Faculty of Physics, Adam Mickiewicz University
Institute of Molecular Physics, Polish Academy of Sciences

The European Conference
PHYSICS OF MAGNETISM'05

ABSTRACTS

Poznań 2005

The European Conference
PHYSICS OF MAGNETISM'05
June 24-27, 2005
Poznań Poland
Abstracts

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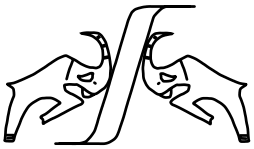

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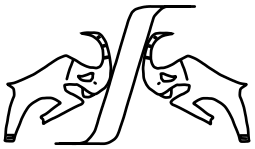

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SCHEDULE

Friday, June 24

8^{55} **OPENING**
R. Micnas, A. Jezierski

I.1 STRONGLY CORRELATED ELECTRONS
Chairmen: R. Micnas, A. Jezierski

9^{00}- 9^{30} **W. METZNER** Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
Magnetic and superconducting correlations in the 2D Hubbard model

9^{30}-10^{00} **B.R. BUŁKA** Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
Correlations in electronic transport through nanostructures

10^{00}-10^{30} **P. HORSCH** Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
Magnetism and charge response in quasi-1d Wigner lattice compounds

10^{30}-11^{00} **B. DĄBROWSKI** Physics Department, Northern Illinois University, DeKalb, USA
Magnetic properties of nonstoichiometric and substituted $SrRuO_3$

11^{05}-11^{30} coffee break

I.2 MOSTLY MAGNETIC NANOSTRUCTURES
Chairman: J. Baszyński

11^{30}-12^{00} **G. BAYREUTHER** Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Regensburg, Germany
Ground state properties and spin excitations in ferromagnetic nanostructures

12^{00}-12^{30} **A. EHRESMANN** Fachbereich Naturwissenschaften, Universität Kassel, Kassel, Germany
In-plane magnetic micro- and nanopatterns: fundamentals, applications, and possibilities

12^{30}-13^{00} **A. MAZIEWSKI** Institute of Experimental Physics, University of Białystok, Białystok, Poland
New spin configurations in nano-sized magnets near reorientation phase transitions

13^{00}-13^{30}	**M. MIGLIERINI**	Department of Nuclear Physics and Technology, Slovak University of Technology, Bratislava, Slovakia

Magnetic microstructure of NANOPERM-type nanocrystalline alloys

13^{35}-15^{00} lunch break

15^{00}-16^{40} **ORAL SESSIONS**

O1 Chairman: K.I. Wysokiński
(O-1-15, O-1-07, O-1-03, O-1-09, O-1-12, O-1-14)

O2 Chairman: A. Ślebarski
(O-4-05, O-2-04, O-2-08, O-2-09, O-3-01)

16^{40}-17^{00} coffee break

17^{00}-18^{30} **POSTER SESSION I** (categories 2, 6, 7)

18^{45}- 20^{15} **WELCOME PARTY**

20^{30} **TRANSPORTATION TO HOTEL**

Saturday, June 25

I.3 HIGH TEMPERATURE SUPERCONDUCTORS

Chairman: S. Robaszkiewicz

9^{00}- 9^{30} **K. MAKI** Department of Physics and Astronomy, University of Southern California, Los Angeles, USA

D-wave density waves in high T_c cuprates and $CeCoIn_5$

9^{30}-10^{00} **C. DI CASTRO** Dipartimento di Fisica, Universita' di Roma "La Sapienza", and Istituto Nazionale per la Fisica della Materia, Rome, Italy

Charge-ordering fluctuations and anomalous Raman response in cuprates

10^{00}-10^{30} **S. MAEKAWA** Institute for Materials Research, Tohoku University, Sendai, Japan

Spin-charge separation and non-linear optical response in one-dimensional cuprates

10^{30}-11^{00} **D. POILBLANC** Laboratoire de Physique Théorique, Université Paul Sabatier and CNRS, Toulouse, France

Doped 2D frustrated quantum magnets: spin-charge separation and non-conventional superconductivity

11^{05}-11^{30} coffee break

I.4 MOSTLY MAGNETIC PROPERTIES

Chairman: H. Szymczak

11^{30}-12^{00} **K. DÖRR** Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden Dresden, Germany

Magnetism in manganites and manganite-titanate biferroics

12^{00}-12^{30} **S. BLÜGEL** Institut für Festkörperforschung, Forschungszentrum Jülich, Jülich, Germany

Magnetic tunneljunctions made from half-metals

12^{30}-13^{00} **H. EBERT** Department Chemistry/Physical Chemistry, Ludwig-Maximilians-University of Munich, Munich, Germany

Relativistic and correlation effects in magnetic solids

13^{00}-13^{30} **R. WIESENDANGER** Institute of Applied Physics and Microstructure Advanced Research Center Hamburg (MARCH), University of Hamburg, Hamburg, Germany

Physics of nanomagnetism revealed by spin-polarized scanning tunneling spectroscopy

13^{35}-15^{00} lunch break

15^{00}-16^{40}	**ORAL SESSIONS** **O3** Chairman: B. Fechner (O-2-05, O-2-10, O-2-11, O-2-12, O-2-15) **O4** Chairman: A. Szytuła (O-1-01, O-1-05, O-1-06, O-1-08, O-1-11)
16^{45}-17^{30}	**TRANSPORTATION TO PALACE IN KÓRNIK**
18^{00}- 21^{00}	**BANQUET**
21^{15}	**TRANSPORTATION TO HOTEL**

Sunday, June 26

I.5 MOSTLY DILUTED MAGNETIC SEMICONDUCTORS, SPINTRONICS AND MIXED VALENCE
Chairman: S. Krompiewski

9^{00}- 9^{30} **T. DIETL** Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
Carrier-controlled ferromagnetic semiconductors

9^{30}-10^{00} **B.L. GALLAGHER** School of Physics and Astronomy, University of Nottingham, Nottingham, UK
GaMnAs materials and nanoscale devices

10^{00}-10^{30} **P. DEDERICHS** Institut für Festkörperforschung, Forschungszentrum Jülich, Jülich, Germany
Percolation effects in dilute magnetic semiconductors

10^{30}-11^{00} **P. WACHTER** Laboratorium für Festkörperphysik, ETH Zürich, Zürich, Switzerland
Superfluidity in condensed excitons below 20 K

11^{05}-11^{30} coffee break

11^{30}-13^{40} **ORAL SESSIONS**
O5 Chairman: A.M. Oleś
(O-1-13, O-7-02, O-7-01, O-2-14, O-6-02, O-2-13, O-3-02)

O6 Chairman: Z. Jacyna-Onyszkiewicz
(O-6-01, O-3-03, O-3-06, O-1-10, O-2-01, O-4-01, O-4-02)

13^{40}-15^{00} lunch break

15^{00}-16^{30} **POSTER SESSION II** (categories: 1, 3, 4, 5)

FREE TIME

Monday, June 27

I.6 SPIN DEPENDENT TRANSPORT, MAGNETIC JUNCTIONS AND MAGNETIC LAYERS

Chairman: J. Barnaś

9^{00}- 9^{30} **A. FERT** Unité Mixte de Physique CNRS-Thomson CSF, Orsay, France
Magnetization reversal by injection and transfer of spin: experiments and theory

9^{30}-10^{00} **S. YUASA** National Institute of Advanced Industrial Science and Technology (AIST) Tsukuba, Japan and PRESTO, Japan Science and Technology Agency (JST), Saitama, Japan.
Giant room-temperature TMR effect in magnetic tunnel junctions with MgO(001) tunnel barrier

10^{00}-10^{30} **B. HILLEBRANDS** Fachbereich Physik, Technische Universität Kaiserslautern, Kaiserslautern, Germany
Propagation, tunneling and phase shift of spin waves at a magnetic field inhomogeneity

10^{30}-11^{00} **H. PUSZKARSKI** Institute of Physics, A. Mickiewicz University, Poznań, Poland
Magnetic excitations in magnonic crystals and in small magnetic particles

11^{05}-11^{30} coffee break

I.7 LOW DIMENSIONAL MAGNETISM

Chairman: L. Kowalewski

11^{30}-12^{00} **R.K. KREMER** Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
Frustrated antiferromagnetic quantum chain systems

12^{00}-12^{30} **J. SZNAJD** W. Trzebiatowski Institute for Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland
Renormalization group approach to weakly interacting spin and Fermion chains

12^{30}-13^{30} **ORAL SESSION** (O-4-04, O-1-02, O-1-04)

13^{30}-15^{00} lunch break

I.8 MOSTLY HEAVY FERMION SYSTEMS
Chairman: R. Troć

15^{00}-15^{30} **F. STEGLICH** Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany
Unconventional forms of superconductivity and quantum criticality in heavy-electron metals

15^{30}-16^{00} **J. SPAŁEK** M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland
Magnetic properties of almost localized Fermions - revisited

16^{00}-16^{30} **SUMMARY** and **CLOSING**

INVITED LECTURES

A.F. Andreev

P.L.Kapitza Institute for Physical Problems, Moscow, Russia

Ground state properties and spin excitations in ferromagnetic nanostructures.

G. Bayreuther
Institut für Experimentelle und Angewandte Physik
Universität Regensburg
D-93040 Regensburg, Germany

The confinement of electrons in one or more dimensions of space in ferromagnetic nanostructures has pronounced consequences for most magnetic properties. The reason is the cooperative or collective nature of ferromagnetism which implies a fundamental influence of the coordination and of local symmetry. On the other hand, with the shrinking dimensions of devices like high density magnetic memories the related phenomena become technologically more and more relevant. In this presentation experimental results on epitaxial ultrathin films and nanostructures are discussed on the following aspects:

enhanced ground state magnetic moments
interface magnetic anisotropies
spin excitations and phase transitions.

Characteristic changes are observed when the transition is made from bulk material to ultrathin films in the monolayer range and from extended films to artificially patterned dot arrays with sub-micrometer dot diameter. In particular, the magneto-crystalline anisotropy at an interface is affected by the reduced symmetry and coordination. In addition to the well-known out-of-plane surface anisotropy an in-plane interface anisotropy is found which shows a universal behavior and has the opposite sign compared to the respective volume anisotropy. It is demonstrated that this effect is exclusively determined by the specific lattice symmetry (bcc or fcc).
Finally, it is shown that reduced dimensions significantly alter the spectrum and energies of spin excitations. Especially, continuously enhanced thermal spin excitations and a lowering of the Curie temperature, T_C, are observed when the film thickness is reduced to a few atomic layers and when a continuous film is patterned into circular dots with decreasing diameter. The effect of magnetic anisotropies on spin wave excitations and on T_C predicted by theory is discussed with respect to second order (uniaxial) and fourth order anisotropies.

Magnetic tunneljunctions made from half-metals

Stefan Blügel
IFF, Forschungszentrum Jülich, D-52425 Jülich, Germany

Half-metallic ferromagnets are ferromagnetic materials showing, in the ideal case, 100% spin polarization at the Fermi level E_F, due to a metallic density of states in one spin direction (usually majority spin) combined with a band gap in the other spin direction (usually minority spin). In principle, half-metallic ferromagnets are ideal spin injectors and detectors, because under moderate voltage they can carry current in only one spin direction. Therefore, they also constitute ideal components for tunneling magnetoresistant (TMR) devices, with two half-metallic leads sandwiching a nonmagnetic semiconducting or insulating spacer. On the other hand, the tunneling current in these TMR devices is very small so that the conventional interpretation in terms of a Landauer-Büttiker picture of ideal interfaces are bound to fail. In this talk we emphasize that interface states at the interfaces of tunneljunctions can have severe implications on the tunnel-magnetoresistance ratio. We propose an antiferromagnetically coupled TMR element made of half-metals without interface state based on an *a priori* understanding of the exchange interactions in such systems, as a paradigm of materials design from first principles.

CORRELATIONS IN ELECTRONIC TRANSPORT THROUGH NANOSTRUCTURES

B.R. Bułka[1], T. Kostyrko[2] and P. Stefański[1]

[1] Institute of Molecular Physics, Polish Academy of Sciences,
ul. M. Smoluchowskiego 17, 60-179 Poznań, Poland

[2] Institute of Physics, A. Mickiewicz University,
ul. Umultowska 85, 61-614 Poznań, Poland

In devices of a nanoscale two phenomena play crucial role in electronic transport: coherent transmission and electronic correlations. Some recent results of coherent transport in a presence of strong electron correlations are presented. In particular we are interested in many-body effects, as the Kondo resonance. As an example a system with two quantum dots connected in series is considered, for which all many-electron correlation functions are determined for an arbitrary number of electrons. The studies predict a new feature in transport resulting from transmission through a triplet state, which can be activated for larger source-drain voltages. An analysis of the spin-spin correlation function allows an insight into formation of the total spin and its influence on transport. The quantum interference effect is also seen in the conductance through the double quantum dot. For a large quantum dot one can expect a discrete set of pointer states, which make conditions for the Fano resonance. Our theoretical results for the conductance are in good agreement with experimental measurements on semi-open quantum dots.

Charge-ordering fluctuations and anomalous Raman response in Cuprates

C. Di Castro
Dipartimento di Fisica, Universita' di Roma "La Sapienza",
and Istituto Nazionale per la Fisica della Materia
Piazzale Aldo Moro 2, I-00185 Roma, Italy

The stripe quantum critical point theory for high T_c superconductors was shown to imply various pseudogap-formation-temperatures with soft and hard pseudogaps, scaling form for optical conductivity and an anomalous isotope effect. We point out here that there is a direct contribution of charge collective fluctuations to the Raman spectra, which becomes a nice probe of the theory. We find that the critical charge collective modes can or cannot be excited depending on the direction of their wavevector and on the polarization of the incoming and outgoing photons. This provides a direct confirmation that the order associated to the quantum critical point near optimal doping of Cuprates occurs at finite wavevectors.

Magnetic Properties of Nonstoichiometric and Substituted $SrRuO_3$

B. Dąbrowski

Physics Department, Northern Illinois University, DeKalb, IL 60115, USA

$SrRuO_3$ has been known for half a century as a strongly-correlated ferromagnetic metal and proposed for use as an electrode material in micro- and nano-electronic circuits. We have discovered that annealing of stoichiometric $SrRuO_3$ perovskites in high-pressure oxygen produces $SrRu_{1-v}O_3$ compounds with vacancies on the Ru-sites. The creation of Ru vacancies rapidly suppresses ordered moment per Ru from 1.6 to 0.8 μ_B and the ferromagnetic ordering temperature, T_C, from 163 K to 45 K with increase of $v \approx 0.09$, whereas the resistivity increases. Subtle structural changes that accompany creation of Ru-site vacancies are different from the typical properties of transition metal perovskites, for which an increased formal oxidation state of the B-site cations normally leads to decreased B-O interatomic distances and contraction of the unit cell volume. The reduced charge screening caused by the Ru-vacancies offsets expected decrease of the average interatomic distance Ru-O and rotation of the RuO_6 octahedra as Sr atoms relax toward Ru-vacancies increases observed volume. Local probes of Ru with XANES, NMR, and EELS find no valence change while isomer shifts of ^{99}Ru from Mossbauer experiments reveal a small change from +4 toward +5 as the T_C decreases.

