic band structures of Tb$_{0.27}$Dy$_{0.73}$(Fe$_{1-x}$Co$_x$)$_2$ intermetallics were calculated by an ab-initio self-consistent Full-Potential Linearized Augmented Plane Waves (FLAPW) method as implemented in the WIEN2K code [10]. The details of calculation process are described elsewhere [4, 5, 8]. Some exemplary results of the FLAPW calculations are presented in Fig.1b, c and d. Specifically, the densities of states (DOS) calculated for Fe, Co (3d electrons) are presented for the Tb$_{0.27}$Dy$_{0.73}$(Fe$_{0.5}$Co$_{0.5}$)$_2$ compound. Fig.1c also contains stoichiometrically weighted DOS (M3d) for Tb$_{0.27}$Dy$_{0.73}$(Fe$_{0.5}$Co$_{0.5}$)$_2$ compound. It can be added that the Fermi energy corresponds to zero value.

A qualitative inspection of the filling process of both 3d-subbands across the series confirmed that the population in the majority 3d-subband (spin up) increases up to $x=0.3$ (a region of weak ferromagnetism) and that over this composition rate it is approximately constant (the majority subband is fully occupied; a region of strong ferromagnetism), while the minority 3d-subband (spin down) population increases across the whole series [5, 8].

![Fig.2. Magnetic hyperfine field $\mu_0 H_{hf}$ (a) at 4.2K, the calculated magnetic moments per atom (b): $m_{Fe}$, $m_{Co}$ and the $m_M$ weighted magnetic moment per transition metal atom vs. the Co content $x$ (bottom axis) or the average number $n$ of 3d electrons (top axis) for the Tb$_{0.27}$Dy$_{0.73}$(Fe$_{1-x}$Co$_x$)$_2$ series [5, 8]. Fig.2b presents magnetic moments $m_{Fe}$ and $m_{Co}$ calculated per Fe and Co atom respectively, and the stoichiometrically weighted $m_M$ magnetic moments per transition metal atom calculated for the Tb$_{0.27}$Dy$_{0.73}$(Fe$_{1-x}$Co$_x$)$_2$ series. The $m_{Fe}$ and $m_{Co}$ magnetic moments were calculated considering both s,p electrons and mainly contributing d electrons. The magnetic moment $m_M$ as a function of $x$ or $n$ resembles a Slater-Pauling dependence.](image)

![Fig.3. Correlation between the experimentally obtained magnetic hyperfine field $\mu_0 H_{hf}$ and the calculated weighted magnetic moment $m_M$ for the Tb$_{0.27}$Dy$_{0.73}$(Fe$_{1-x}$Co$_x$)$_2$ series [5, 8].](image)
In Fig. 3 the correlation between the experimental \( \mu_0 H_{hf} \) magnetic hyperfine field and the calculated \( m_M \) weighted magnetic moment per transition metal atom is presented. It is to notice that \( \mu_0 H_{hf} \) field matches well the average magnetic moment \( m_M \) of the transition metal atom separately in regions of the weak and the strong ferromagnetic type behaviour of the M-sublattice. The slope rate \( \mu_0 H_{hf}/m_M \) for the weak ferromagnetic case is approximately three times higher then the slope rate of the strong ferromagnetic case.

The presented here results can be helpful both in band type calculations and for practical applications of the Terfenol-D-type \( \text{Tb}_{0.27}\text{Dy}_{0.73}(\text{Fe}_{1-x}\text{Co}_x)_2 \) compounds, which are to be treated as particulate constituents of magnetoelectric composites.

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Assessing night time surface fluxes of CO$_2$ and CH$_4$

in the Krakow area

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Quantification of surface fluxes of CO$_2$ and CH$_4$ plays a key role in assessing atmospheric budgets of these gases over continental areas. The preferred approach is a direct flux measurement on the landscape scale via eddy covariance method. However, direct measurements of surface emissions of CO$_2$ and CH$_4$ into the atmosphere in densely populated areas using this method are complicated mostly due to large heterogeneity of urban land cover. The commonly used methodology of assessing urban fluxes of CO$_2$ relies on statistics of spatial and temporal distribution of fuel consumption. Reliability of this method strongly depends on the completeness and overall quality of the relevant statistical data. In order to validate the inventory data, independent methods based on atmospheric measurements have been suggested. This work presents an attempt to quantify surface fluxes of CO$_2$ and CH$_4$ in urban environment by combining the measurements of atmospheric mixing ratios of these gases with measurements of the mixing layer height performed with the aid of a sodar system.

The study was performed in Krakow, southern Poland (50.067°N, 19.913°E, 220 m a.s.l.), between May 2005 and May 2009. The presented method of assessing night-time surface fluxes of CO$_2$ and CH$_4$ is based on parallel measurements of the mixing height within the Planetary Boundary Layer (PBL) and the atmospheric mixing ratios of these gases measured at certain elevation above the local ground. The mixing height within the PBL was monitored using VHS sodar (Version 3) built by the Krakow Branch of the Institute of Meteorology and Water Management. The ground-based inversion is mainly observed during night-time. Usually, it develops after sunset and disappears ca. 1.5-2 hours after sunrise. The analysis of the sodar data from 1994 to 2008 showed that the ground-based inversion in Krakow is almost always observed between 8 p.m. and 3 a.m. UTC, regardless of seasons. The measurements of atmospheric mixing ratios of CO$_2$ and CH$_4$ were performed inside the university campus, on the western side of the city center, surrounded by recreation area and sport complex. Strong anthropogenic sources of CO$_2$ and CH$_4$ were absent in immediate vicinity of the measurement site, thus no filtering procedure has been applied to the mixing ratio record. The measurements of CO$_2$ and CH$_4$ mixing ratios were performed with the aid of automatic GC system (HP6890) equipped with Ni catalyst and FID detector. Atmospheric concentrations of trace gases within the PBL are controlled to a large extent by intensity of vertical mixing processes [1].

During the day, when strong thermal convection prevails, CO$_2$ and CH$_4$ emitted from the surface are diluted in a large volume of well-mixed PBL. Therefore, relatively low concentrations of these gases, close to the background values typical for the free troposphere, can be observed during the day. In late afternoon, after the sunset, the vertical temperature profile in the atmosphere is changing, largely reducing the vertical mixing. During the periods of low wind speed, when advection is small, this leads to accumulation of trace gases emitted from the surface and their concentrations within the PBL start to increase.