By using "design rules" of the synthesis and magnetic interactions for perovskites we have established that Cr substitution into Ru site of $SrRuO_3$ increases T_C to 188 K at the solubility limit of12%. The ^{53}Cr and ^{99,101}Ru NMR studies reveal that the electronic configurations of Cr and Ru are $3d^3$ ($t_{2g}^{3\uparrow}$) and $4d^4$ ($t_{2g}^{3\uparrow 1\downarrow}$), respectively. Compared with $SrRuO_3$, the spin-down electron in Ru 4d shell is more itinerant in $SrRu_{0.875}Cr_{0.125}O_3$ which is consistent with a broadened conduction band and a possible minority band $Cr(d^3)$-O^{2-}-$Ru(d^4)$ double-exchange-like interaction. The exchange interaction involves the Cr^{3+} into the ferromagnetic ordering and enhances the ordering temperature. This picture is supported by a steady decrease of the ordered moment per Ru/Cr.

Neutron powder diffraction analysis revealed that below T_c = 163 K the *b* and *c* lattice parameters and the unit cell volume are virtually temperature independent for the stoichiometric material. We show that this previously reported invar-effect below the ferromagnetic ordering temperature originates from freezing of the octahedral tilting about the [001] axis. The invar-effect is much less pronounced in the Ru-deficient samples with decreased T_c 's = 135 K and 82 K. We show that the invar-effect gradually disappears also for the Cr-substituted samples with increased T_c 's.

Supported by the NSF-DMR-0302617 and by the US Department of Education

This research was conducted in collaboration with O. Chmaissem, S. Kolesnik, P.W. Klamut, S. Mini, Y. Ito, M. Maxwell, J. Mais, and T. Maxwell, Physics Department, Northern Illinois University, DeKalb, IL 60115, USA; J.D. Jorgensen, M. Avdeev, P. Barnes, and S. Short, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA; Z.H. Han, J.I. Budnick, and W.A. Hines, Department of Physics, University of Connecticut, Storrs, CT 06269, USA; M. De Marco, D. Coffey, and R. Heary, Physics Department, Buffalo State College, Buffalo, New York 14222, USA; S. Toorongian and M. Haka, Nuclear Medicine Department, State University of New York, Buffalo 14260, USA.

PERCOLATION EFFECTS IN DILUTE MAGNETIC SEMICONDUCTORS

Peter H. Dederichs*, K. Sato and H. Katayama-Yoshida** **

*Research Center Jülich, Germany, **Osaka University, Japan

We discuss the origine of ferromagnetism in dilute magnetic semiconductors with wide band-gaps such as (Ga,Mn)N or (Zn,Cr)Te as compared to the ferromagnetism in systems like (Ga,Mn)As or (In,Mn)As. While in the later case, the ferromagnetism is caused by Zener's p-d exchange, in systems like (Ga,Mn)N and (Zn,Cr)Te the main interaction is Zener's double exchange. The electronic structure calculations are performed by using the KKR-Green function method in connection with the CPA to describe the substitutional disorder of the transition metal atoms. We use both the local density approximation (LDA) and the LDA+U method to describe correlation effects. The exchange interaction constants Jij between two magnetic ions are calculated by embedding the two ions i and j into an effective CPA-medium. The Curie temperatures are calculated from the Heisenberg model by Monte Carlo simulations using Binder's cumulant method. The general trend for impurity band systems is, that the exchange interactions Jij are very strong, but short ranged. Therefore the interaction is dominated by a strong nearest neighbour interaction. This has important consequences. For instance, in dilute systems percolation of the strong nn interactions cannot be achieved, since the concentrations are far below the percolation threshold. Therefore the ferromagnetism is dominated by the weak longer-ranged interactions and the Curie temperatures are very low.

CARRIER-CONTROLLED FERROMAGNETIC SEMICONDUCTORS

Tomasz Dietl

Laboratory for Cryogenic and Spintronic Research, Institute of Physics, Polish Academy of Sciences, al. Lotnikw 32/46, PL 02-668 Warszawa, Poland; also Chair of Condensed Matter Physics, Institute of Theoretical Physics, Warsaw University, Poland (dietl.edu.pl)

Recent advances in understanding of carrier-controlled ferromagnetism in tetrahedrally coordinated diluted magnetic semiconductors and their nanostructures will be reviewed with a focus on the phenomena important for prospective spintronic devices. Experimental results for III-V materials, where the Mn atoms introduce both spins and holes, will be compared to the case of II-VI compounds, in which the Curie temperatures TC above 1 K have been observed for the uniformly and modulation-doped p-type heterostructures but not in the case of n-type films. The experiments demonstrating the tunability of TC by light and electric field will be presented. The tailoring of domain structures and magnetic anisotropy by strain engineering and confinement will be discussed emphasizing the role of the spin-orbit coupling in the valence band. Recent progress in search for semiconductors with TC above room temperature and hopes associated with compounds containing magnetic ions other than Mn will be presented.

This work is partially supported by ERATO Semiconductor Spintronics Project of Japan Science and Technology Agency, KBN grant, and Humboldt Foundation; for review, see, T. Dietl and H. Ohno, MRS Bulletin, October 2003, p. 714, and for recent preprints, T. Dietl et al., http://www.arxiv.org/find/cond-mat.

MAGNETISM IN MANGANITES AND MANGANITE-TITANATE BIFERROICS

K. Dorr and C. Thiele

[a]IFW Dresden, Postfach 270116 Dresden, 01171 Dresden, Germany

Ferro- or antiferromagnetic manganites (La,A)MnO_3 have been investigated mainly for two reasons during the last decade: First, the high spin polarization of conduction electrons in the conducting manganites might be useful in spintronics devices. Second, the competition of charge, orbital and lattice degrees of freedom leads to a variety of different ground states which are controllable by external parameters like magnetic or electric fields, pressure und lattice strain in thin films or light. In our work, epitaxial thin film systems of manganites and titanates ($SrTiO_3$ and ferroelectric $PbZr_{0.48}Ti_{0.52}O_3$ (PZT))have been prepared by the off-axis pulsed laser deposition (PLD) method that allows to grow coherently strained and smooth films. Investigations on tunnel trilayers of $La_{0.7}Ce_{0.3}MnO_3$-$SrTiO_3$-$La_{0.7}Ca_{0.3}MnO_3$ indicate the electron-doped and minority-carrier nature of the Ce-doped manganite. Epitaxial bilayers of a manganite and PZT show both, biaxial strain induced by the PZT inverse piezoelectric effect and an electrical field effect modulating the manganite carrier density near the interface. Additionally, piezoelectric substrates have been employed to reproducibly control the strain state of manganite films deposited on top. Data on electrical transport and magnetism of these biferroic thin film systems will be discussed.

Relativistic and correlation effects in magnetic solids

H. Ebert, J. Minar, S. Chadov and A. Perlov

Department Chemistry / Physical Chemistry
University of Munich, Germany

The interplay of magnetic ordering and spin-orbit coupling leads to a large variety of phenomena that are even of great technological importance. Corresponding well known examples are the magneto-crystalline anisotropy or orbital contributions to the magnetic moments and hyperfine fields. As a peculiar spin-orbit induced ground state property one may add the occurrence of a field gradient in cubic ferromagnets. Besides the galvano-magnetic effects spin-orbit coupling in addition gives rise to many interesting effects in electron spectroscopy. A theoretical approach is presented that allows a detailed investigation of these spin-orbit induced phenomena in magnetic solids. This is achieved by using the spin-polarized relativistic version of multiple scattering or Korringa-Kohn-Rostoker (SPR-KKR) formalism on the basis of local spin density functional theory (LSDA). Corresponding applications to a variety of transition metal bulk, surface and cluster systems will be presented. To allow for a more detailed discussion of the results a simplified analytical approach will be used. As LSDA turns out to provide often an insufficient basis -in particular when dealing with magnetic properties connected with the orbital degree of freedom of an electron- various schemes that are designed to allow for an improved treatment of correlation effects will be presented together with corresponding results.

In-plane Magnetic Micro- and Nanopatterns: Fundamentals, Applications, and Possibilities

A. Ehresmann
Universität Kassel, Fachbereich Naturwissenschaften, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Ion bombardment in an external magnetic field has become an excellent tool to modify the magnetic properties of magnetic thin film systems showing the exchange bias effect. Additionally this novel technique enables lateral magnetic patterning of these layer systems without topography contrast. Magnetic patterns can be achieved either by focussed ion beam techniques or by combining lithography techniques with broad ion bombardment. To understand the fundamental effects of ion bombardment induced magnetic modifications in exchange bias layer systems, the involved modification processes will be discussed in the context of a tentative model. Some applications of ion bombardment induced magnetic patterning (IBMP) will be shown and some further application possibilities will be discussed.

MAGNETIZATION REVERSAL BY INJECTION AND TRANSFER OF SPIN: EXPERIMENTS AND THEORY.

A. Fert[1], M. AlHajDarwish[2], J. Barnaś[3], O. Boulle[1], J. Bass[2], V. Cros[1], J.M. George[1], M. Gmitra[3], J. Grollier[1], G. Faini[4], A. Hamzic[1], H. Jaffrés[1], F. Petroff[1], W.P. Pratt[2], I. Weymann[3]

[1]Unité Mixte de Physique CNRS-Thomson CSF, 91404 Orsay, France,

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[4] L2M-CNRS, 92250 Bagneux, France

The magnetization of a ferromagnetic body can be reversed without applying a magnetic field but only by transferring spins from a spin-polarized electrical current. A reversal can be obtained either by the coherent precession of the magnetic moment generated by the transfer of spin, or by the motion of domain walls induced by the spin-polarized current. In other conditions the magnetization can also be maintained in precession by spin transfer. This maintained precession generates oscillations of the current in the microwave frequency range. Several theoretical approaches, extending the initial theories (Slonczewski, Berger), have been recently developed.

The first part of the lecture describes experiments of both types, that is current-induced reversal by coherent precession and current-induced domain wall motion. The first type of experiment is performed on F/N/F submicronic pillars fabricated by an e-beam lithography method (F = ferromagnetic metal or semiconductor, N = nonmagnetic metal or semiconductor). In the second type of experiments, the magnetic configuration of spin valves is switched by current-induced domain wall motion in the soft layer between two pinning centers. This type of current-induced magnetic switching, as it requires smaller current densities than the magnetization reversal in pillars and can also be obtained by very short current pulses, is promising for applications.

In the second part of the talk, I summarize the theoretical issue and describe the model we have developed to unify the interpretation of CPP-GMR and spin transfer experiments on pillars. This model is based on a self-consistent calculation of the longitudinal and transverse components of the spin current throughout the multilayered structure in the limit of quasi-interfacial spin transfer. The torques acting on the magnetic layers are derived from the transverse component of the spin current injected into each layer. I will also discuss the different behaviors expected in different ranges of applied field (direct reversal or maintained precession).

GaMnAs Materials And Nanoscale Devices

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By careful control of MBE growth conditions and post growth annealing procedures we have produced GaMnAs epilayers which high conductivities and Curie temperature up to 173K. We demonstrate that the improvement in material properties resulting from annealing is due to the out diffusion of interstitial Mn (PRL 94, 127202 (2005)) . We find that compensation is very low in best samples. We show that our measured Curie Temperatures, Hall conductivities and AMR are in good agreement with the mean field theory. We also find that there is no evidence of a fundamental magnetisation deficit in our material.

We also present the observation of a large tunneling anisotropic magnetoresistance (TAMR) in thin (Ga,Mn)As epilayers with lateral nanoconstrictions (PRL 92 037201 (2004)). The observation establishes the generic nature of the recently discovered TAMR effect, which originates from spin-orbit coupling in a ferromagnet and is not specific to a particular tunneling geometry. The lateral geometry allows us to directly link normal anisotropic magnetoresistance (AMR) and TAMR. This indicates that TAMR may be observable in other materials showing room temperature AMR, and suggest a re-examination of previous tunneling and nanocontact results.

PROPAGATION, TUNNELING AND PHASE SHIFT OF SPIN WAVES AT A MAGNETIC FIELD INHOMOGENEITY

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We show experimentally and by numerical simulation, that spin waves propagating in a magnetic film can pass through a region of a magnetic field inhomogeneity or, alternatively, can be reflected by this region depending on the sign of the inhomogeneity. If the region is reflecting and narrow enough, spin wave tunneling takes place. We investigate the tunneling mechanism and demonstrate that it has a magnetic dipole origin. While travelling through a region of inhomogeneous field, spin waves undergo a phase shift. We show, that this can be used for designing phase shifters and spin-wave logic elements.

MAGNETISM AND CHARGE RESPONSE IN QUASI-1D WIGNER LATTICE COMPOUNDS

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Doped edge-sharing Cu-O chain compounds are ideal realizations of 1D Wigner lattices. Such doped edge-sharing chains are found in the recently synthesized $Na_3Cu_2O_4$ and $Na_8Cu_5O_{10}$ systems [1], and they are also structural elements in the widely studied composite compounds $Sr_{14-x}Ca_xCu_{24}O_{41}$. As a result of the geometrical structure (90 degree Cu-O-Cu coordination) the hopping matrix elements and hence the kinetic energy is small compared to the Coulomb energy. At low temperature the charge order resulting from Coulomb interaction $V_l \sim 1/l$ generates Heisenberg chains with varying distance between spins, i.e., dictated by the Coulomb interaction. We analyse the strikingly different magnetic properties of $Na_3Cu_2O_4$ and $Na_8Cu_5O_{10}$ adopting the picture of *modulated Heisenberg chains*. We discuss the role of quantum charge fluctuations on magnetism. Spin-charge coupling is manifested in the fluctuation of spin positions, which results in a doping dependence of exchange interactions.
In the final part, we turn to the charge dynamics of Wigner lattices. Charge excitations are described as fractionally charged domain walls in these systems. We present a detailed discussion of domain-wall excitation spectra, excitonic states, and of the temperature dependence of optical conductivity [2].

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Frustrated Antiferromagnetic Quantum Chain Systems

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Antiferromagnetic (afm) S=1/2 Heisenberg chain systems with uniform nearest-neighbour exchange coupling are best understood. The ground state and the excitation spectrum are well known and the experimental observations are in good agreement with theory. Additional next-nearest neighbour exchange along the chains which can be described by the Majumdar-Ghosh Hamiltonian $H = J_{nn} \sum_i (S_i S_{i+1} + \alpha S_i S_{i+2})$ with α=J_{nnn}/J_{nn} gives rise to a more complex behaviour, since next-nearest neighbour interaction may lead to magnetic frustration. I review the magnetic properties of the afm S=1/2 Cu^{2+} chain systems $LiCuVO_4$ and CuX_2 (X=Cl, Br) for which afm *incommensurate* long-range ordering has been observed by neutron diffraction at low temperatures. The appearance of incommensurate ordering is ascribed to competing *nn* and *nnn* exchange interaction which is also evidenced in the bulk magnetic properties.