The rate of increase of the mean concentration of the given trace gas within the mixing layer is controlled by the actual height of the mixing layer and the net flux of this gas to this layer. During stable atmospheric conditions, with low wind speeds, a distinct vertical gradient of CO$_2$ and CH$_4$ concentration is usually established within the PBL. As the measurements of mixing ratios are performed close to the surface, a correction factor relating the average increase of the concentration within the PBL ($dnc/dt$) to the increase of the concentration observed close to the ground level (ca. 20 m) is required. This correction factor was calculated using an analytical dispersion model [2]. The value of the correction factor derived for stable-stratified PBL and the aerodynamic surface roughness of a big city (one to a few meters) was equal 6.5. After applying the correction factor $k$, the formula for calculating surface fluxes of CO$_2$ and CH$_4$ reads as follows:

$$\frac{h}{k} \frac{dnc_{surf}}{dt} = F_{in} \tag{1}$$

where:
- $h$ – PBL height
- $k$ – correction factor
- $c_{surf}$ – Concentration of CO$_2$ (CH$_4$) at the measurement height
The surface fluxes of CO\textsubscript{2} and CH\textsubscript{4} were calculated using eq. (1) for late evening and night hours, when an increase of the measured mixing ratios of these gases was observed. The calculations were performed under the following assumptions: (i) the CO\textsubscript{2} and CH\textsubscript{4} emitted into the atmosphere during the periods for which calculations were performed, was accumulating within the PBL (no transport between the PBL and the free troposphere), (ii) only the nights with wind speed below 1 m/s were chosen to fulfill the closed-system assumption (no significant advection, adding or removing trace gases from the atmosphere below PBL within the city), (iii) major removal processes of CO\textsubscript{2} and CH\textsubscript{4} are not active at that time, (iv) the mean concentration of CO\textsubscript{2} and CH\textsubscript{4} within the PBL is derived from vertical concentration profiles calculated using analytical dispersion model. The nighttime surface fluxes of CO\textsubscript{2} and CH\textsubscript{4} obtained with the procedure outlined above were subject to two-step data selection scheme. In the first step, only values representing the nights with the linear regression coefficient calculated for the increase of CO\textsubscript{2} and CH\textsubscript{4} concentration $R^2>0.8$ were selected. In the second step, the values of surface CO\textsubscript{2} and CH\textsubscript{4} fluxes representing the nights with standard deviation of the mean PBL height greater than 30 m were removed from the remaining dataset. Subsequently, the monthly mean values of the CO\textsubscript{2} and CH\textsubscript{4} surface fluxes were calculated. For some months, the adopted data selection procedure significantly reduced the number of available data, leading to substantial increase of the uncertainty of the monthly mean values. Figure 1 a and b present mean monthly fluxes of CO\textsubscript{2} and CH\textsubscript{4}, respectively, calculated with the aid of the procedure outlined above.

The calculated mean monthly surface fluxes of carbon dioxide (Fig.1a) reveal distinct seasonality, with a minimum of ca. 2 mmol m\textsuperscript{-2} h\textsuperscript{-1} occurring during winter and a maximum of ca. 20 mmol m\textsuperscript{-2} h\textsuperscript{-1} in summer. This strong seasonality is most probably induced by seasonally modulated biospheric component, originating from soil respiration. The measured surface fluxes of CO\textsubscript{2} during summer were comparable with the soil respiration fluxes obtained from regular observations carried out in Southern Poland region between 1998 and 2000 using the enclosure method. The reported monthly mean respiration fluxes of CO\textsubscript{2} for summer months (MMJJ) for three typical areas (grassland, mixed forest and agricultural field) were equal 11.5±0.2, 19.8±0.4 and 13.4±0.2 mmol·m\textsuperscript{-2}·h\textsuperscript{-1}, respectively [3]. The mean CO\textsubscript{2} flux representing summer months (MMJJ) calculated using eq.(1) is equal 15.6±0.9 mmol·m\textsuperscript{-2}·h\textsuperscript{-1}. It lies within the range of respiration CO\textsubscript{2} fluxes quoted above. This points to a dominant role of the biospheric component in the derived nighttime fluxes of CO\textsubscript{2} in the investigated urban setting, at least during the summer months.

Contrary to the CO\textsubscript{2} flux, the calculated surface fluxes of CH\textsubscript{4} (Fig. 1b) do not reveal any distinct seasonality. The mean value of the CH\textsubscript{4} flux calculated for the whole analysed period (May 2005 – December 2008) is equal 97.2±5.4 μmol m\textsuperscript{-2} h\textsuperscript{-1}. Multiplying the mean CH\textsubscript{4} flux by the surface area of the city (326.8 km\textsuperscript{2}), one arrives at the total mean emission of methane into the atmosphere in Krakow in the order of $(6.2±0.4)\times10^{9}$ m\textsuperscript{3} yr\textsuperscript{-1}. Leakages of the city gas network are thought to be the main source of this methane. This has been confirmed by carbon isotope analyses of atmospheric methane and the methane being distributed within the network. The carbon isotope composition of methane emitted by the hypothetical methane source in Krakow, derived from carbon isotope analyses of atmospheric methane and the two-component mixing model, is equal ca. -54.2‰ [4]. Measurements of carbon isotopic composition of methane present in the city gas yield the value of -54.4±0.6‰ which is virtually identical with the isotopic signature of the hypothetical methane source within

$$F_n = \text{surface flux of CO}_2 (\text{CH}_4) \text{ to the atmosphere.}$$

Fig. 1. The monthly means of surface night-time fluxes of CO\textsubscript{2} (a) and CH\textsubscript{4} (b) in Krakow for the period May 2005 -May 2009.
The leakages of CH$_4$ estimated by Kuc et al. for the period 1996-1997 [4] were in the order of 2.15x10$^7$ m$^3$ yr$^{-1}$, a significantly higher value than that derived in the present study. This apparent reduction of CH$_4$ leakages is most probably linked to major improvements of the distribution infrastructure of the city gas network in the course of the last decade, as testified by the gas operator.

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## Third-party funds
Badania finansowane ze źródeł zewnętrznych

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### PROJEKTY ZAMAWiane

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Books published in Poland

1. Z. STĘGOWSKI

2. NGUYEN DINH CHAU

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1. P. PANASIUK, K. SAEED

2. W. SIKORA, L. PYTLIK

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4. M. SMOLEŃ, K. CZOPEK, P. AUGUSTYNIAK

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2. K. SAEED, K. SURMACZ


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16. L.PETRYKA, R.HANUS, M.ZYCH, M.ŚLEZIAK
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17. A.ZIĘBA
    Effective number of observations and unbiased estimators of variance for autocorrelated data - an overview
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18. J.CHOWANIEC, M.DULIŃSKI, P.MOCHALSKI, J.NAJMAN, I.ŚLIWKA, A.ZUBER
    Water Ages in Thermal System of the Podhale Basin (Inner Carpathians, Southern Poland)
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19. A.ZUREK, K.RÓŻAŃSKI, P.MOCHALSKI, T.KUC
    Assessment of Denitrification Rates in Fissured-Karstic Aquifer near Opole (South-West Poland): Combined
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20. A.JUNG
    Praktyki studenckie z zakresu inżynierii biomedycznej - nowe doświadczenia
    Inżynieria Biomedyczna, 16 (2010) 48-49
   Maximum Entropy Approaches to Living Neural Networks
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22. B.F.O.COSTA, J.CIEŚLAK, S.M.DUBIEL
   Study of a sigma-phase formation in an equiatomic Fe-V alloy

23. R.GOZDYRA, S.M.DUBIEL, J.CIEŚLAK
   Iron in ferrous gluconate and Ascofer®

24. W.SIKORA, J.MALINOWSKI
   Symmetry Analysis in Parametrisation of Complex Systems

25. A.KUNA, W.SIKORA
   The symmetry analysis of structural deformations related to the hydrogen implementation in borohydrides

   Influence of Cd²⁺ on the spin state of non-heme iron and on protein local motions in reactions centers from purple photosynthetic bacterium Rhodospirillum rubrum

27. A.PAJA
   Electron transport in disordered metallic nanosystems

28. P.KUCZERA, B.KOZAKOWSKI, J.WOLNY, W.STEURER
   Real space structure refinement of the basic Ni-rich decagonal Al-Ni-Co phase

29. B.ŁABNO, L.PYTLIK, J.WOLNY, J.ADAMOWSKI, M.DUDA
   Configuration energy analysis of β-Mg₂Al₃ cluster structure

30. J.WOLNY, M.DUDA, B.KOZAKOWSKI
   Simple model of Mg₂Al₃: β and β’ phases

31. A.P.PIKUL, Ł.GONDEK, D.KACZOROWSKI, A.SZYTUŁA
   Magnetic behavior in TmCu₃Ge₂

32. M.SZCZERBOWSKA-BORUCHOWSKA, J.CHWIEJ, P.DUMAS, B.TOMIK, D.ADAMEK, M.LANKOSZ
   Revealing the presence of creatine in human spinal cord in amyotrophic lateral sclerosis, by infrared microspectroscopy
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   Magnetism of ultra-thin iron films seen by the nuclear resonant scattering of synchrotron radiation  

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   Study of Vitamins and Dietary Supplements Containing Ferrous Fumarate and Ferrous Sulfate Using Mössbauer Spectroscopy  
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36. P. GUZDEK, J. PSZCZOŁA, P. STOCH, A. STOCH  
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37. E. ABAT, [ET AL.], T. Z. KOWALSKI, B. MINDUR  
   Combined performance studies for electrons at the 2004 ATLAS combined test-beam  

38. A. MANKA-KRASÓN, K. KUŁAKOWSKI  
   Assortativity in random line graphs  

39. J. NIZIOL, Z. ESSAIDI, B. SAHRAOUI  
   Third order NLO properties of modified azo-azulenes  
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40. V. ANISHCHIK, V. UGOV, N. KVASOV, Y. PETUKHOU, V. ASTASHYNSKI, A. KUZMITSKI, P. ZHUHOKSKI, CZ. KARWAT, J. ŻUKROWSKI, J. FEDOTOVA  
   Silicide formation on silicon by dense compression plasma treatment  
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41. M. SIKORA, O. MATHON, P. VAN DER LINDEN, J. M. MICHALIK, J. M. DE TERESA, CZ. KAPUSTA, S. PASCARELLI  
   Field-induced magnetostructural phase transition in $Ca_2FeReO_6$ studied via XMCD under 30 T pulsed magnetic field  

42. H. FIGIEL, Ł. GONDEK, M. ZIAREK, N. B. SELVARAJ, N. KARDJILOV  
   Zastosowanie radiografii oraz tomografii neutronowej w badaniach dla potrzeb energetyki wodorowej  

43. M. KOWALIK, M. SIKORA, A. KOŁODZIEJCZYK, CZ. KAPUSTA  
   XANES and X-RAY Photoemission of the $La_{0.67}(Ca,Pb)_{0.33}(Mn_{1-x},Fe_x)O_3$ Compounds  

44. J. FIEDOR, R. HAESSNER, H. SCHEER, L. FIEDOR  
   Investigations of antioxidant properties of carotenoids in model systems  
   Proceedings of Natural Pigment Conference for South-East Asia,  (2010) 25-29
1. WASILEWSKA-RADWAŃSKA M., MATUSIAK K., STĘPIEŃ A.

2. BOLEWSKI A., CIECHANOWSKI M., DYDEJCZYK A., KREFT A.

3. A. KORUS, M. KOTARBA, M. DZIENIEWICZ, H. SECHMAN
Conferences presentations and seminars

Invited lectures

1. RÓŻAŃSKI K.
   Environmental tracers in groundwater hydrology.
   Seminar at Thailand Institute of Nuclear Techniques
   Bangkok, February 15, 2010

2. RÓŻAŃSKI K.
   Environmental isotopes in precipitation- determining water balances of lakes and surface water bodies.
   Workshop on flow-path characterization, Munich, June 29, 2010

3. RÓŻAŃSKI K., ZIMNOCH M., NĘCKI J.
   Greenhouse gases in urban atmosphere of Krakow: assessing local loads and fluxes
   Coordination meeting of COST-ABBA Project, June 21, 2010

4. RÓŻAŃSKI K.
   Antropogeniczné zmiany klimatu – mit czy rzeczywistość?
   Posiedzenie Konwentu AGH, Kraków, 4 października 2010

5. RÓŻAŃSKI K., NĘCKI J., CHMURA Ł., ZIMNOCH M.,
   Pomiar stężeń gazów cieplarnianych na stacji Kasprowy Wierch
   Spotkanie Grupy Inicjatywnej Projektu ICOS-PL, Mierzęcin, 16 września 2010

6. RÓŻAŃSKI K.
   Spatial and temporal variability of stable isotope composition of precipitation and atmospheric moisture.
   Workshop SINA2010, Vienna, November 25-26, 2010
   (przewodnictwo sesji)

7. SZCZERBOWSKA-BORUCHOWSKA M.
   Biochemical imaging of brain tumors using synchrotron radiation microprobe.
   Synchrotron Radiation for Bio-Imaging at PETRA III
   Hamburg, 29-30. 03. 210

8. ADAMEK D., SZCZERBOWSKA-BORUCHOWSKA M., LANKOSZ M.
   Toward “fingerprinting” of brain tumours based on the synchrotron radiation x-ray fluorescence, Fourier transform infrared microspectroscopy (FTIRM) and discriminant analysis
   Intercongress Meeting of the European Society of Pathology
   31 August – 3 September 2010, Krakow, Poland

9. WASILEWSKA-RADWAŃSKA M.
   Higiena radiacyjna w Unii Europejskiej i w USA – stan obecny i perspektywy
   XV Zjazd Polskiego Towarzystwa Badań Radiacyjnych im. Marii Skłodowskiej-Curie.
   Siedlce, 20-23.09.2010

10. JANUSZ TOBOŁA
    Electronic structure of thermoelectric and magnetocaloric systems
    5th European School in Materials Science
    Slovenia/Ljublana 24-29.05.2010
Contributed presentations