Spin-Charge Separation and Non-Linear Optical Response in One-Dimensional Cuprates

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The spin-charge separation is one of the key concepts in strongly correlated electron systems in one-dimension[1]. This also provides an opportunity for much debate on high temperature superconductivity. The Mott gap, i.e., the charge excitation gap in strongly correlated electron systems is in contrast to the energy gap in band insulators. Recent experiments have revealed that Mott inlsusulators in one-dimension exhibit the strikingly large non-linear optical response. Here, we theoretically examine the spin-charge separation and the linear and non-linear responses in one-dimensional Mott insulators and clarify the nature of the photo-excited states. In particular, we focus on the followings: (i) the linear absorption which is characterized by the odd-parity excited states, (ii) the two-photon absorption (TPA) which is characterized by the even-parity excited states, and (iii) the third-harmonic generation (THG). The theoretical results are compared with the experimental ones. We discuss the similarity and dissimilarity of the electronic and optical properties in one- and two-dimensional Mott insulators based on the spin-charge separation.

This work has been done in collaboration with T. Tohyama, H. Matsueda and N. Bulut.

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D-wave density waves in high T_c cuprates and $CeCoIn_5$

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As is well known there are many parallels between high T_c cuprate superconductors and heavy fermion compound $CeCoIn_5$;quasi two dimensional Fermi surfaces,vicinity of antiferromagnetism and d-wave superconductivity. Recently giant Nernst effect and angle dependent magnetoresistance (ADMR) are observed in the pseudogap phases in both high T_c cuprates and $CeCoIn_5$. We shall describe these phenomena in terms of d-wave density waves. Also some properties of the gossamer superconductivity (d-wave superconductivity in the presence of d-wave density wave) will be explored.

New spin configurations in nano-sized magnets near reorientation phase transition

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By micromagnetic simulations and analytically we study the ground and metastable magnetic states of ultrathin magnets (with thickness d) in the form of films and laterally size-limited samples: semi-infinite films, wires (width w) and disks (radius r). Nanostructures are discussed with low-perpendicular magnetic anisotropy determined by the quality factor Q - the ratio between magnetic anisotropy and demagnetization energies. Simulations are based on real material parameters, determined for ultrathin Co with defined Q(d) dependence. Domain structure existence decrease Q when the transition into in-plane phase undergoes down to $Q^* < 1$ [1]. Out-of-plane magnetization component exists at the edge of semi-infinite film when $Q > Q_{edge}$ ($Q_{edge} < Q^*$). Perpendicular magnetization states can be achieved by properly decreasing lateral nanostructure size in whole Co ultrathin thickness regime. Q dependent different scenarios of magnetization distribution changes decreasing parameters w or r are discussed for nanostructure with defined d. Novel nanometer-scale magnetization distributions are discussed such as: domain-like distribution with an oscillating out-of plane magnetization component and decaying amplitude; out-of plane component patterned vortex.

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MAGNETIC AND SUPERCONDUCTING CORRELATIONS IN THE 2D HUBBARD MODEL

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The functional renormalization group (fRG) is an ideal tool for dealing with the hierarchy of energy scales and competition of different interactions in correlated electron systems. Starting point is an exact hierarchy of flow equations which yields the gradual evolution of the effective low-energy action from the microscopic model Hamiltonian as a function of a continuously decreasing energy cutoff. Truncated at one-loop level the fRG yields a systematic and unbiased weak coupling stability analysis, where the competition and mutual feedback of particle-particle and particle-hole channels is consistently taken into account. The latter channel drives in particular magnetic, the former superconducting correlations. For the weakly interacting 2D Hubbard model detailed information on the dominant low-energy effective interactions and correlations has been obtained from numerical solutions of the one-loop flow equations. These calculations conclusively established the existence of d-wave superconductivity in the 2D Hubbard model at weak coupling. In a regime with strong antiferromagnetic correlations the spectral function for single-particle excitations obtained from the two-loop self-energy exhibits pseudogap features near van Hove points or other hot spots on the Fermi surface.

Magnetic Microstructure of NANOPERM-type Nanocrystalline Alloys

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A brief description of the influence of structural modifications caused by temperature of annealing (i.e. number of nanocrystallites) as well as by temperature of measurement upon magnetic behaviour of nanocrystalline alloys of the NANOPERM family prepared from amorphous precursors will be given. Results of nuclear and atomic based techniques of (subatomic) structural characterization comprising Mössbauer spectrometry, XRD, TEM, HREM, DSC, and AFM will be correlated with magnetic data obtained from macroscopic measurements.

Doped 2D frustrated quantum magnets: spin-charge separation and non-conventional superconductivity

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Dynamics of mobile holes in two-dimensional frustrated quantum magnets is investigated. Numerical evidences are provided for spin-charge separation under doping the Kagome lattice, a featureless spin liquid. On the contrary, in the checkerboard lattice, a candidate of broken-symmetry Valence Bond Crystal, a small quasi-particle weight exists for some crystal momenta, a finding interpreted as a restoration of weak holon-spinon confinement (1). Amplification of pairing occurs in this case (for $t > 0$) due to a localisation process that blocks single hole tunneling between the plaquettes of the Valence Bond Solid while hole pairs can delocalize (2). This scenario can give rise to new singlet pairing channels with s-, d- or g-wave symmetries. I also argue that the formation of a spatially-extended region where the plaquette solid melts around the hole can lead to an effective correlated hopping responsible for the two hole boundstate.

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MAGNETIC EXCITATIONS IN MAGNONIC CRYSTALS AND IN SMALL MAGNETIC PARTICLES

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Magnetic normal modes, vital for the problem of thermal noise in small magnetic elements used in writing/reading devices, are investigated here in finite thin films, cube grains and rods. We show how a strong inhomogeneity of the demagnetizing field in these structures induces amplitude bulk localization of magnetostatic modes. Moreover, a new type of magnetostatic modes (*comb modes*) is found in a spectrum of elongated axially magnetized rods, with two clearly discernible regions: a zone of fast amplitude oscillations inside the rod, and slow-oscillation narrow regions at the borders. Absorbing virtually no energy from an *applied* alternating field, comb modes have no significant contribution to the magnetic noise. A separate issue to be raised in this study is that of magnetic excitations propagating in *magnonic crystals* (MC), *i.e.* hypothetical macrocrystals with periodically inhomogeneous magnetic structure, topologically equivalent to well known photonic crystals [1]. Magnonic spectra are investigated in 1D, 2D and 3D structures, and conditions of opening of energy gaps forbidden to magnonic propagation are determined in particular. A confrontation of our 3D MC theory with recent experimental results (spin-wave spectra measurements through neutron scattering) obtained in certain low-doped manganites allows us to suggest a hypothesis that these materials can be regarded as magnonic crystals *existing in nature*.

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MAGNETIC PROPERTIES OF ALMOST LOCALIZED FERMIONS - REVISITED

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The properties of almost localized fermions became a subject of a renewed interest in recent years. This is caused by the discovery of the spin-dependent heavy masses predicted some time ago [1] as well as of critical behavior near metal-insulator transition of the Mott-Hubbard type [2]. We discuss these properties within our earlier approach [3] and include the quantum Gaussian fluctuations. A strong metamagnetic behavior is connected to the spin-dependent masses. Effect of the orbital degeneracy on these effects is also briefly mentioned within an original rotationally invariant version of the extended Hubbard model containing the Hund's rule coupling.

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[2]P. Limelette et al., Science **302**, 89 (2003).
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UNCONVENTIONAL FORMS OF SUPERCONDUCTIVITY AND QUANTUM CRITICALITY IN HEAVY-ELECTRON METALS

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Some recent observations made on the isostructural compounds $CeCu_2Si_2$ and $YbRh_2Si_2$ are discussed. We first address the interplay of superconductivity in $CeCu_2Si_2$ with both a spin-density-wave-type quantum critical point (QCP) at low pressure [O. Stockert et al., PRL **92**, 136402 (2004)] and a weak valence transition of Ce at high pressure [H. Q. Yuan et al., Science **302**, 2104 (2003)]. We then turn to $YbRh_2Si_2$ displaying a novel type of QCP [J. Custers et al., Nature **424**, 524 (2003); S. Paschen et al., Nature **432**, 881 (2004)], which appears to be detrimental to superconductivity.
Work done in collaboration with:
J. Custers, P. Gegenwart, C. Geibel, F. M. Grosche, R. Küchler, K. Neumaier, S. Paschen, J. Sichelschmidt, G. Sparn, Y. Tokiwa, H. Wilhelm, S. Wirth, H.Q. Yuan, P. Coleman, C. Pépin, Q. Si and G. Zwicknagl

Renormalization Group Approach to Weakly Interacting Spin and Fermion Chains

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The properties of many real materials are dominated by the presence of weakly coupled chains. We propose a method based on the real space renormalization group transformation which can be used to study critical behavior and thermodynamics of a broad class of the weakly interacting classical and quantum spin chains with $S \geq 1/2$ in an magnetic field as well as fermion chains. The method is presented and examined for the standard Ising model on a rectangular lattice and then applied to the weakly interacting quantum anisotropic Heisenberg model and spinless fermion system. We discuss a dimensional crossover in coupled spin chains. We also show that the characteristic feature of a strongly correlated spinless fermion chain is a double peak structure of the specific heat as a function of temperature and a small interchain (transverse) hopping leads to a phase transition from a metallic to a charged ordered phase.

SUPERFLUIDITY IN CONDENSED EXCITONS BELOW 20 K

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In superconductivity the electrical conductivity is diverging at the critical temperature, in superfluidity the heat conductivity is diverging. Therefore, the measurement of heat conductivity and thermal diffusivity is giving the essential information if superfluidity occurs. Superfluidity needs a "fluid" to start with and in a solid this means a condensed state of bosons. Such bosons are Coulomb coupled electron-hole states, excitons, which can condense. In materials, which exhibit intermediate valence, 4f holes can be very heavy with masses around $100\,m_e$ and, nevertheless, the compounds can be narrow gap semiconductors. Such a material is $TmSe_{0.45}Te_{0.55}$ and its thermal properties have been measured as function of temperature (4 K) and pressure (17 kbar). Below 20 K the heat conductivity and the thermal diffusivity diverge exponentially with decreasing temperature, being indicative of superfluidity. Above this temperature the condensed excitons can order in a Wigner lattice, couple to phonons, and thus, creating exciton-polarons with very anomalous specific heat and sound velocities with a special dispersion. For the first time stable exciton condensation with permanent superfluidity has been observed.

Physics of Nanomagnetism revealed by Spin-Polarized Scanning Tunneling Spectroscopy

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In order to probe and tailor magnetic properties at the spatial limit we have combined the scanning tunneling microscope (STM) with spin-sensitivity [1-3]. This is achieved by the use of ferro- [4-6] and antiferromagnetically [7,8] coated probe tips offering a high degree of spin-polarization of the electronic states involved in the tunneling process. Spin-polarized Scanning Tunneling Microscopy (SP-STM) and Spectroscopy (SP-STS) has allowed the visualization of atomic-scale spin structures [2,9] and the investigation of the spin-dependent local density of states spatially resolved [10]. Magnetic domain imaging with sub-nanometer-scale spatial resolution has been demonstrated for magnetic transition metal as well as rare earth metal films. Ultra-sharp domain walls were discovered in ultra-thin iron films on W(110) substrates [11]. In a recent SP-STM experiment we could prove that single monolayers of Fe on W(001) substrates exhibits a c(2x2) antiferromagnetic ground state with perpendicular anisotropy in contrast to a single Fe monolayer on W(110) which is ferromagnetic with in-plane anisotropy [12]. Spin-dependent scattering at single oxygen impurities on Fe/W(110) was visualized in real-space reflecting the orbital nature of the electronic states involved as well as their spin character [13]. Finally, applications of SP-STM for studying spin states of single magnetic impurities will be discussed.

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GIANT ROOM-TEMPERATURE TMR EFFECT IN MAGNETIC TUNNEL JUNCTIONS WITH MgO(001) TUNNEL BARRIER

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Magnetic tunnel junctions (MTJs) consisting of ferromagnetic electrodes separated by a tunnel barrier exhibit the tunneling magnetoresistance (TMR) effect. While a magnetoresistance (MR) ratio up to 70% has been obtained at room temperature (RT) in MTJs with an amorphous Al-O tunnel barrier, a much higher MR ratio is theoretically expected in fully-epitaxial MTJs with a crystalline MgO(001) tunnel barrier. We fabricated the fully epitaxial Fe(001)/MgO(001)/Fe(001) MTJs with MBE and micro-fabrication techniques and achieved a giant MR ratio up to 188% at RT.[1,2] We observed even higher MR ratio up to 271% at RT (353% at 20 K) in fully-epitaxial bcc Co(001)/MgO(001)/Fe(001) MTJs. We also fabricated MTJs consisting of a highly-oriented poly-crystalline MgO(001) barrier and amorphous CoFeB ferromagnetic electrodes with sputtering deposition technique. The CoFeB/MgO(001)/CoFeB MTJs also exhibited a giant TMR effect above 200% at RT.[3] A crystalline MgO(001) tunnel barrier seems to be essential for the giant TMR effect because an amorphous MgO tunnel barrier yielded a much lower MR ratio. These results are of great importance not only for industrial applications but also for the physics of spin-dependent tunneling.

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CONTRIBUTIONS

O-1-01

PHASE DIAGRAM OF HEAVILY DOPED ($x > 0.5$) $La_{1-x}Sr_xMnO_3$

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A vast majority of research of $La_{1-x}Sr_xMnO_3$ manganites was done for $x < 0.5$. Data on $0.5 < x \leq 1$ materials are sparse because of inherent difficulty in synthesizing them. The occurrence of a rich phase diagram for $x > 0.5$ was evidenced by structural and magnetic measurements. For the present, first specific heat studies of $x = 0.55$, 0.7, and 0.9 compositions, highly stoichiometric samples were prepared. Specific heat was measured from 2 K to 395 K on heating and on cooling, in zero magnetic field and in $B = 7$ T. Orders of particular phase transitions and specific heat anomalies accompanying them were studied. For $x = 0.55$, the second order paramagnet-ferromagnet phase transition, visible as the λ-anomaly at 267 K, and the first-order transition from ferromagnetic to A-type antiferromagnetic state, associated with the structural transition from a tetragonal to an orthorhombic structure, were observed. The latter, visible as a δ-type anomaly at 216 K, was very sensitive to magnetic field (7 T lowered the transition temperature by 26 K). For $x = 0.7$ and 0.9, the second-order transition from the paramagnetic to the C-type antiferromagnetic state, occurring at 265 K and 205 K, respectively, was studied. For $x = 0.7$, it was a purely magnetic transition, whereas for $x = 0.9$, it was coupled with the structural transition from a cubic to a tetragonal phase.