1. **K. ŚWIENTEK**
   Forward Calorimetry Readout and DAQ status for FCal Collaboration
   ILD Workshop 2010, 4th Workshop on ILD
   Francja/Paryż 2010-01-28 2010-01-30
   ORAL

2. **M. LANKOSZ, Z. STĘGOWSKI, M. SZCZERBOWSKA-BORUCHOWSKA, M. CZYŻYCKI**
   Analysis of levels, speciations and chemical environments of selected elements in brain gliomas
   XFEL user meeting and hasylab user meeting
   Niemcy/Hamburg 2010-01-26 2010-01-30
   ORAL

3. **A. ŻEBA**
   Efektywna liczba obserwacji i estymacja odcylenia standardowego dla danych skorelowanych (referat przeglądu)
   IX Sympozjum Niepewność Pomiarów
   Polska/Świnoujście 2010-02-15 2010-02-19
   POSTER

4. **M. IDZIK**
   Detektory dla obszaru małych kątów w zderzaczach liniowych e+e-, Detektor LumiCal przy ILC
   Seminarium Zakładów Cząstek i Oddziałów Fundamentalnych UW oraz IPJ w Warszawie
   Polska/Warszawa 2010-02-26 2010-02-26
   ORAL
5. **J. FIEDOR, R. HAESSNER, H. SCHEER AND L. FIEDOR**
Investigations of Antioxidant Properties of Carotenoids in Model Systems
Natural Pigments Conference for South-East Asia
Indonezja/Malang  2010-03-20 2010-03-21
POSTER

Sub-lattice magnetism in sigma-phase Fe-V compounds 4th Seheim
Conference on Magnetism,
Frankfurt Niemcy/Frankfurt  2010-03-27 2010-04-01
ORAL

Pressure effect on the crystal lattice of unconventional superconductor UCoGe.
40 Journies des Activites and 2 Workshop on Activite Targets
Szwajcaria/Genewa  2010-03-27 2010-04-01
ORAL

High-pressure hydrogen doping into the UTGe compounds.
40 Journies des Activites and 2 Workshop on Activite Targets
Szwajcaria/Genewa  2010-03-27 2010-04-01
POSTER

Synchrotron based techniques in the investigation of mechanisms underlying the neurodegenerative changes induced by pilocarpine evoked epileptic seizures and mechanical brain injury
Synchrotron Radiation for Bio-Imaging at PETRA III
Niemcy/Hamburg  2010-03-28 2010-03-31
ORAL

Synchrotron based techniques in the investigation of mechanisms underlying the neurodegenerative changes induced by pilocarpine evoked epileptic seizures and mechanical brain injury
Synchrotron Radiation for Bio-Imaging at PETRA III
Niemcy/Hamburg  2010-03-28 2010-03-31
POSTER

11. **J. CIEŚLAK, J. TOBOLA, S. M. DUBIEL AND W. SIKORA**
Theoretical calculations of magnetic properties of $\sigma$-Fe$_5$Co$_4$ alloy
Fourth Seheim Conference on Magnetism
Niemcy/Frankfurt  2010-03-28 2010-04-01
ORAL

Biomolecular changes of rat brain tissue after pilocarpine induced seizures – synchrotron FTIR microspectroscopy study
Synchrotron Radiation for Bio-Imaging at PETRA III
Niemcy/Hamburg  2010-03-29 2010-03-30
POSTER

Radiocarbon dating of woolly rhinoceroses and plant remnants in pleistocene sediments from starunia (the velyky lukavets river valley, sw Ukraine)
10th international conference methods of absolute chronology
Polska/Gliwice 2010-04-22 2010-04-24
ORAL
14. **A. JUNG, P. KRISPER, D. SCHNEDITZ**  
Wpływ wybranych parametrów na ocenę efektów pozaustrojowej terapii wątroby  
XVI Krajowa Konferencja Biocybernetyki i Inżynieria Biomedyczna  
Polska/Warszawa 2010-04-26 2010-04-29  
ORAL

15. **M. BONCZYK, Z. GORCZYCA, P. WACHNIEW, P. WACH-JANKOWSKA**  
Short-term and short-range variations of $^{222}$Rn concentrations and fluxes from soil in Krakow, Poland  
European Geoscience Union General Assembly 2010  
Austria/Vienna 2010-05-02 2010-05-07  
POSTER

Annual variations of $^{222}$Rn concentration in soils in Krakow, Poland  
European Geoscience Union General Assembly 2010  
Austria/Vienna 2010-05-02 2010-05-07  
POSTER

17. **K. SAEED**  
Algorytm do identyfikacji człowieka na podstawie obrazu twarzy w różnych warunkach  
Metody biometryczne i kryptograficzne w zintegrowanych systemach bezpieczeństwa  
Polska/Warszawa 2010-05-07 2010-05-07  
ORAL

18. **Ł. GONDEK, H. FIGIEL**  
Neutron imaging of metal-hydride based hydrogen storage systems  
15th International Seminar on Neutron Scattering Investigation in Condensed Matter  
Polska/Poznań 2010-05-12 2010-05-15  
POSTER

19. **M. CZYŻYCKI, M. LANKOSZ, D. WĘGRZYNEK**  
Quantitative elemental imaging with X-ray fluorescence  
Micro-analytical techniques based on nuclear spectrometry for environmental monitoring and material studies  
Austria/Wiedeń 2010-05-16 2010-05-22  
ORAL

20. **K. MATUSIAK, A. JUNG**  
Zastosowanie modelowania kompartmentowego do szacowania dawek promieniowania jonizującego w diagnostyce medycznej MCSB 2010  
VII Konferencja Modelowanie Cybernetyczne Systemów Biologicznych  
Polska/Kraków 2010-05-21 2010-05-22  
ORAL

Growth and structure characterization of iron oxide films on Pt(111)  
High-Field Nanoscience Workshop  
Polska/Wrocław 2010-05-27 2010-05-28  
POSTER

22. **J. TOBOLA, P. ZWOLENSKI, S. KAPRZYK**  
Theoretical search for efficient dopants in Mg$_2$X (X=Si, Ge, Sn) thermoelectric materials  
The 29th International Conference on Thermoelectrics  
Chiny/Shanghai 2010-05-30 2010-06-03  
ORAL
23. K. Drogowska, M. Krupiński, A. Polit, Y. Zabila, M. Perzanowski, M. Marszałek, 
Structure and surface morphology of FePd thin alloy films 
9th Prague Colloquium on f-electron Systems 
Czechy/Praga 2010-05-30 2010-06-04 
POSTER

24. J. Fiedor, M. Baster, L. Fiedor, Kvetoslava Burda 
Temperature Effect on Organization of Photosynthetic Membranes of Rhodobacter sphaeroides studied by 
AFM technique 
International Nanomeasurement Conference 
Polska/Kraków 2010-06-03 2010-06-04 
POSTER

Xanes and x-ray photoemission study of the La0.67(Ca,Pb)0.33(Mn1-xFex)O3 compounds. 
10th International School and Symposium on Synchrotron Radiation in Natural Sciences ISSRNS 2010. 
Polska/Szklarska Poręba 2010-06-06 2010-06-11 
POSTER

Stable isotope composition of atmospheric CO2 at high mountain site (Kasprowy Wierch, southern Poland). 
Atmosphere Chemistry and Physics Symposium 
Szwajcaria/Interlaken 2010-06-06 2010-06-12 
ORAL

27. Ł. Chmura, J. M. Necki, M. Zimnoch, K. Rozanski, A. Vermeulen 
Comparison of the filtration procedures for CO2 and CH4 mixing ratio datasets from the high-mountain station 
Kasprowy Wierch, southern Poland 
Symposium on Atmospheric Chemistry and Physics at Mountain Sites 
Szwajcaria/Interlaken 2010-06-07 2010-06-11 
POSTER

28. T. Śležak, M. Zając, M. Śležak, K. Matlak, N. Spiridis, K. Freindl, D. Wilgocka-Śležak, 
R. Rüffer and J. Korrecki 
Depth-resolved magnetization structure at the spin reorientation transition in Fe/W(110) ultrathin films studied 
by the nuclear resonant scattering of synchrotron radiation 
10th International School and Symposium on Synchrotron Radiation in Natural Sciences ISSRNS 2010. 
Polska/Szklarska Poręba 2010-06-07 2010-06-11 
POSTER

29. P. Wachniew, M. Bodziony, P. Mazur, E. Lokas 
Chemical transformations of surface and subsurface waters in the proglacial zone 
International Polar Year Oslo Science Conference 
Norwegia/Oslo 2010-06-08 2010-06-12 
ORAL

Diurnal variation of trace gas concentrations measured at Kasprowy Wierch station, Tatra, 
Poland Symposium on Atmospheric Chemistry and Physics at Mountain Sites 
Szwajcaria/Interlaken 2010-06-08 2010-06-10 
POSTER

31. J. Wolny, P. Kuczera, R. Strząłka 
Application of the average unit cell concept to the 3d aperiodic Amman tiling 
11th International Conference on Quasicrystals 
Japonia/Sapporo 2010-06-11 2010-06-22 
POSTER
32. **P. KUCZERA**
The structure of decagonal Al-Ni-Co superstructure type I
11th International Conference on Quasicristals
Japonia/Sapporo 2010-06-11 2010-06-22
ORAL

33. **J. TOBOŁA, J LESZCZYNSKI, K KUTORASINSKI, B LENOIR**
Tuning of thermoelectric properties in double doped skutterudites
CIMTEC 2010 –12th International Conference on Modern Materials and technologies (5th Forum on New Materials)
Włochy/Riva del Garda 2010-06-13 2010-06-18
ORAL

34. **J. TOBOŁA, J LESZCZYNSKI, K KUTORASINSKI, B LENOIR**
Tuning of thermoelectric properties in double doped skutterudites
CIMTEC (5th Forum on New Materials)
Włochy/Montecatini Terme 2010-06-13 2010-06-18
ORAL

35. **M. DUDA, J. WOLNY**
Stable configurations of atoms in MgAl2 phases
11th International Conference on Quasicristals
Japonia/Sapporo 2010-06-13 2010-06-18
POSTER

36. **M. RYBAK, K. KUŁAKOWSKI,**
Critical mass effect in the contact process of decision making SOLSTICE 2010-2nd Summer Solstice International Conference on discrete models of complex systems
Francja/Nancy 2010-06-14 2010-06-18
POSTER

37. **M. PONIEDZIAŁEK, B. SZAFRAN,**
Anomalous current injection and interlaced Fano resonances of conductance of three terminal quantum ring.
Jaszowiec 2010
Polska/Krynica 2010-06-18 2010-06-25
POSTER

38. **M. LANKOSZ, M. SZCZERBOWSKA-BORUCHOWSKA, A. WANDZILAK,M. CZYŻYCKI,**
**P. WRÓBEL, D. ADAMEK, E. RADWAŃSKA, K. RICKERS, D. ZAJĄC**
Pilot studies of levels, speciation and chemical environments of iron and zinc brains cancers
European Conference on X-RaySpectrometry
Portugalia/Coimbra 2010-06-20 2010-06-25
ORAL

Monte Carlo simulation code for confocal 3D micro-XRF analysis of stratified materials European Conference on X-RaySpectrometry
Portugalia/Coimbra 2010-06-20 2010-06-25
ORAL

40. **P. RYDYGIER, P. WIACEK, T. FIUTOWSKI, W. DABROWSKI,**
Low Power, High Dynamic Range, Sample and Hold Circuit and Analogue Multiplexer for Multi-channel Recording of Neuronal Signals
17th International Conference Mixed Design of Integrated Circuits and Systems
Polska/Wroclaw 2010-06-23 2010-06-26
POSTER
41. P. GAWROŃSKI, K. KUŁAKOWSKI,
Crowd dynamics - being stuck
Conference on Computational Physics
Norwegia/Trodheim 2010-06-23 2010-06-26
POSTER

42. W. SIKORA, J. CIEŚLAK, S. DUBIEL, J. TOBOŁA,
Theoretical calculations of magnetic properties of \(\sigma\)-Fe\(_{54}\)Cr\(_{46}\) alloy
52 Konwersatorium Krystalograficzne
Polska/Wrocław 2010-06-24 2010-06-25
POSTER

43. W. SIKORA, A. KUNA,
The symmetry analysis of structural deformations in Mg(BH\(_4\))\(_2\) borohydride
52 Konwersatorium Krystalograficzne
Polska/Wrocław 2010-06-24 2010-06-25
POSTER

44. J. WOLNY, M. DUDA,
Stable configurations of atoms in Mg\(_2\)Al\(_3\) phases
52 Konwersatorium Krystalograficzne
Polska/Wrocław 2010-06-24 2010-06-25
POSTER

45. J. WOLNY, P. KUCZERA, R. STRZAŁKA
Application of the average unit cell concept to the 3d aperiodic amman tiling
53 Konwersatorium Krystalograficzne
Polska/Wrocław 2010-06-24 2010-06-25
ORAL

46. S. DUBIEL, B. F. O. COSTA, J. CIEŚLAK,
Debye temperature in Fe-rich Fe-Cr alloys Materials Topical Group - W WALloys-ODS-REMEV
Monitoring Meeting CEIT
Hiszpania/San Sebastian 2010-06-27 2010-07-02
ORAL

47. S. DUBIEL, J. CIEŚLAK, H. REUTHER
Determination of short-range-order in Fe-Cr alloys* Materials Topical Group-W Walloys-ODSF-REMEV
Monitoring Meeting CEIT
Hiszpania/San Sebastian 2010-06-28 2010-07-02
ORAL