O-1-02

NON-FERMI LIQUID GROUND STATE IN CeRhSn: EFFECT OF GRAIN BOUNDARY DEFECTS ON THE ELECTRIC TRANSPORT BEHAVIOR

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The compound CeRhSn exhibits a non-Fermi liquid (NFL) character of the temperature dependence for low-temperature physical properties. The susceptibility χ and specific heat C divided by temperature, C/T, can be fitted to T^{-n} behavior with the value of the power-law exponent $n \cong 0.5$ suggesting that the NFL behavior can be described by the Griffiths-McCoy model. The resistivity is indeed NFL in character (i.e., $\rho \sim T^{\epsilon}$), however, the power-law that should extend over several decades in temperature is dependent on the T-range ($\epsilon \cong 1$ down to ~ 3 K, while $\rho \sim T^{1.7}$ for $0.1 < T < 3$ K). Measurements by an atomic force microscopy show the nanometre-sized grains consisting of the crystalline components separated by the grain boundary/interface, which are strongly inhomogeneous and off-stoichiometry. We argue that there is possible a ballistic transport of electrons through an interface which strongly modifies the $\rho(T)$ dependence of the polycrystalline CeRhSn sample.

O-1-03

Resonant magnetic excitations in high-T_c cuprates: influence of orthorhombicity and upward dispersion

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Recent inelastic neutron scattering (INS) experiments in the superconducting (SC) state of YBCO [1] detected a new resonant magnetic excitation at incommensurate momenta, but at frequencies *larger* than $\Omega_{res}(\mathbf{Q})$. We show that a new resonant magnetic excitation at incommensurate momenta, observed recently by inelastic neutron scattering experiments on $YBa_2Cu_3O_{6.85}$ and $YBa_2Cu_3O_{6.6}$, is a *spin exciton*. We identify several features that distinguish this novel mode from the previous resonance mode observed near $\mathbf{Q} = (\pi, \pi)$[2]. Furthermore, we have analyzed the in-plane magnetic anisotropy in high-T_c superconductors with orthorhombic distortions and compared our results with INS data on fully untwinned YBCO [3].

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[3] I. Eremin and D. Manske, Phys. Rev. Lett. **94**, 067006 (2005).

O-1-04

Low-field magnetic investigations of the superconducting state in $PrOs_4Sb_{12}$

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Superconductivity in the filled skutterudite compound $PrOs_4Sb_{12}$ appears to be unconventional, as inferred form, e.g., the lack of a coherence peak near T_c=1.85 K in the inverse nuclear-spin-lattice-relaxation time of Sb nuclei. Furthermore, spontaneous magnetic moments develop just below T_c, indicative of time reversal symmetry breaking. From measurements of dc isothermal magnetization curves for a $PrOs_4Sb_{12}$ single crystal, we have obtained the temperature dependence of the lower critical field $H_{c1}(T)$. Unexpectedly, a pronounced enhancement of $H_{c1}(T)$ emerges upon cooling below around 0.6 K (i.e., $T/T_c \simeq 0.3$). In addition, the critical current, estimated from remnant magnetization measurements, also increases faster upon lowering the temperature below 0.6 K. These experimental findings clearly point at another phase deep in the superconducting state of $PrOs_4Sb_{12}$. We will also discuss flux dynamics in $PrOs_4Sb_{12}$: while there is no obvious anomaly at $T/T_c \simeq 0.3$, vortex creep is extremely weak already below T_c. The very strong pinning in this material is in agreement with theoretical expectations for superconductors with broken time reversal symmetry.

O-1-05

PRESSURE EFFECTS ON MAGNETIC PROPERTIES OF MANGANITES NEAR PERCOLATION THRESHOLD

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Effects of hydrostatic pressure up to 11 kbar on magnetic properties of $La_{1-x}Ca_xMnO_3$ ($x = 0.18, 0.20, 0.22$) and $Pr_{1-x}Sr_xMnO_3$ ($x = 0.22, 0.24, 0.26$) single crystals were studied near percolation threshold x_c which is observed at $x = 0.22$ and at $x = 0.24$ for La and Pr based manganites, respectively. In both systems magnetic ordering temperature T_c of the Mn spin sublattice increases upon applying the pressure. The pressure coefficient dT_c/dP for both systems enhances significantly near x_c and then the changes are much smaller with increasing doping. It was found that in the case of $Pr_{1-x}Sr_xMnO_3$ system the nature of the ferro-to-paramagnetic transition of the Mn spin system evaluates with increasing doping from a continuous second order transition ($x < x_c$) to a more abrupt first order-like transition ($x > x_c$). For $Pr_{0.76}Sr_{0.24}MnO_3$ sample an applied pressure changes the character of the phase transition from nearly a continuous one at $P = 0$ to more abrupt, almost discontinuous one at $P = 11$ kbar.

O-1-06

INFLUENCE OF CHEMICAL SUBSTITUTIONS ON ANISOTROPIC UPPER CRITICAL FIELD IN MgB_2: IMPACT OF FERMI SURFACE CHANGES

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Specific band structure of MgB_2, with two bands π and σ involved in superconductivity, leads to high critical temperature, T_c, of 39 K and temperature and field dependent anisotropy of superconducting parameters. Chemical substitutions lead to modification of band structure and therefore influence all superconducting parameters, especially T_c, the upper critical field, H_{c2}, and its anisotropy, γ_H. Magnetic investigations of $Mg_{1-x}Al_xB_2$ crystals show the slight increase of $H_{c2||c}$ for the samples with small x, significant reduction of γ_H at lower temperatures for Al substituted samples as compared to this of unsubstituted crystals. In $Mg(B_{0.94}C_{0.06})_2$ single crystals $H_{c2||c}(0) \cong 85$ kOe is more than twice as large as that one of $\cong 31$ kOe in unsubstituted MgB_2. Anisotropy of H_{c2} decreases to about 4 at low temperatures, the value considerably lower than that in MgB_2, and its temperature dependence is much less pronounced. The corresponding $H_{c2||ab}(0) \approx$ 330-350 kOe is likely close to the maximum enhancement of H_{c2} due to chemical substitutions. The enhancement of H_{c2} can be explained as a disorder effect only if the main result of disorder is to make the π bands more dirty while not affecting the σ bands as much. However, in addition to disorder and weakened electron-phonon coupling, the impact of the Fermi level shifting into a region with lower σ Fermi surface velocities has to be taken into account in the analysis of H_{c2} data as well.

O-1-07

MICROSCOPIC THEORY OF MAGNETIC INTERACTIONS IN $KCuF_3$ AND $LaMnO_3$ — THE ROLE OF CHARGE TRANSFER

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Magnetic interactions in correlated insulators with orbital degrees of freedom are described by superexchange spin-orbital models, which are characterized by nontrivial quantum effects [1]. We analyze the spin interactions in A-type antiferromagnetic phase of $KCuF_3$ with one hole in e_g orbital ($S = 1/2$) and of $LaMnO_3$ with $t_{2g}^3 e_g$ high-spin ($S = 2$) electronic configuration. The spin exchange constants along cubic axes J_{ab} and J_c sensitively depend on three parameters: (i) overall energy scale $J = 4t^2/U$, where t is $(dd\sigma)$ hopping and U is on-site Coulomb repulsion, (ii) the Hund's exchange $\eta = J_H/U$, and (iii) the parameter $R = 2U/(2\Delta + U_p)$, where Δ and U_p are charge transfer (CT) energy and Coulomb repulsion on oxygen, and (iv) on the e_g orbital order. One finds that quasi one-dimensional spin interactions $J_c \gg |J_{ab}|$ in $KCuF_3$ are intrinsically related to its CT type insulating state. On the contrary, the effects of CT superexchange terms are moderate in a Mott insulator $LaMnO_3$. Finally, using partial optical sum rules [2], we discuss experimental constraints on the microscopic parameters of $LaMnO_3$.

[1] L. F. Feiner, A. M. Oleś, and J. Zaanen, Phys. Rev. Lett. **78**, 2799 (1997).

[2] G. Khaliullin, P. Horsch, and A. M. Oleś, Phys. Rev. B **70**, 195103 (2004).

O-1-08

HALL EFFECT IN THE LOW CHARGE-CARRIER DENSITY FERROMAGNET $UCo_{0.5}Sb_2$

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The Hall coefficient R_H of ferromagnetic $UCo_{0.5}Sb_2$ ($T_C = 74.5$ K) has been measured on a single crystal in the temperature range 2 - 300 K and in magnetic fields up to 7 T. The values of the normal R_0 and anomalous R_s coefficients were estimated by comparing the $R_H(B)$ with magnetization $M(B)$ data. Both $-R_0$ and R_s show a maximum near T_C and a minimum at $T_{min} \approx 20$ K. Below T_{min}, R_0 and R_s tend to a saturation. The ratio R_s/R_0 reaches a value of ~ 1000 for $T \leq T_C$ and of ~ 21000 at higher temperatures, implying that R_H is dominated by R_s. The negative sign of R_0 is found to be unchanged down to 2 K, which is indicative of electron-type carriers. The carrier concentration $n_e = |1/eR_0|$ is found to decrease rapidly when the system undergoes the ferromagnetic ordered state, i.e., it varies from 0.785 e/f.u in the paramagnetic state to about 0.024 e/f.u at 2 K. The charge mobility μ_e was evaluated from the $R_H(1\mathrm{T})$ and electrical resistivity ρ values. $\mu_e = R_H(1\mathrm{T})/\rho$, passes over a maximum (≈ 450 cm^2/Vs) at T_{min} and falls down by as many as two orders of magnitude for $T = 2$ K (≈ 3.7 cm^2/Vs). Since the effective mass $m^* = 3\gamma\hbar^2/(3\pi^2 n_e)^{1/3}k_B^2$ shows weak temperature dependence (from 53.8 m_e at T_{min} to 69.5 m_e at 2 K), the decline in μ_e with decreasing temperature seems to be associated with an enormous decrease of the carrier collision time.

O-1-09

Quantum fluctuations of the ultracold atom-molecule mixtures

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We investigate emergence of the quantum coherence in the ultracold mixture of fermionic atoms and bosonic dimer molecules. Interactions between these species can be there experimentally controlled via tuning the external magnetic field. In consequence the fermionic atoms and their bosonic counterparts can be driven to a correlated behavior which resembles the usual BCS to BEC crossover scenario. We analyze this issue in some detail. In particular we comment on the recent experiments using the fast sweep across the Feshbach resonance which induce the fluctuations analogous to the superradiant state originally discussed by von Dicke.

O-1-10

ELECTRONIC STATES OF MAGNETITE FROM ELECTRON PHOTOEMISSION SPECTROSCOPY

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The core- level and valence band photoemission spectra for epitaxial thin film and bulk single crystal of magnetite were measured by the X-ray (XPS) and the angle- resolved ultraviolet (ARUPS) photoemission spectroscopy. The 3d electron on-site correlation energy, the 3d-2p electron charge transfer energy and the hybridisation energy between Fe-3d and O-2p states were obtained. They were calculated from the energy separations between the Fe-2p main lines and their satellite lines and from the iron and oxygen Auger spectra together with the relevant valence band spectra according to the Zaanen, Sawatzky and Allen (ZSA) theory. The ARUPS spectra were compared to the accessible band structure calculations. Type of insulating gap in these oxides was discussed.

O-1-11

NEW ORTHOROMBIC MULTIFERROICS $R_{1-x}Y_xMnO_3$ $(R = Eu, Gd)$

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A competition of exchange interactions in orthorhombic manganites $RMnO_3$ induced by decreasing of the rare-earth ion ionic radii causes a sinusoidal antiferromagnetic ordering resulting in appearance of electric polarization below incommensurate-commensurate (IC-C) transition at $T_{lock} < T_N \sim 45K$. In this work we have realized the tendency to form multiferroic states in the single crystals of substituted compounds $Eu_{1-x}Y_xMnO_3$ $(0.2 \leq x \leq 0.5)$ and $Gd_{1-y}Y_yMnO_3$ $(0 \leq y \leq 0.2)$. While slightly substituted $(x \leq 0.1)$ compounds exhibited a spontaneous transition from the IC to the canted antiferromagnetic (CAF) state at $T_{CA} < T_N$, the IC-C phase transition at $T_{lock} = 30K$ was observed for x=0.2, followed by the transition to the CAF phase at $T_{CA} \sim 22K$. For $x \geq 0.3$ and $y \geq 0.05$ only the IC-C transitions were found while the CAF phase disappeared at all. Various phase transitions were observed in the pulsed magnetic fields up to 250 kOe along a, b, c-axes by magnetization, magnetostriction and electric polarization measurements. The polarization showed a strong dependence on a preliminary poling in an electric field $E \sim 1500\ V/cm$ that indicated on an existence of a spontaneous electric polarization below T_{lock}, which was suppressed by $H \parallel c$ or changed by $H \parallel a, b$.

O-1-12

Andreev reflection at ferromagnetic metal- triplet superconductor junctions

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Properties of tunneling conductance spectra of a ferromagnetic-insulator-anisotropic spin triplet superconductor junction are theoretically investigated. The Andreev reflection and transmission of quasiparticles at the interfaces, parallel and perpendicular to the c-axis of the superconductor Sr_2RuO_4, are discussed for unitary $p-$wave $d_z(\vec{k}) = \hat{z}\Delta_0(\sin(ak_x) + i\sin(ak_y))$,and $f-$wave $d_z(\vec{k}) = \hat{z}\Delta_0(\sin(ak_x) + i\sin(ak_y))\cos(ck_z)$. Moreover, selected non-unitary $f-$ wave pairing states are discussed, as well. The choice of symmetry pairing is motivated by recent experiments on Sr_2RuO_4. Asymmetry of the Andreev reflection amplitude with respect to the boundary normal is analyzed. The behaviour of the resonance peak in this reflection is also performed. The essential influence of the magnitude and direction of the exchange field on the conduction spectrum is investigated. Especially the evolution of a zero-conductance peak into a zero conductance deep has been shown.

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O-1-13

ORBITAL-SELECTIVE MOTT TRANSITIONS IN THE ANISOTROPIC TWO-BAND HUBBARD MODEL AT FINITE TEMPERATURES

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The anisotropic degenerate two-orbital Hubbard model is studied within dynamical mean-field theory at low temperatures. High-precision calculations on the basis of a refined quantum Monte Carlo (QMC) method reveal that two distinct orbital-selective Mott transitions occur for a bandwidth ratio of 2 even in the absence of spin-flip contributions to the Hund exchange. The second transition – not seen in earlier studies using QMC, iterative perturbation theory, and exact diagonalization – is clearly exposed in a low-frequency analysis of the self-energy and in local spectra.

O-1-14

Single particle spectral weight and ARPES spectra from cuprates in the bond-ordered, bond-centered stripe phase

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Motivated by recent inelastic neutron scattering experiments on cuprates, we discuss the formation of bond order in the stripe phase. We suggest that spin-Peierls order appears in hole-rich domain walls (DWs) formed between hole-poor regions in which long-range antiferromagnetic (AF) correlations exist. On the example of a single stripe we analyze the stability of such structures. The motion of a hole inside the DW which takes the form of a bond ordered ladder is in principle unrestricted. The hopping of a hole in domains is to some extent obscured by the fact that a moving hole spoils AF correlations. By analyzing the energy dispersion of a quasiparticle propagating along the bond-centered, bond-ordered stripe and of a quasiparticle propagating along the site-centered stripe we deduce that bond ordered stripes are stable at and above the total doping level 1/8 and the linear stripe-filling level 1/2. Later we compute the electronic structure and the single-particle spectral density of a stripe array formed by ladder-like DWs and by AF domains of width 2 lattice spacings and compare them with ARPES spectra from some doped cuprates belonging to the 214 family of compounds. The intensity map plotted in the coordination frame momentum-energy reproduces quite well the ARPES spectra of Nd doped LSCO systems obtained at the doping level of 15%.

O-1-15

FLUCTUATION OF COOPER PAIRS

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Low-field part of microwave absorption (MA) line results from vortex currents in type II superconductors, thus from the broken Cooper pairs (PC). Because of strongly damped vibrations of vortexes in weak junctions, AC Josephson absorption is non-resonant and results from energy dissipation of ac field, which is proportional to the concentration of normal electrons from broken Cooper pairs. Josephson junctions system (JJS) is well isolated form the lattice, so there is a local temperature different from the temperature of the lattice, $T_{JJS} \neq T_{lat.}$. When Cooper pairs (which have spin S=0) break, electrons with the spin of S=1/2 should give resonant absorption. There is an anomalous temperature dependence of EPR line intensity due to electrons, which at low temperature are paired. It will be shown that resonant absorption manifests itself on Josephson hysteresis in oscillating electromagnetic field at 22 and 15 MHz.

P-1-01

Tunneling of correlated electrons through a narrow domain wall in magnetic nanowires

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Electron transmission through a narrow domain wall in a ferromagnetic one dimensional metal is studied taking into account both potential and spin dependent scattering at the wall. This introduces transmission amplitudes with or without spin reversal. We consider a model electron-electron interaction which is local and includes a spin dependent term. Then, the correction to the bare scattering amplitudes is calculated to first order in the electron-electron interaction, within a Hartree-Fock theory. Such correction diverges logarithmically with the bandwidth cutoff. Using a poor man's renormalization group approach for the electron interactions, where the coupling constants and transmission amplitudes are renormalized as the bandwidth cutoff is progressively reduced, we obtain analytical expressions for the conductance at any temperature. We also compare our results to those obtained from bosonization techniques and discuss the implications to domain wall movement.

P-1-02

DYNAMIC RESPONSE OF MAGNETIC IONS IN THE COLOSSAL MAGNETOREZISTANCE MANGANITES $La_{1-X}Ca_XMnO_3$

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We present a detailed study of nonlinear dynamic susceptibility of the polycrystalline perovsckite manganites $La_{1-X}Ca_XMnO_3$ ($0.30 \leq x \leq 0.66$), below and above transition temperature as function of frequency and temperature. Near by $x = 0.5$ the system changes from ferromagnetic and conducting to antiferromagnetic and insulating with large hysteretic behavior in $M(T)$ and $\rho(T)$. The Curie temperatures determined from dynamic susceptibility analysis were compared to the data obtained previously by electrical and static magnetic measurements, and a new phase diagram was drawn. A sharp negative peak in $\chi'_3(T)$ curves was found for the samples with $x = 0.3$ - 0.51. The data suggest the presence of correlated magnetic clusters near by the magnetic transition.

P-1-03

KONDO PHENOMENA OF STRUCTURAL DEFECTS IN USbTe FERROMAGNET

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USbTe is a ferromagnet (T_C = 123.4 K) crystallising in tetragonal PbFCl-type structure. Its isostructural compounds UPS and UAsSe, showing low-T turn-up of electrical resistivity, were found to be two-level-system Kondo (i.e. orbital-Kondo, OK) ferromagnets. We have shown previously (phys. stat. sol. (a) **196** (2003) 352) that resistivity along a-axis - $^a\rho$(T) - for USbTe, unlike that for UPS and UAsSe revealed coherent low-T electronic scattering and unlike typical ferromagnetic metal shows unusually convex shape between 50 K and T_C.
To explain this unusual behaviour we have measured resistivity along c-axis - $^c\rho$(T) - for USbTe and showed that having $^a\rho$(T) and $^c\rho$(T) we can resolve the temperature dependent resistivity of USbTe into components corresponding to particular mechanism of electronic scattering. It occurred that OK effect is responsible for unusual transport properties of USbTe ferromagnet. The OK electronic scattering contributes to the resistivity component ρ_K(T). It reaches maximum at T^* = 78 K and goes to zero at the lowest temperatures. Such temperature is assumed to be the Kondo temperature in case of Kondo paramagnetic systems showing transition to coherent electronic scattering and we propose to classify the USbTe as the coherent orbital-Kondo ferromagnet.

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P-1-04

HALF-FILLED STRIPES IN THE t-t'-U HUBBARD MODEL

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Using a self-consistent Hartree-Fock (HF) approximation we investigate the relative stability of various stripe phases in the extended t-t'-U Hubbard model. They involve nonmagnetic filled stripes (one doped hole per site in a domain wall) stabilized by transverse charge fluctuations [1], and half-filled stripes (one doped hole per two atoms in a domain wall) involving an on-wall spin-density wave. In spite of better optimizing the potential energy the latter represent only locally stable solutions, both for the t-t'-U Hubbard model at half-filling, and $t' = 0$ off half-filling. However, previous HF studies of the filled stripes have shown that a negative ratio of next nearest-neighbor to nearest-neighbor hopping $t'/t < 0$, relevant to the doped CuO_2 planes of high-T_c superconductors, gives a positive kinetic energy contribution, expelling holes from antiferromagnetic domains and reinforcing the stripe order [2]. Guided by this observation we show here that half-filled stripes accommodate holes markedly easier than the filled ones. Consequently, the former take over in the regime of $t'/t \simeq -0.3$ appropriate for $YBa_2Cu_3O_{6+x}$.

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P-1-05

INFLUENCE OF Ti ON THE MAGNETIC STATE OF $CaRu_{1-x}Ti_xO_3$

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The magnetic ground state of the ternary ruthenate $CaRuO_3$ is rather controversial. There are indications that it is a non-Fermi liquid metal. It has been considered a paramagnet, however, in the light of the most recent experimental sudies it appears to be a material at the verge of magnetic ordering that readily evolves into a magnetically ordered one. Substitution of Ru by nonmagnetic Ti atoms was found to induce ferromagnetism in this material with maximum effect for 40% of Ti.
Polycrystalline samples of $CaRu_{1-x}Ti_xO_3$ with x=0, 0.005, 0.03 and 0.07 have been prepared and pressed into pellets that were sintered at 1100-1200^{o}C for 72 h in air. We have measured the specific heat in the temperature region of 3-300 K in magnetic field of 0, 0.5 and 1 T, as well as the ac-susceptibility up to 120 K at frequencies of 100 Hz, 1 and 3 kHz.
No specific heat anomaly has been observed neither for $CaRuO_3$ nor for the Ti containing samples but clear cusp was visible in the real part as well as in the imaginary part of ac-susceptibility at 30 K for the samples with Ti. These results are indicative of spin glass behaviour, together with the observed increase of magnetization below 30 K.

P-1-06

Two-band ferromagnetic Kondo lattice model on a ladder with quantum mechanical $S = 3/2$ core spins

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We present a numerical study of the ferromagnetic Kondo lattice model with quantum mechanical $S = 3/2$ core spins. We treat two orbitals per site on a ladder using the density matrix renormalization group. We examine parameters relevant to manganites for the undoped case of quarter-filling. We investigate the influence of the superexchange parameter J' between core spins and find that a small increase of J' is sufficient to induce a transition from ferromagnetic (FM) to antiferromagnetic (AFM) ordering. This transition is accompanied by a change of orbital order from alternating orbital occupation to predominant occupation of the in-plane orbital. Furthermore, we consider the influence of doping on the magnetic and orbital order and compare these results to an effective spin-orbital-model that takes the multiplet structure of the Mn ions correctly into account.

P-1-07

SPIN WAVE AND MIXED SPIN-AND-ORBITAL EXCITATIONS IN $KCuF_3$

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We consider an effective spin-orbital model [1], which describes interactions between Cu^{2+} ions in d^9 configuration and investigate spin and mixed spin-and-orbital excitations in $KCuF_3$ for antiferromagnetic ground state with the ferro type of orbital order of occupied e_g orbitals. Spin excitations couple to mixed spin-and-orbital excitations in the spin-orbital superexchange model, as shown using the random phase approximation (Tjablikov decoupling) within the Green's function scheme [2]. Here we employ Holstein-Primakoff method for spin and orbital operators and derive the spin wave and spin-and-orbital wave excitations using the bosonic representation. The results demonstrate that this approach gives equivalent results to those of Ref. [2]. In addition, we include the charge transfer term which originates from two-hole charge excitations at a common neighboring $2p_\sigma$ orbital of a common fluorine ion in between two copper ions, and modifies the spin-orbital model. Implications of this new superexchange term on spin and spin-and-orbital excitations are discussed in antiferromagnetic phases with different orbital order.

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P-1-08

HOMES RELATION IN ATTRACTIVE HUBBARD MODEL IN $D = \infty$

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Lack of the recognized theory of high-temperature superconductivity (HTS) has led to an intense experimental and theoretical search for some universal relationships, which might unravel the physics behind HTS. One of the most known is so called Uemura relation, $\rho_s(0) \propto T_c$, where ρ_s is superfluid density and T_c is the superconducting transition temperature. Recently Homes *et al.* (Nature **430**, 539 (2004)) reported a new universal scaling relation, $\rho_s \propto \sigma(T_c) \cdot T_c$, where $\sigma(T)$ is dc conductivity. On the other hand there are also reports, citing data denying the universality of this new relation and ascribing the cases where the relation does appear to some well known mechanisms. In this situation theoretical calculations of the effect would be very interesting. Unfortunately calculating transport properties like $\sigma(T)$ is not a simple task. The present paper shows the results of calculations of the Homes relation for the attractive Hubbard model in the limit of infinite dimensions $d = \infty$, where calculations are simplified but the results can still be an approximation for the $d = 3$ case.

P-1-09

DOUBLE EXCHANGE MODEL IN CUBIC VANDATES

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Following the idea of the double exchange (DE) mechanism, we pose a question how the C-type antiferromagnetic (AF) order (ferromagnetic chains staggered in two other directions) of undoped $LaVO_3$, stabilized by the superexchange spin-orbital model [1], is modified under doping. In particular, we investigate the role of the DE mechanism for stability of *metallic and antiferromagnetic* phase, which was observed experimentally in $La_{1-x}Sr_xVO_3$ in the range of doping $0.178 < x < 0.26$. The DE model treats electrons in d_{xy} orbitals as classical $S = 1/2$ spins, which interact by Hund's exchange J_H with $d_{yz/zx}$ electrons in partly filled t_{2g} orbitals. Including the orbital degeneracy of doped holes and strong Coulomb repulsion U between t_{2g} electrons, we investigate the magnetic interactions and determine the phase diagram of the model using mean-field approximation and slave boson method. We demonstrate that C-type AF and metallic phase can be stabilized. The generic role of degenerate t_{2g} orbitals in the present DE model with orbital degeneracy is discussed and contrasted with the conventional DE model, which involves partly filled e_g orbitals and is used to describe doped manganites.

[1] G. Khaliullin, P. Horsch, and A. M. Oleś, Phys. Rev. Lett. **86**, 3879 (2001).

P-1-10

The properities of a charge density wave phase in the anharmonic Holstein-Hubbard model : A variational approach.

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The Holstein-Hubbard model with anharmonic phonons is treated within a variational canonical transformation framework. The non-perturbative nature of this method allows a reliable inclusion of the effects of anharmonicity. An effective electron Hamiltonian is derived, in which importantly the anharmonicity produces relatively large correlated hopping terms. The half-filled $n = 1$ case is studied, in which the ground state is a charge density wave phase. The ground state order parameter and critical temperature dependence on the anharmonicity parameter α is calculated. A reasonable agreement with earlier Quantum Monte Carlo method results is shown.

P-1-11

FINITE SIZE CORRECTIONS IN THE TWO-LEVEL BCS MODEL

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The properties of nanoscale materials differ from those observed in bulk systems due to discrete structure of their energy spectrum. In this work the small superconducting grains modelled by two level system has been studied. The finite size correctionns to the ground state energy, the average number of particles in each level and other characteristics of the system has been studied by means of direct solution of the Richardson's model. We compare our results with those found in the literature and obtained by other techniques.

P-1-12

Stability of charge-stripe phases in a system of spinless fermions or hardcore bosons

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We consider two strongly correlated two-component quantum systems, consisting of quantum mobile particles and classical immobile particles. The both systems are described by Falicov–Kimball-like Hamiltonians on a square lattice, extended by direct short-range interactions between the immobile particles. In the first system the mobile particles are spinless fermions while in the second one they are hardcore bosons. We construct rigorously ground-state phase diagrams of the both systems in the strong-coupling regime and at half-filling. Two main conclusions are drawn. Firstly, short-range interactions in quantum gases are sufficient for the appearance of charge stripe-ordered phases. By varying the intensity of a direct nearest-neighbor interaction between the immobile particles, the both systems can be driven from a phase-separated state (the segregated phase) to a crystalline state (the chessboard phase) and these transitions occur necessarily via charge-stripe phases: via a diagonal striped phase in the case of fermions and via vertical (horizontal) striped phases in the case of hardcore bosons. Secondly, the phase diagrams of the two systems are definitely different. However, if the strongest effective interaction in the fermionic case gets frustrated gently, then the phase diagram becomes similar to that of the bosonic case. Influence of the hopping anisotropy on striped phases has been considered.