48. M. KRAWCZYK
Communities in five networks: a meta-analysis
The International Sunbelt Social Network Conference
Włochy/Trento 2010-06-28 2010-07-04
ORAL

49. P. HOTTOWY, BEGGS J M, CHICHLINSKY E J, DĄBROWSKI W., FIUTOWSKI T.,
GUNNING D E, HOBBS J, JEPSON L, KACHIGUINE S, MATHIESON K, RYDYGIER P, SHER A,
SKOCZEN A., LITKE A M
512-electrode MEA System For Spatio-TempORAL Distributed Stimulation and Recording of Neural Activity
7th International Meeting on Substrate-Integrated Microelectrode Arrays
Niemcy/Reutlingen 2010-06-29 2010-07-03
ORAL
50. P. Gawroński, Blanco Juan Mari, Chizhik Alexander and Gonzalez Julian
   Remagnetization process of a Fe-rich amorphous wire under time dependent tensile stress
   European Conference on Magnetic Sensors and Actuators
   Turcja/2010-07-02 2010-07-07
   POSTER

51. M. Jedrychowski, J. Tarasiuk, B. Bacroix
   Investigation of deformed and recrystallized textures in zirconium
   International Conference on Recrystallization and Grain Growth. Rex and GGIV
   Wielka Brytania/Sheffield 2010-07-04 2010-07-09
   POSTER

52. J. Tarasiuk, B. Bacroix, Kr. Wierzbowski, S. Wroński, Ph. Gerber
   Room temperature recovery in rolled polycrystalline copper after many years
   International Conference on Recrystallization and Grain Growth. Rex and GGIV
   Wielka Brytania/Sheffield 2010-07-04 2010-07-09
   ORAL

53. P. Gawroński, Zhukova Valentina, Zhukov Arcady and Gonzalez Julian
   Magnetic properties of Fe$_{75}$B$_{15}$Si$_{10}$ microwires
   International Workshop on Magnetic Wires
   Turcja/Bodrum 2010-07-08 2010-07-09
   POSTER

54. K. Kułakowski, M. J. Krawczyk, P. Gawroński,
   Hate: no choice. Agent simulations.
   XVII ISA World Congress of Sociology
   Szwecja/Goeteborg 2010-07-11 2010-07-18
   ORAL

55. A. Mańka-Krasoń, K. Kułakowski,
   Ising antiferromagnetism of random networks with tunable clusterization
   New Frontiers in complex network:Statphys24 satellite meeting
   Korea Płd./Seul 2010-07-12 2010-07-16
   POSTER

56. K. Koźla, H. Figiel, J. Przewoźnik, Ł. Gondek, A. Szytula
   Structural and magnetic properties of PrPdInH and NdPdInH hydrides.
   International Symposium on Metal-Hydrogen Systems 2010
   Rosja/Moskwa 2010-07-19 2010-07-23
   POSTER

57. M. Ornat, A. Paja,
   The effect of hydrogenation on the electrical resistivity of disordered alloys
   International Symposium on Metal-Hydrogen Systems 2010
   Rosja/Moskwa 2010-07-19 2010-07-23
   POSTER

58. A. Żywczac, D. Shinya, Ł. Gondek, A. Takasaki and H. Figiel
   Hydriding Ti$_{45}$Zr$_{38}$Ni$_{17}$-M$_{x}$ (M - 3d metals) intermetallic compounds
   International Symposium on Metal-Hydrogen Systems 2010
   Rosja/Moskwa 2010-07-19 2010-07-23
   POSTER
59. **Nivas Babu Selvaraj, Ł. Gondek, N. Kardjilov, H. Figiel**

Visualising hydrogen absorption/desorption in a MH storage tank using Neutrons
International Symposium on Metal-Hydrogen Systems 2010
Rosja/Moskwa 2010-07-19 2010-07-23
ORAL

60. **A. Szkudlarek, A. Fernández-Pacheco, J. M. de Teresa, R. Córdoba, M. R. Ibarra**

Magnetization reversal in cobalt nanostructures created by focused-electron-beam-induced-deposition.
ECCL 2010 meeting
Polska/Sterdyń 2010-08-16 2010-08-24
ORAL

61. **R. Strzałka**

The difficult world of quasicrystals
International Conference of Physics Students
Austria/Graz 2010-08-17 2010-08-23
ORAL

62. **P. Pedra**

Archimedes Sandbox
International Conference of Physics Students
Austria/Graz 2010-08-17 2010-08-23
ORAL

63. **M. Kuś**

Singing sand
International Conference of Physics Students
Austria/Graz 2010-08-17 2010-08-23
ORAL

64. **K. Burda, M Lipińska, A Orzechowska, J Fiedor, A I Chumakov, T Ślęzak, M Zając, K Matla, J Korecki, K Strzałka, L Fiedor**

Spin states of the non-heme iron and collective motions of the protein matrix in type II bacterial reaction centers.
15th International Congress of Photosynthesis Beijing 2010
Chiny/Beijing 2010-08-22 2010-08-27
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65. **A. Halas, M Lipińska, A Orzechowska, J Fiedor, A I Chumakov, T Ślęzak, M Zając, K Matla, J Korecki, K Strzałka, L Fiedor, and K Burda**

Spin states of non-heme iron and protein local motions in reaction centers from purple photosynthetic bacterium Rhodospirillum rubrum modified by Cd²⁺
15th International Congress of Photosynthesis Beijing 2010
Chiny/Beijing 2010-08-22 2010-08-27
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66. **A. Orzechowska, M Lipińska, J Fiedor, A I Chumakov, T Ślęzak, M Zając**

The influence of Cu²⁺ ions on the spin state and dynamics of non-heme iron in photosynthetic reaction centers from Rhodobacter sphaeroides
15th International Congress of Photosynthesis Beijing 2010
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67. **K. DROGOWSKA, Z. TARNAWSKI, NHU-TARNAWSKA HOA., BRUDNIK A., SOKOŁOWSKI M., ZAKRZEWSKA K., BALOCH A.**
   Application of RBS, GIXR and optical reflectivity in the studies of Ti/TiO$_2$/Ti thin films deposited on Si(111)
   27th European Conference on Surface Science
   Holandia/Groningen 2010-08-29 2010-09-03
   POSTER

68. **M. SIKORA, CZESLAW KAPUSTA, JANUSZ PRZEWOŹNIK, JOANNA STĘPIEŃ, K. SCHNEIDER, D. POMYKALSKA, M. BUČKO, M. RĘKAS**
   Magnetic moments and valence of Mn in the yttrium stabilized zirconia
   EPS CMD23
   Polska/Warszawa 2010-09-01 2010-09-01
   ORAL