P-1-13

CHARGE KONDO STATE IN THE (HARD CORE) BOSON-FERMION MODEL

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We study the phase diagrams and thermodynamic properties of a system of coexisting local pairs and itinerant electrons described by the (hard-core) boson-fermion model. The model considered takes into account both the intersubsystem charge exchange coupling I_0 as well as the density-density interaction V_0. Up to now the studies of the model have been concentrated on the superconducting (SC), charge ordered (CDW) and nonordered (normal) phases. Here we will discuss the conditions of occurrence and the properties of the so called charge Kondo state (CKS). One finds that such a state can be realized in the present model if the charge exchange interaction is increased. The CKS being an analogue of the magnetic Kondo state in the systems of the periodic Kondo lattice is characterized by a compensation of a local charge moment (isospin singlet) and it can compete with the superconducting and charge orderings. Within an extended mean-field approximation a mutual stability of CDW, SC and CKS states are determined at $T = 0$ for various lattice structures in the case of half-filled fermionic and bosonic bands. The effects of increasing temperature on the properties of CKS are also discussed.

P-1-14

PHASE DIAGRAMS OF THE EXTENDED HUBBARD MODEL WITH TRANSVERSE (XY-TYPE) SPIN-EXCHANGE INTERACTION

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The ground state properties of the extended Hubbard model with transverse (XY-type) spin-exchange interaction (J_{ij}^{xy}) are studied. The case of ferromagnetic ($J_{ij}^{xy} > 0$) and antiferromagnetic ($J_{ij}^{xy} < 0$) exchange couplings are considered. The analysis of the model is performed for d-dimensional hypercubic lattices, including $d = 1$ and $d = \infty$, by means of the (broken symmetry) Hartree-Fock approximation and, for $d = \infty$, by the slave-boson mean-field method. Some rigorous results derived for the strong coupling regime of the model for $d = 1$ are also presented. At half filling the ground state phase diagram for $d = 1$ is shown to consist of ten different phases, including site and bond located antiferromagnetic (SDW) and charge density wave (CDW) states, ferromagnetic XY (F) state, the superconducting s-wave (SS) and p-wave (TS) states, as well as several mixed phases with coexisting site and bond orderings. For $d = \infty$ the corresponding diagram is simpler and consists of the phases involving exclusively site located orderings. The obtained phase diagram for $d = 1$ is in agreement with results of recent studies based on the continuum-limit approach and the density-matrix renormalization group method.

P-1-15

Two dimensional model for correlated e_g electrons in doped nickelates

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The magnetic and orbital instabilities in e_g band are relevant for the appearence of novel phases with orbital and magnetic order, discovered in doped nickelates such as $La_{2-x}Sr_xNiO_4$ [1]. We investigate this problem using two-dimensional Hubbard type model with two e_g orbitals, with anisotropic hopping (dependent on orbital-phases) and with intraorbital Coulomb and Hund's exchange interactions. The insulating undoped phase corresponds to two electrons per site.

The calculations were carried on 8×8 cluster: first, using Hartree-Fock approximation; next, including the correlations implemented within (space-nonhomogeneous) Local-ansatz-like method. Comaprison with mean-field (Hartree) results [2] is made. For parameters of the model Hamiltonian which, presumably, are applicable to nickelates we found that for the dopings ranging from 1/8 to 1/2 the most stable phases consist of ferromagnetically ordered lines of spins with antiferromagnetic coupling between them (C-AF phase). It was found that the correlations renormalised the HF ground state energies but in no case was the renormalised HF ground state switched with higher laying metastable states. It was also found that the orbital ordering in space is weak but couples to the spin order.

[1] J. M. Tranquada, et al., Phys. Rev. B **67**, 012404 (2003).
[2] R. Frésard, M. Raczkowski,, and A. M. Oleś, Phys. Stat. Sol. (b) **242**, 370 (2005).

P-1-16

BCS-Bose condensation crossover in anisotropic superconductors

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We analyze the crossover from BCS to local pair (LP) superconductivity for the $d_{x^2-y^2}$-wave pairing symmetry in the ground state. The thermodynamic and spectroscopic characteristics of the extended Hubbard model with intersite electron pairing are obtained for the $2D$ square lattice. The two crossover scenarios, density driven and interaction driven, are compared. The influence of the next-nearest neighbors hopping (t_2) on the crossover is discussed. For $|t_2/t| < 0.5$ crossover is simultaneous with the vanishing of nodal points in the quasiparticle energy, whereas for $|t_2/t| > 0.5$ the crossover is similar to that of s-wave type. The vanishing of nodal points is clearly reflected in superconducting characteristics.

P-1-17

. Charge transport within dynamical mean-field approach

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The main goal of this paper is to employ the dynamical mean-field theory in the limit of the infinite spatial dimensions and discuss transport properties of strongly correlated systems. The dynamical mean-field method (DMF) maps the Hubbard model onto a single impurity Anderson model, which has to be solved self-consistently.To solve the Anderson model, we employ the iterative perturbation theory (IPT) developed in [1]. Within the IPT, the self-energy is expressed to the second order contribution with respect to the on site Coulomb repulsion. In the DMF approach, in the limit of infinite spatial dimensions, the self-energy and all vertex functions are local and thus the transport quantities can be calculated from the single-particle spectral function. Different density of states are used to study a crossover from coherent Fermi liquid excitations to incoherent excitations. This crossover is seen as a nonmonotonic temperature dependence of various transport quantities such as the resistance, thermopower, and Hall coefficient. The calculations are performed for arbitrary doping over a wide range of temperatures.

1. H. Kajueter and G. Kotliar, Phys. Rev. Lett. **84**,131 (1996).
2. J.K. Freericks, Pys. Rev. B**70**, 195342 (2004).

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P-1-18

INFLUENCE OF THE SHORT RANGE ORDER (SRO) ON THE ELECTRICAL CONDUCTIVITY OF THE MAGNETIC BINARY ALLOYS IN THE PARAMAGNETIC STATE

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The model of the magnetic binary alloy which contains interacting itinerant electrons and localized spins was considered. The interaction between two kinds of electrons was assumed to be in the simple local exchange form. The complicated many body problem was reduced to the one particle one with the help of Coherent Potential Approximation (CPA). Itinerant electron selfenergy was calculated using standard Green's function technique with taking into account short range order within the localized spin system. Electrons' states were strongly affected by the magnetic ordering and correlations within localized moments (when $T > T_C$). The DC electrical conductivity expressed by Kubo-Grennwood alloy formula was calculated and analysed in detail in the paramagnetic region. The temperature derivative of the resistivity $\frac{d\rho}{dT}$ was found to be neither constant nor equals to zero but was negative or positive in dependence on the model parameters and had the structure just nearby the $T_C + 0^+$. Our investigations have shown that SRO in the localized spin subsystem has significant influence on the resistivity in the temperature range $[T_C, 2T_C]$.

P-1-19

DEVIATIONS FROM THE MATTHIESSEN'S RULE IN MAGNETIC DISORDERED ALLOYS: THEORETICAL INVESTIGATIONS

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The model of the magnetic disordered alloys, including the itinerant electrons, localized spins and phonons, was elaborated in details in the paramagnetic region with the use of the Coherent Potential Approximatiom (CPA) approach. The expression for the DC electrical conductivity was taken from the Kubo-Greenwood formula for the alloys. The separate (residual, phonon and magnetic) contributions to the resistivity for the temperatures above Curie transition temperature for different sets of the model parameters were calculated. The linear temperature dependence of the phonon contribution to the resistivity was reproduced except from the anomalous behaviour observed for the parameters sets for which the Fermi level locates near the bands edges. For the same parameters sets our calculations showed the largest deviations from the Matthiessen's rule. Our model calculations confirmed the Matthiessen's rule generalized to the case of the three, residual, phonon and magnetic contributions to the resistivity of the magnetic disordered alloys with the partially filled band when the Fermi level locates far from the bands edges.

P-1-20

Superconductivity in Strontium Ruthenate

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We analyze the possibilities of triplet pairing in Sr_2RuO_4 based upon a three orbital and three dimensional model. Depending on the orbital dependent effective interactions we find two possible gap models. In the first model the orbital dependent interlayer attraction influences the quasi-particle spectra which have horizontal line or point nodes on the α and β sheets and no nodes on the γ sheet. In the other model there is no interlayer interaction coupling and all bands are fully gaped. For both models we show the quasi-particle density of states and the eigenvalues on the Fermi surface. The corresponding calculated specific heat results are also compared to the experimental data.

P-1-21

SIMPLE TOOLS TO UNDERSTAND CORRELATED SYSTEMS WITH ORBITAL DEGENERACY

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Correlated e_g electrons exhibit a series of fascinating properties, in particular in cuprates and nickelates. Here we present simple calculations meant to estimate the phase diagram of the two-band Hubbard model. It is known to be very rich, in particular for e_g electrons in the vicinity of quarter-filling [1,2]. Indeed, in mean-field theory, various orbitally polarized ferromagnetic and antiferromagnetic phases appear when the Hubbard U, the Hund's rule coupling J_H and the crystal field are varied. In particular ferromagnetism (antiferromagnetism) is favored for $J_H/U < (>)\ 0.2$.

Here we show that the same tendency is reproduced when diagonalizing small clusters. Moreover the phase diagram is very sensitive to the type of considered orbitals, being e_g or t_{2g}. The limits of a hopping expansion are also discussed.

[1] L. F. Feiner, A. M. Oleś, and J. Zaanen, *Phys. Rev. Lett.* **78**, 2799 (1997).

[2] R. Frésard, M. Raczkowski, and A. M. Oleś, *Phys. Stat. Sol.* (b) **242**, 370 (2005).

O-2-01

INTRINSIC MECHANISM OF ANOMALOUS HALL EFFECT IN A TWO-DIMENSIONAL MAGNETIC SYSTEM WITH IMPURITIES

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We discuss the mechanism of anomalous Hall effect related to the contribution of electron states below the Fermi surface (induced by the Berry phase in momentum space). Our main calculations are made within a model of two-dimensional electron gas with spin-orbit interaction of the Rashba type, taking into account the scattering from impurities. We demonstrate that such an "intrinsic" mechanism can really dominate but there is a competition between the geometric Berry-phase-induced term σ_{xy}^{II} in the Hall conductivity, and the impurity-induced term σ_{xy}^{I}, related to the contribution of states in the vicinity of Fermi surface. We also show that the contribution to the Hall conductivity from electron states close to the Fermi surface has the intrinsic property as well, and it does not vanish in the clean limit
The main effect of impurity-related conribution is a possible change of sign for the off-diagonal conductivity. The resulting magnitude and sign of the Hall conductivity strongly depend on the electron density in the system.

O-2-04

IMPORTANCE OF SPIN FLUCTUATIONS IN COUPLED TWO-DIMENSIONAL MAGNETIC TRILAYERS

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Two ultrathin ferromagnetic films of Co and Ni separated by a non-magnetic spacer of Cu are taken to study the spin-spin correlations of weakly coupled ferromagnets. The Ni film thickness ranging between $d_{Ni} = 2 - 6$ monolayers (ML) is chosen to study the 2D $\rightarrow$ 3D dimensional crossover in ferromagnets. X-ray magnetic circular dichroism is the ideal technique to study the temperature dependence of the magnetization of Co and Ni separately. The spacer thickness ranges from $d_{Cu} = 2 - 8$ ML to monitor the oscillatory behavior of the interlayer exchange coupling. The measured temperature-dependent magnetizations and the corresponding Curie temperatures are accompanied by a microscopic many-body Green's function theory. Both experiment and theory give firm evidence that for nanostructured magnets a static mean field description is insufficient. It is demonstrated that higher order spin-spin correlations are important and explain the observed increase of the Curie temperature by up to ~ 200 % due to the interlayer exchange coupling. The results are visualized in a three-dimensional diagram for the first time as a function of *both* the Ni thickness *and* the Cu spacer thickness.
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O-2-05

"CHARGE SENSING" EFFECTS IN CONDUCTANCE THROUGH QUANTUM DOTS AND POINT CONTACTS

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We investigate the influence of charge dynamics on electronic transport through large quantum dots (QD) and point contacts (QPC). Because of the complex energetic structure of the large dot and high anisotropy of hybridization of its levels with electrodes, some electron charge can be accumulated within the dot area. It influences in capacitative way the active in transport levels, which is manifested by saw-like pattern in the conductance curve. This effect is called "charge sensing". Additionally, when a small hybridization is present between transmitting channel and levels accumulating charge, Fano resonances emerge in conductance. Their shape is also influenced by charge sensing. We derive this effect starting from microscopic Hamiltonian. Similar effects have been also experimentally observed in conductance through QPC when a QD is present in the close vicinity of QPC. Our calculations are in good correspondence with these data and capture the basic physics behind.

O-2-07

SPIN MODES IN SATURATED ELLIPICAL DOTS

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Brillouin light scattering spectra have been measured in arrays of permalloy elliptical dots 15 nm thick, with major and minor axes 500 and 200 nm long. A magnetic field of fixed magnitude (1.5 kOe) is applied along the easy and the hard axis. Several peaks are resolved in both configurations. They are interpreted within the framework of the recently introduced dynamical matrix model, in terms of modes localized at the dot ends, or extending throughout the whole dot. Hybridization between these two families is discussed in dependence of the direction of the applied field.

O-2-08

ASYMMETRIC MAGNETIZATION REVERSAL IN EXCHANGE-BIASED Co/Pt MULTILAYERS

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A detailed study of the magnetization reversal process in [2 nm Pt/t nm Co]$_3$/10 nm IrMn/2 nm Pt multilayers with 0.4 nm $\leq$ t $\leq$ 0.9 nm is presented. The films with t = 0.4 nm exhibit a square hysteresis with full out-of-plane remanence and a perpendicular exchange bias field ($\mu_0 H_{eb}$) of 10.2 mT. For t $\geq$ 0.5 nm, however, the magnetization curves are highly asymmetric. Kerr microscopy images reveal that the reversal process is different in the two branches of the hysteresis curves: In one of the branches magnetization reversal proceeds by the nucleation of numerous small inverse domains, whereas in the other a few inverse domains steadily grow by domain wall propagation. This asymmetry is explained by a lateral variation in the perpendicular exchange bias direction due to the growth of IrMn onto multidomain ferromagnetic Co/Pt multilayers. Annealing at 220^{o}C for 1 hour in a perpendicular applied field of 0.8 T removes the switching asymmetry. For these films a maximum exchange bias field of 16.3 mT is obtained for t = 0.7 nm. This indicates that the relation $\mu_0 H_{eb} \sim 1/t$ does not hold for Co/Pt multilayers with small Co layer thickness.

O-2-09

MAGNETIZATION DYNAMICS OF PERPENDICULAR EXCHANGE–BIASED (Pt/Co)–Pt–IrMn MULTILAYERS STUDIED BY MOKE MICROSCOPY AND MAGNETOMETRY

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The magnetization dynamics of [2 nm Pt/5 nm Co]$_3$/t *nm* Pt/10 nm IrMn/2 nm Pt multilayers, in which a ferromagnetic multilayer with perpendicular magnetic anisotropy is separated from an IrMn antiferromagnet by a thin Pt insertion layer with 0.1 nm $\leq$ t $\leq$ 1.2 nm, has been investigated by Kerr magnetometry and Kerr microscopy. The insertion of 0.1 nm thick Pt enhances the exchange bias field ($\mu_0 H_{eb}$) from 20 mT to 28 mT above which it decreases exponentially with increasing Pt layer thickness. We show from relaxation measurements of the magnetization $M(t)$as well as by direct observation of magnetic domains, that the magnetization reversal at maximum H_{eb} takes place by the nucleation of isolated cylindrical domains with different nucleation density sites for the forward and backward branches of the hysteresis loop. For a Pt layer thickness larger than 0.4 nm magnetization reversal proceeds by domain wall movement. All the results will be quantitatively analyzed using Fatuzzo[1] theory. The origin and magnitude of the activation energies for the domain nucleation and domain wall movement processes will be discussed.

[1] E. Fatuzzo, Phys.Rev. 127 (1962) 1999

O-2-10

Wave-packet dynamics of Bloch electrons — role of Berry phase

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Motivated by a recent proposal on the possibility of observing a monopole in the band structure, and by an increasing interest in the role of Berry phase in spintronics, we reconsidered the problem of adiabatic motion of a wave packet of Bloch functions, under a perturbation varying slowly and incommensurately to the lattice structure. We showed, using only the fundamental principles of quantum mechanics, that the effective wave-packet dynamics of Bloch electrons is conveniently described by a set of equations of motion (EOM) in which a *nonabelian* Berry phase associated with an internal degree of freedom appears. We then apply our wave-packet dynamics to the analyses on transport phenomena such as charge/spin Hall-type/polarization currents. We also discuss its relevance to the physics of orbital current as well as transport through a magnetic domain wall, which may serve as a probe for detecting and controling Berry phase.

O-2-11

FERROMAGNETIC (Eu,Gd)Te SEMICONDUCTOR LAYERS

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In (Eu,Gd)Te magnetic semiconductor alloys the substitution of Gd^{3+} ions for Eu^{2+} ions creates a high concentration of quasi-free electrons and transforms EuTe (a well known antiferromagnetic compound) into a ferromagnetic (driven by RKKY interaction) n-type semiconductor alloy. This material is expected to have a very high degree of electron spin polarization and can serve as a spin injector in model semiconductor spintronic heterostructures. We studied the electron concentration induced magnetic transition in monocrystalline layers of (Eu,Gd)Te grown by MBE technique. By variation of Gd content and stoichiometry both n-type and insulating layers of (Eu,Gd)Te were obtained with ferromagnetic state found only in conducting layers. The ferromagnetic transition in (Eu,Gd)Te is also observed in electron transport as a peak of resistivity at the Curie temperature and a strong negative magnetoresistance. The magnetic properties of (Eu,Gd)Te layers will be discussed based on experimental studies of magnetization, ac magnetic susceptibility, and ferromagnetic resonance revealing the ferromagnetic transition temperature T_c=11-15 K as well as a dominant easy-plane type of magnetic (shape) anisotropy with negligible in-plane magnetocrystalline anisotropy.

O-2-12

Kondo effect in the presence of ferromagnetism

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We study the Kondo effect in a quantum dot (QD), which is coupled to ferromagnetic leads, and analyze its properties. Based on a scaling analysis we first show that a splitting of the Kondo resonance similar to the usual magnetic-field-induced splitting will appear due to exchange interaction with leads. The most important result is that this splitting can be fully compensated by an appropriately tuned external magnetic field and the strong coupling limit of the Kondo effect can be restored. We adapt the NRG method to the case of a QD coupled to ferromagnetic leads. We show that the Kondo effect in the presence of ferromagnetic leads has unique properties such as a strong spin polarization of the density of states at the Fermi level. In addition, we find, surprisingly, that even in the presence of strong spin asymmetry in the QD spectral function at the Fermi level, the ground state of the system has a fully compensated local spin and displays Fermi liquid behavior. We also analyze the nonlinear transport through the QD. We find that for parallel alignment of the lead magnetizations the zero-bias anomaly is split. This splitting can be removed by appropriately tuning of a magnetic field. In the antiparallel configuration of the lead magnetizations and symmetric coupling no splitting occurs. New experimental results for a single C_{60} molecule confirm our theoretical predictions.

O-2-13

SPIN TRANSPORT IN DISORDERED SINGLE-WALL CARBON NANOTUBES CONTACTED TO FERROMAGNETIC LEADS

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Recent conductance measurements on multi-wall carbon nanotubes (CNTs) show that they effectively behave similar to disordered single-wall CNTs [1]. This is due to the fact that electric current flows essentially through the outermost shell and is strongly influenced by inhomogeneous electrostatic potential coming from the inner tubes. Here we present theoretical studies of spin-dependent transport through disorder-free double-wall CNTs as well as single-wall CNTs with Anderson-type disorder. The CNTs are end-contacted to ferromagnetic electrodes modelled as fcc (111) surfaces [2]. Our results shed additional light on the giant magnetoresistance effect in CNTs. Some reported results concern realistically long CNTs, up to several hundred nanometers.

[1] R. Egger and A. O. Gogolin, Phys. Rev. Lett. 87, 066401 (2001); B. Stojetz et al., cond-mat/0410764, (2004).
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O-2-14

ELECTRONIC STRUCTURE AND PARITY EFFECTS IN CORRELATED NANOSYSTEMS

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We discuss the spectral, transport and magnetic properties of quantum nanowires composed of single atoms and containing either even or odd numbers $N \leq 13$ of valence electrons. In our approach we combine **E**xact **D**iagonalization and **Ab I**nitio calculations (EDABI method [1]). The analysis is performed as a function of the interatomic distance. The momentum distribution differs drastically for those obtained for even N with those for odd N, whereas the Drude weight of the optical conductivity evolves smoothly. An appearance of magnetic, Slater-type splitting in electronic structure is demonstrated and explained [2]. A nontrivial role of boundary conditions is stressed.

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O-2-15

Monte- Carlo Simulation of Solid State and Melting of 2D Confined Magnetic Particles

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Numerous systems correspond to confined magnetic particles interacting through dipolar interactions : magnetic particles, flux lines in superconductors, charged colloids. Because of the long range dipolar interaction, the ground state and excited states of such 2 D system are not simply found. Here from careful extended Monte-Carlo simulations the ground state is obtained and shown to be derived from a triangular lattice with a few layers stuck to the confinement boundary. The most common solid state obtained by relaxation from a random configuration is found to be an excited state composed of many triangular crystallites separated by lines of alternate topological defects with five and seven nearest neighbors. The melting of these two solid phases gives finally a common liquid phase as expected. But the melting of the ground state happens as a sharp first order transition while the melting of the excited state happens as a continuous vitreous transition which starts at low temperature with the motion of topological defects on their defect lines, while the rest of the sample remains solid, as a two component medium. These results are compared to experimental and numerical results of corresponding experiments with such Wigner glass and Wigner crystal. The elastic properties of these solid states are also considered.

O-2-16

On the prospects of probing surface magnons using Atomic Beam Spin Echo

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The Atomic Beam Spin Echo technique is a novel, powerful tool for investigating surface dynamics, including quasi- and inelastic processes. In this atom interferometry method, we combine the exclusive surface sensitivity of thermal atom scattering with the neV resolution of in-beam magnetic resonance techniques. Using ^{3}He atoms as a non-magnetic probe, we succeeded to resolve time correlations at the surface in the ps through ns range. In a theoretical study we have recently shown that, by using the spin magnetic moment of atomic hydrogen, this method may be applied to the study of fast surface magnetization dynamics including surface magnons. In particular, we show that this method may be used for the determination of surface magnon dispersion curves since they produce a unique signature in the expected spin echo signal. We will present data from first atomic hydrogen spin echo experiments and address its perspectives.

P-2-01

IMAGING MAGNETIC MICROSTRUCTURES WITH THE USE OF ELECTRONS

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Magnetic domains can be observed by a number of methods, involving different physical principles of magnetic contrast formation. The subject of interest of the present paper is studying magnetic microstructures by some of the techniques which make use of electrons. In this context, we refer to the examples of magnetic microstructure images of cobalt monocrystals, Nd-Fe-B permanent magnet and a thin permalloy film, while the methods used are the type-I magnetic contrast technique of scanning electron microscopy (SEM), the colloid-SEM method and the Fresnel mode of transmission electron microscopy (TEM). It is shown that the SEM type-I magnetic contrast and the colloid-SEM method have quite different probing depths and consequently provide useful complementary information on the magnetic microstructure at the surface of bulk materials which exhibit an out-of-plane component of magnetization. Improved results were achieved with the colloid-SEM technique, both from the viewpoint of the spatial resolution and the quality of the original images obtained. It is demonstrated that TEM is a very valuable method for investigating the magnetic microstructure of thin magnetic films, mainly because of its high spatial resolution and high sensitivity to small variations in the magnetization.

P-2-02

Domain structure of NiFe/Au/Co/Au multilayers with perpendicular anisotropy

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The magnetic properties of sputtered $[Ni_{80}Fe_{20}(2\ nm)/Au(t_{Au})/Co(t_{Co})/Au(t_{Au})]_{15}$ multilayers with t_{Au}=1.5-3 nm and t_{Co}=0.6-1.5 nm were investigated with magnetic force microscopy. The NiFe layers possessed in-plane anisotropy while the sandwiching of Co layers between Au layers ensured their perpendicular anisotropy through the influence of a surface anisotropy. It led to the formation of maze configuration of stripe domains. The stripe domains period λ strongly depends on t_{Co} changing from 0.9 to 0.3 μm when t_{Co} changes from 0.6 to 0.8 nm. λ increases with the Au layers thicknesse, too. Both dependencies can be qualitatively understood by the model of Draaisma and de Jonge [1]. It describes however, a multilayer with all sublayers possessing perpendicular anisotropy in contrast to our case. Therefore the exact estimate of the effective magnetic anisotropy with the above model is not possible. The values of stray fields acting on Py layers, in the range of 100 kA/m, estimated from magnetoresistive dependencies are in qualitative agreement with those evaluated from the model of infinitely long stripe domains with domain widths taken from magnetic force microscopy measurements.

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P-2-03

Superconducting and magnetic properties of large-angle bismuth bicrystals

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Magnetic moment measurements in large-angle ($\Theta > 30^o$) bicrystals of bismuth with crystallite interface (CI) of twisting type were performed by use of a Cahn balance, PPMS and SQUID magnetometers. Bicrystals were obtained by zone recrystallization method using double seed technique. The magnetic properties of bicrystals essentially differ from well-known results on single-crystal bismuth (the paramagnetism of charge carriers become stronger, the diamagnetism rise, etc). Two superconducting phase at CI of bicrystals with $T_c \sim 8.4$ K (for some bicrystals $T_{onset} \sim 16$ K) and $T_c \sim 4.3$ K was observed (ordinary rhombohedral Bi is not a superconductor). It was shown that one of them (phase with $T_c \sim 8.4$ K is localized in central part of CI and have an upper critical field ~ 2.5 T, and a coherence length ~ 12 nm. Also it was found that in adjacent layers (width of layer $L_a \sim 20$ nm) of CI the density of electrons is lower than in central part and is significant the proximity effect.

P-2-04

Magnetic domain structure of micro-patterned PtMn/CoFe exchange bias bilayers

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Using magnetron sputter deposition a number of glass/Ta 70 Å/PtMn 200 Å/CoFe 40 Å/Ta 40 Å samples with large exchange bias field were prepared for magnetic pattering investigations. By means of optical lithography and physical etching several patterns with decreasing lateral sizes of either the elements or the spacing between the elements were prepared. The largest square is 50×50 μm^2 and the smallest only 1 μm^2. The separating lines range from 10 μm to 2 μm width. The magnetic characterization of the samples was done by VSM and MOKE. Kerr microscopy and MFM investigations in an applied magnetic field have been performed in order to get a deeper understanding of the domain pattern. All images show a monodomain magnetization state in zero magnetic field. The shape of the structure itself dose not influence the magnetization direction. The shape anisotropy contribution is thus smaller than the unidirectional anisotropy given by the exchange bias. In addition 5 keV He^+ ion irradiation was used to decrease exchange bias field value and thereby modify the ratio between unidirectional and shape anisotropy. The magnetic domain structure is investigated as a function of this ratio.

P-2-05

Electrical Transport in Strained $La_{0.7}Ca_{0.3}MnO_3$ Films

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Magnetotransport properties of 15 nm $La_{0.7}Ca_{0.3}MnO_3$ thin films deposited on (100) LaAlO3 substrate were investigated. Fine balance between the charge ordered insulating phase and ferromagnetic metallic phase results in the number of glassy features: significant hysteresis phenomena, memory effects and long-time relaxation of resistivity at turning on and off of magnetic field in wide temperature range 10 - 220 K. In this temperature range the resistance of the $La_{0.7}Ca_{0.3}MnO_3$ films decreases significantly with current, exhibiting a nonlinear conduction, which cannot be explained by homogeneous Joule heating of the films. Effect of current on the resistance follows the temperature dependence of magnetization. Magnetotransport properties of strained thin films are discussed in the frame of cross-coupling of charge, spin and strain.

P-2-06

ELECTRIC CHARGE TRANSPORT IN HOLMIUM THIN FILMS AT LOW TEMPERATURES AND IN MAGNETIC FIELD

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High precision electrical resistance measurements were performed on holmium bulk and thin film samples prepared in ultrahigh vacuum in the temperature range between 4.2 K and 300 K, and in magnetic field up to 5 T. A "knee-like" resistance anomaly was observed near the magnetic phase transition from paramagnetic state to basal-plane spiral antiferromagnetic structure ($T_N = 128.9$ K) in the bulk and below 122 K in thin Ho films having a thickness between 98 nm to 215 nm. Numerical analysis of experimental R vs. T data yielded the transition to magnetic cone-shape structure in bulk Ho at $T_C = 19$ K. Application of magnetic field parallel to the substrate at temperatures below ~ 150 K caused a decrease of resistance with increasing field. Moreover, a suppression of the T_N value up to ~ 5 K with increasing field up to 5 T was observed. An unexpected resistance minimum at ~ 9 K and a slope's change of the R vs. T curve near ~ 170 K was observed in 215 nm thin film. X-ray diffraction of Ho films revealed diffraction peaks originating from the h.c.p. structure of Ho and those from holmium dihydride.