69. **B. WIENDELCHA, STANISŁAW KAPRZYK, JANUSZ TOBOŁA,**
   Magnetism of the superconducting weak ferromagnet Y$_3$Co$_3$
   17th International Conference on Solid Compounds of Transition Elements
   Francja/Annecy 2010-09-05 2010-09-10
   POSTER

70. **J. TOBOŁA, P. ZWOLENSKI, STANISŁAW KAPRZYK,**
   Theoretical search for efficient dopants in Mg2X (X= Si, Ge, Sn) thermoelectric materials
   SCTE 2010 Solid Compounds of Transition Elements
   Francja/Annecy 2010-09-05 2010-09-11
   POSTER

71. **J. CIEŚLAK, S. DUBIEL, W. SIKORA, J. TOBOŁA,**
   Theoretical calculations of magnetic properties of $\alpha$-Fe$_{54}$Cr$_{46}$ alloy
   17th International Conference on Solid Compounds of Transition Elements
   Francja/Annecy 2010-09-05 2010-09-10
   ORAL

72. **DINH CHAU NGUYEN, NOWAK J., RAJCHEL L.**
   $^{226}$Ra, $^{228}$Ra and their activity ratio in polish carpathian mineral waters of different chemical composition
   LSC 2010 Advances in Liquid Scintillation Spectrometry
   Francja/Paryż 2010-09-06 2010-09-10
   ORAL

73. **J. NOWAK, DINH CHAU NGUYEN, RAJCHEL L.**
   Natural radioactivity of thermal waters of Podhale trough-preliminary results
   XXXVIII International Association of Hydrogeologists Congress
   Polska/Kraków 2010-09-12 2010-09-17
   POSTER

74. **J. CIEŚLAK, S. DUBIEL, J. TOBOŁA,**
   Experimental and theoretical study of the phase in Fe-Cr and Fe-V alloys 3rd Joint International Conference on Hyperfine Interactions and Intern Nuclear Quadrupole Interactions
   Szwajcaria/Genewa 2010-09-13 2010-09-17
   POSTER

75. **P. ARMATYS, J. NIZIOŁ, E. GONDEK, A. DANIEL, M. POKLADKO, J. SANETRA**
   Organiczne ogniwa słoneczne typu heterozłącze objętościowe.2 Badania eluipsometryczne cienkich warstw polymerów o zastosowaniach elektro-optycznych. 3 Zastosowanie materiałów organicznych w fotowoltaice.
   XVII Ogólnopolska Konferencja Kryształy Molekularne
   Polska/Polanica Zdrój 2010-09-13 2010-09-18
   POSTER
76. J. NIZIOŁ, P. ARMATYS, M. POKLADKO, E. GONDEK, A. DANEL, J. SANETRA
XVII Ogólnopolska Konferencja Kryształy Molekularne 2010 
Polska/Polanica Zdroj 2010-09-13 2010-09-18 
POSTER

77. P. ARMATYS, JACEK NIZIOŁ, E. GONDEK, A. DANEL, M. POKLADKO, J. SANETRA
Organiczne ogniwa słoneczne typu heterozłącze objętościowe 
XVII Ogólnopolska Konferencja KRYSZTAŁY MOLEKULARNE 
Polska/Polanica Zdroj 2010-09-13 2010-09-18 
POSTER

78. M. KRAWCZYK, K. KULAKOWSKI, 
Networks of ground states of frustrated systems 
ECCS 10 European Conference on Complex Systems 
Portugalia/Lisbona 2010-09-13 2010-09-17 
POSTER

79. P. WACH-JANKOWSKA, M. BONCZYK, P. WACHNIEW, Z. GORCZYCA, M. GĄSIOREK 
Annual variations of $^{222}$Rn concentration in soils in Krakow 
10th International Workshop on the Geological Aspects of Radon Risk Mapping 
Czechy/Praga 2010-09-22 2010-09-25 
POSTER

80. M. JABŁONSKA, T. SKÓRKA, U. TYRANKIEWICZ, H. FIGIEL, 
Application of cluster analysis for the assessment of the left ventricle long-axis orientation in mice with heart failure 
VI Sympozjum Magnetic resonance in chemistry, physics and biological sciences 
Polska/Warszawa 2010-09-22 2010-09-24 
ORAL

81. J. ŚWIEBOCKA-WIEK, H. FIGIEL, 
Application analysis of adaptive weight smoothing algorithm and wavelet transform for the noise removing in magnetic resonance imaging 
VI Sympozjum Magnetic resonance in chemistry, physics and biological sciences 
Polska/Warszawa 2010-09-22 2010-09-24 
ORAL

82. T. KUC, W. POHORECKI, B. OSTACHOWICZ, P. BILSKI 
Novel methods of tritium production rate measurements in hcl tbm mock-up experiment with liquid scintillation technique. 
26th Symposium on Fusion Technology 
Portugalia/Porto 2010-09-27 2010-10-01 
ORAL

83. T. SZUMLAK 
First Results from the LHCb Vertex Locator 
8th International Conference on Radiation Effects on Semiconductor Devices and Materials 
Włochy/Florencja 2010-10-12 2010-10-15 
ORAL

84. J. NOWAK, DINH CHAU NGUYEN, L. RAJCHEL 
Wstępne pomiary naturalnej promieniotwórczości wód termalnych z polskich Karpat wewnętrznych 
Polska/Zakopane 2010-10-14 2010-10-16 
POSTER
85. J. TOMKOWICZ, J. GONZALEZ, K. KUŁAKOWSKI,
Asymmetric hysteresis loops of systems of bistable nanoscopic wires
5th International Conference on Surfaces
Francja/Reims 2010-10-19 2010-10-21
ORAL

86. A. KUNA, W. SIKORA,
Structural phase transitions of light metal borohydrides the symmetry analysis
European Integrated Center for the Development of New Metallic Alloys and Compounds (C-MAC)
Niemcy/Drezno 2010-11-15 2010-11-18
POSTER

87. S. WROŃSKI, K. WIERZBANOWSKI, A. BACZMAŃSKI, S. WROŃSKI, P. LIPINSKI AND A. LODINI
Predictions of mechanical properties of b-Al-Mg alloy- Example of compression and rolling
C-MAC Days2010
Niemcy/Drezno 2010-11-15 2010-11-18
POSTER

88. P. KOCJAN, K. SAEED,
Wyznaczenie poszczególnych cech antropometrycznych twarzy oraz ich dalsza obróbka z wykorzystaniem macierzy Toeplitza.
BIOMETRIA 2010
Polska/Warszawa 2010-12-01 2010-12-01
ORAL

89. W. ŁUŻNY, K. PIWOWARCZYK,
Hydrogen bonds in camphorsulfonic acid doped polyaniline VIII International Conference on X-Ray Investigations of Polymer Structure
XIPS 20-10
Polska/Wrocław 2010-12-08 2010-12-10
POSTER

90. A. BERNASIK, J. HABERKO, J. RYSZ, M. MARZEC, A. BUDKOWSKI AND W. ŁUŻNY
Morphology of Pani(CSA)-Pš Thin Films Studied by Means of Scanning Probe Microscopy.
Polska/Wrocław 2010-12-08 2010-12-10
ORAL
Scientific events

Titles, positions, etc.

FULL PROFESSOR POSITION

Jarosław Pszczoła
1.12.2010

ASSOCIATE PROFESSOR POSITION

Bartłomiej Szafran
1.1.2010

Ryszard Radwański
7.10.2010 (Uniwersytet Pedagogiczny w Krakowie)

Habiliations and PhD Defenses

HABILITATIONS

Dariusz Węgrzynek
18.10.2010

Andrzej Bernesik
26.04.2010

Filipowicz Mariusz
25.10.2010 (Wydział Energetyki i Paliw AGH)

PHD DEFENSES

Katarzyna Grymek-Wąchocka
„Badanie in vitro wpływu mutacji cichych na oligomeryzację receptorów błonowych z zastosowaniem technik fluorescencyjnych”
- promotor - prof. dr hab. Marta Dziedzicka-Wasylewska
- obrona - 1.02.2010r

Monika Klisch (wyróżnienie)
„Kompleksowe badania izotopowe laminowanych osadów jeziora Gościąź”
- promotor - prof. dr hab. inż. Kazimierz Różański
- obrona - 22.03.2010r

Łukasz Chmura
„Gazy cieplarniane w atmosferze Polski Południowej zmienność czasowo-przestrzenna w okresie 1994 – 2007”
- promotor - prof. dr hab. inż. Kazimierz Różański
- obrona - 22.03.2010r

Dariusz Orzechowski
„Analiza dyfrakcyjna układów aperiodycznych”
- promotor - prof. dr hab. Janusz Wolny
- obrona - 25.10.2010r
Wojciech Tabiś (wyróżnienie)
„Badanie dynamicznych zmian struktury krystalicznej w magnetycie”
- promotor - dr hab. inż. Andrzej Kozłowski
- obrona - 22.11.2010r

Karolina Półtorak
„Front-end electronics in submicron CMOS technologies for tracking detectors in future particle physics experiments”
- promotor - prof. dr hab. inż. Władysław Dąbrowski
- obrona - 20.12.2010r

Organized Conferences

INTERNATIONAL CONFERENCE ON COMPUTER INFORMATION SYSTEMS AND INDUSTRIAL MANAGEMENT APPLICATIONS WITH APPLICATIONS TO AMBIENT INTELLIGENCE AND UBIQUITOUS SYSTEMS
Cracow, October 8 - 10, 2010

WORKSHOP ON TIMING DETECTORS: ELECTRONICS, MEDICAL AND PARTICLE PHYSICS APPLICATIONS
Cracow, November 29 - December 1, 2010

Faculty Seminars

2010/01/15
"GMT (Greenwich Mean Time) – Historia”, prof. dr hab. Kazimierz Przewłocki (WFIiS AGH)

2010/01/29
1) "An Overview of Teaching and Research Activities at Ca’ Foscari University of Venice”,
2) "Static program analysis using abstract interpretation”, prof. Agostino Cortesi (Ca’ Foscari University of Venice)

2010/03/05
"A Topic Toward Advanced AI – KANSEI”, Prof. Tomomasa Nagashima (Design and Manufacturing at the Graduate School of Engineering, Muroran Institute of Technology, Japan)

2010/03/19
"Fizyczne aspekty radioterapii wiązkami jonów”, doc. dr hab. Paweł Olko (Zakład Fizyki Radiacyjnej i Dozimetrii IFJ)

2010/03/26
"Nauki obliczeniowe jako propozycja makrokierunku”, dr hab. inż. Krzysztof Banaś, prof. AGH (WIMiIS AGH)

2010/04/16
"Statystyka danych samoskorelowanych”, prof. dr hab. inż. Andrzej Zięba (KFMS WFIiS AGH)

2010/04/23
"Strange behaviour at the band edges of amorphous semiconductors and a stranger idea about the Schrödinger equation”, Prof. Gwynne James Morgan (University of Leeds)
2010/04/30
"Struktura Mg2Al3 - układu o gigantycznej komórce elementarnej", prof. dr hab. Janusz Wolny (Katedra Fizyki Materii Skondensowanej WFiIS AGH)

2010/05/14
"Rola wybranych układów redoksowych w biofizyce stresu oksydacyjnego komórki upigmentowanej. Podejść systemowe", dr Zenon Matuszak (KFMiB WFiIS AGH)

2010/05/21
"O największej molekule mionowej", dr Wilhelm Czapliński (KZFJ WFiIS AGH)

2010/05/28
"W poszukiwaniu sensu w świecie widzialnym", prof. Andrzej Śluzek (Nanyang Technological University Singapore)

2010/06/11
"Konfokalna mikroskopia rentgenowska", dr Dariusz Węgrzynek (KFMiB WFiIS AGH)

2010/06/25
"Mechanical properties of biomaterials studied with AFM", Prof. Jose Luis Toca-Herrera (Parque tecnologico de San Sebastian, Spain)

2010/10/08
"Seminarium dziekańskie", prof. dr hab. inż. Wojciech Łużny, dr hab. Andrzej Lenda oraz dr inż. Krzysztof Małarz (WFiIS AGH)

2010/10/15
"Czy będzie lepiej - szkolnictwo wyższe w świetle nowych rozwiązań prawnych", prof. dr hab. inż Marek Przybylinski (WFiIS AGH)

2010/10/22
"30 lat badań nadprzewodnictwa w Zakładzie (Katedrze) Fizyki Ciała Stałego", prof. dr hab. Andrzej Kołodzieczyk (KFCS WFiIS AGH)

2010/10/29
"Właściwości magnetyczne i elektronowe wybranych perowskitów manganowych domieszkowanych żelazem i cyną", dr Janusz Przewoźnik (KFCS WFiIS AGH)

2010/11/05
"Towards the Evolution of Smart Information Systems: Challenges, Perspectives, Directions", prof. Ajith Abraham (MIR Laboratories, USA)

2010/11/19
"Modulacje magnetyczne i strukturalne w tlenowych związках manganu", dr hab. Radosław Przeniosło, prof. UW (Instytut Fizyki Doświadczalnej, Wydział Fizyki Uniwersytetu Warszawskiego)

2010/11/26
"Studnie kwantowe, a anizotropia magnetyczna", prof. dr hab. inż. Marek Przybylinski (KFCS WFiIS AGH, Max-Planck-Institut fur Mikrostrukturphysik, Halle, Niemcy)

2010/12/03
"Biofotonika i nowe metody obrazowania medycznego", dr hab. Maciej Wojtkowski (Instytut Fizyki Uniwersytetu Mikołaja Kopernika)

2010/12/10
"Present status of LHC, upgrade plans and future accelerators", Prof. Frederick Bordry (CERN)