P-2-07

Spin accumulation, spin currents, and torque, in the problem of motion of a sharp domain wall in magnetic nanowires

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We consider the motion of a sharp domain wall in magnetic nanowires with electric current. The width of the domain wall is much smaller than the electron wavelength, which is typical for magnetic semiconductors. We calculate the distributions of the spin density and the spin current related to different modes of the scattering states. The accumulated transverse components of the spin density and the spin current oscillate in the vicinity of the wall and they essentially affect its dynamics whereas the longitudinal part of the spin current is responsible for another component of the spin torque creating a force for the current-induced motion of the domain wall along the nanowire.
We also analyze the dynamics of the sharp domain wall using the standard Landau-Lifshits-Gilbert formalism and the two-component spin torque calculated for this model. We demonstrate that the domain wall changes its shape depending on the velocity of the motion, and we calculate this velocity as a function of the electric current.

P-2-08

The influence of roughness on some magnetic properties of layered structures of Fe, Co separated by Cu or Au

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The system of two magnetic (M) layers divided by nonmagnetic (N) spacer is considered. Roughness in the interface region is introduced employing model proposed by Bruno and Chappert [1, 2]. Presence of roughness leads to modification of the interface exchange parametr and interface anisotropy in comparison to samples with ideal interface. The magnetisation distribution and Curie temperature has been calculated using Green function formalism [3] for systems consisting of Fe or Co standing for M and Cu or Au standing for N, respectively. Parameters corresponding to GaAs have been taken into account to characterize the substrate. The results obtained show decreasing of Curie temperature and shift of magnetisation curve with incresing of roughess parameter.

P-2-09

Spin wave parameter in the system of non-equivalent exchange coupled-layers

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The system of two ferromagnetic layers described by different exchange parameters and indirectly coupled by nonmagnetic spacer has been considered in low temperature region. Special attention has been paid to the influence of anisotropy in the surface and interface region on the temperature dependence of magnetisation. The range of interaction parameters for which the Bloch's $T^{3/2}$ was fulfilled has been determined employing Green function formalism. It has been shown that the spin wave parameter B was fluctuating as a function of spacer thickness and its value was increasing with decreasing of thickness of constituent layers. Significant influence of the substrate on the amplitude of B parameter has been also found.

P-2-10

AN EXTENDED BOLTZMANN FORMALISM FOR TRANSPORT DESCRIPTION IN THIN Fe-Cr-Fe TRILAYERS

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We present the calculations of Giant Magnetoresistance (GMR) for the thin trilayers nFe/3Cr/nFe where $1 \leq n \leq 8$ for the slab geometry. All parameters used for calculations, i.e., the layer potential, the relaxation time, the effective mass and the Fermi energy are determined on the basis of ab initio calculations for the electronic structure of the considered trilayer when the spin polarisation is taken into account. The comparison of semiclassical approach based on the Boltzmann formalism is given. The value of the specularity factor in the Fuchs-Sondheimer theory responsible for scattering electrons from metallic surface is found in an analytical way. The results show an increase of GMR for the samples with different ferromagnetic layer thickness when compared with those obtained from the standard Boltzmann theory.

P-2-11

SPIN -MIXING INTERFACE CONTRIBUTION TO MAGNETORESISTANCE IN TRILAYER

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We discuss the transport properties of trilayer $A(n)/A_cB_{1-c}/B(p)/A_cB_{1-c}/A(n)$ including the structure with two mixed interfaces $A_cB_{1-c}(S^A = 1,\ S^B = 1/2)$ for arbitrary concentration c of A-spins. The existence of enhanced or diminished interface magnetism leads to a strong inhomogenity of the potential in the interface region. The complex interface potential behaviour constitutes the additional source of electron scattering at the interface and contributes significantly to GMR-effect in trilayer. The matching conditions for electron distribution functions as well as the value of the magnetoresistance are presented. The obtained results are compared with those of different model results accessible in literature.

P-2-12

EFFECT OF STRUCTURAL DISORDER ON THE ELECTRONIC STRUCTURES, MAGNETIC, MAGNETO-OPTICAL AND OPTICAL PROPERTIES OF Ni_2MnGa AND Co_2MnGa HEUSLER ALLOY FILMS

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Amorphous (disordered) as well as $L2_1$-type (ordered) Ni_2MnGa and Co_2MnGa alloy films have been fabricated by flash evaporation onto substrates cooled by liquid nitrogen and warmed up to 720 K, respectively. The ordered films exhibit the physical [magneto-optical (MO), optical and magnetic] properties close to the properties of corresponding bulk alloys. The nature of the interband absorption peaks in the optical conductivity spectra for the ordered alloys was interpreted in terms of their band structures. The significant effect of the structural disorder on the optical, MO and magnetic properties of Ni_2MnGa and Co_2MnGa was experimentally observed and discussed in terms of electronic structure of alloys. Thus, for example, the disordered Ni_2MnGa films show no ferromagnetic ordering down 5 K, while Co_2MnGa ones noticeable reduce their magnetization.

P-2-13

Simulated and Measured Hysteresis Curves for Permalloy Based Thin Films

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A computer micromagnetic simulator was used to obtain the hysteresis curves for thin films of permalloy (NiFe) and NiFe/Cu/NiFe multilayers. The thickness of the permalloy layers was ranged between 10 and 100 nm. The thickness of the Cu interlayer was 4 nm. The magnetic measurements were made with a Vibrating Sample Magnetometer. The agreement between measured and simulated curves is very good when the permalloy layer is thinner than 100 nm. For a 10 nm NiFe layer the simulation gives a coercive field of 15 Oe. For a NiFe(10 nm)/Cu(4nm)/NiFe(10 nm) we obtained from simulation a coercive field of about 50 Oe and a value for the remnant to saturation magnetisation ratio of about 0.36. The measured values for the same parameters were 60 Oe and 0.32 respectively. To obtain these values we used a grid or two grids of 12x12 single domains, square shape, whose dimensions are inspired from the film structure. For the NiFe/Cu/NiFe multilayer, each single domain is 10 nm thick and 95 nm each side. The distance between the adjacent domains was 5 nm. The thickness of the Cu layer is, in our simulation, the distance between the two grids. Between the top and the bottom layers we introduced coupling fields that have random values from 30 to 60 Oe. The data are very sensitive on the right choice of the parameters used for simulation.

P-2-14

Magnetic interlayer coupling across parabolic quantum well

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The physics of quasi-2D electron gas /2DEG/ has been influencial in condensed matter magnetism research since the discovery of the oscillatory interlayer coupling in magnetic superlattices. In case of rectanglar profiles of the quantum-wells /QW/ formed by the superlattice potential the theory of interlayer coupling was elaborated over ten years ago. However, there is only limited progress in description of magnetic interactions in the nonsquare-QW superlattices [1], [2]. In our contribution we will present theory of interlayer coupling in the case of parabolic QW system. Contrary to the conventional models based on perturbative or total energy approaches we exploit the similarities of the quasi-2DEG oscillations within parabolic QW to the de Haas-van Alphen effect [3]. We derive formula for the interlayer coupling parameters as the function of potential barrier heights and the nonmagnetic layer thickness. Applications of the results obtained to the description of real systems will be widely discussed.

[1] Z. Bak, R. Jaroszewicz, W. Gruhn : J. Mag. Mag. Mater. **213**, 340 (2000).
[2] Z. Bak Solid State Commun. **118**, 43 (2001).
[3] D. M. Edwards: Phys. Rev. Lett. **67**, 493 (1991)

P-2-15

MAGNETIZATION DISTRIBUTION IN ULTRATHIN MAGNETIC FILM NEAR PHASE REORIENTATION WITH REGARDS TO THE SECOND MAGNETIC ANISOTROPY CONSTANT

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Wide scale thickness and field-driven evolution of magnetization distributions in ultrathin magnetic films was recently studied[1]. It was shown that the sinusoidal-like domains appearance shifts the reorientation phase transition (RPT) aside the smaller values of Q (=K1/2Ms^2) the relation between anisotropy and demagnetizing energies). Here, by micromagnetic simulations and analytically we study the magnetic states of laterally infinite ultrathin films of different values of Q and K2 (the second anisotropy constant). We show that influence of positive K2 results in a prolongation of the stability region of the sinusoidal domain structure and in an additional shift of Q determining the RPT. The metastability states coexistence of the in-plane and perpendicular magnetic phases, were studied for negative values of K2. Domains sizes and domain phases liability boundaries were determined.

[1]M. Kisielewski, A. Maziewski, T. Polyakova, and V. Zablotskii. Phys. Rev. B 69, 184419 (2004).

P-2-16

Magnetic viscosity in soft magnetic nanocrystalline FeNbB alloys

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The attention of the present work is focused on the study of the magnetic viscosity at elevated temperatures in the nanocrystalline ternary $Fe_{80.5}Nb_7B_{12}$ alloy with a low and medium volumetric fraction of nanocrystalline particles. An analysis of the logarithmic-like time creep of magnetization below and above the Curie temperature of the amorphous matrix, T_c*(am)*, enabled us to calculate the corresponding values of the fluctuation field, H_f, and the activation volume, V_{act}, of the soft magnetic specimens. We have found that slightly below T_c*(am)*, the estimated activation volume is rather large and involves more than 10^2 grains. Above T_c*(am)*, V_{act} is strongly reduced but it is still larger than the size of single nanocrystalline grains. This indicates that above T_c*(am)*, the bcc-Fe particles are still interacting and V_{act} involves several grains coherently reversing their magnetic moments.

P-2-17

MICROSTRUCTURE AND EXCHANGE COUPLING PARAMETERS OF MTJ WITH CoFeB BOTTOM ELECTRODE

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In this study we report the relationship between texture degree of antiferromagnetic and ferromagnetic pinned bilayer induces by different seed-buffer layers, and the exchange bias and the interlayer-Néel coupling fields. MTJs with the structure: substrate Si(100)/SiOx/buffer/IrMn/CoFeB/AlOx/NiFe/Ta were deposited using two types buffers: Cu and Ta/Cu/Ta/Cu. Samples were annealed in vacuum at temperatures ranging from 150°C to 350°C. XRD analysis reveals that the texture of the sample with Cu buffer is characterized by lower texture degree than of the sample with Ta/Cu/Ta/Cu buffer. Major and minor hysteresis loops show that values of exchange bias and Néel coupling fields increase with increasing annealing temperature and are higher for the stronger textured samples. The texture of the IrMn increases slightly, while of the CoFeB increases significantly with the annealing temperature. The roughness, measured by AFM, depends on the type of the buffer and is higher for strong textured Ta/Cu/Ta/Cu buffer. The comparison of junctions with CoFe and CoFeB bottom electrode shows that addition of 5% B in CoFe layer makes the surface of pinned layer smoother. This leads to smaller Néel coupling field, which is desirable for application of MTJ in MRAM.

P-2-18

STRUCTURE AND MAGNETIC ANISOTROPY EVOLUTION IN Au/Co/Au SANDWICHES UPON THERMAL TREATMENT

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Co ultra-thin films sandwiched between Au layers are one of the most intensively studied magnetic systems due to the existence of perpendicular anisotropy. Despite large lattice mismatch of 14% between the constituent layers the structure of Au/Co/Au sandwiches is coherent. As a consequence the induced tensile strains in Co layer contribute to a magnetoelastic component of magnetic anisotropy in this system. The aim of this study is the investigation of thermal treatment influence on crystalline structure and magnetic properties of Au(111)/Co(0001)/Au(111) sandwiches MBE grown on sapphire substrate covered with Mo buffer. After annealing at 250^{o}C the RHEED pattern of Co layer reveals the loss of lattice coherence and additionally the results of synchrotron radiation reflectometry studies suggest breaking of Co layers continuity. These structural observations are correlated with magnetic properties examined by magnetooptical Kerr effect. Annealing at 150^{o}C does not affect substantially the perpendicular anisotropy. Treatment at 250^{o}C switches the magnetisation vector from perpendicular to in-plane orientation. Achieved results are supported by theoretical considerations in terms of magnetoelastic and diffusion contributions.

P-2-19

MAGNETIC DOMAIN STRUCTURE IN ULTRATHIN Co WEDGES GROWN ON VICINAL SAPPHIRE SUBSTRATES

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In the present work we report on magnetic domain structures in ultrathin hcp Co(0001) films grown by molecular beam epitaxy, on vicinal sapphire substrates in the wide Co thickness range. The following nanostructures were deposited on sapphire single-crystal (11$\underline{2}$0) wafers with 1 and 5 deg miscut angles: (i) first buffer layer of 20 nm Mo(110), (ii) second buffer layer of 10 nm Au(111), (ii) a Co wedge with thickness range 0-2.3 nm; (iii) 8nm thick Au cover layer. The measurements were performed at room temperature by means of the polar Kerr effect in polarizing optical microscope. The evolution of the domain structures during the magnetization reversal processes was studied. The Co-thickness dependence of the local coercivity field was determined. Preferential orientation of domain wall was observed. Ordering of domain wall was correlated with magnetization easy axis orientation. The preferention and the coercivity field depend on both Co thickness and the miscut angle.

P-2-20

MAGNETIC ANISOTROPY CHANGES IN ULTRATHIN Co FILMS GROWN ON VICINAL SAPPHIRE SUBSTRATES

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The aim of the work is to study of the magnetic anisotropy of ultrathin hcp Co magnetic films epitaxially MBE grown on vicinal $Al_2O_3(11\underline{2}0)$ substrate with miscut angles of 1° and 5°. The epitaxial samples with the following structure: (i) first buffer layer of 20 nm Mo(110) deposited at $T = 1000$°C, (ii) second buffer layer of 10 nm Au(111) deposited at room temperature and annealed at $T = 200$°C for 30 minutes, (iii) 2 nm of Co layer, (iv) covered by a 8 nm thick Au layer. RHEED was used to check the growth process of the samples. Measurements were performed at room temperature using MOKE magnetometer and FMR X-band spectrometer. Magnetization processes were studied in both longitudinal and polar MOKE experiments. Changes of in-plane magnetic anisotropy symmetry were deduced from shape analysis of the magnetization curves and angular dependence of the resonance field measured in the sample plane. Two-fold and four fold symmetry was observed for different miscut angle, respectively. The experimental data, will be discussed taking into account the following energy contributions: (i) demagnetization term; (ii) surface and bulk uniaxial anisotropy; (iii) and step-induced uniaxial anisotropy. Magnetic anisotropy constants are fitted for different miscut angles.

P-2-21

Current-induced conductance jumps in $La_{0.7}Sr_{0.3}MnO_3$ manganese point-contacts

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The conductance switching processes are studied as a function of the DC current (up to 10^8 A/cm^2) passing through nanoconstruction of a mechanically controllable junction (MCJ). The current-voltage ($I-V$) curves of the MCJ are non-ohmic with a parabolic form of the differential conductance (dI/dV) versus the voltage, typical of an electron tunnelling process. By fitting of the $I-V$ curves to the Simmons theory the barrier width (1-1.6) nm and height (0.4-0.7) eV as well as the effective tunnelling area (1-10)$\times 10^{-9}$cm^2 were estimated for the junctions. We interpret the jumps in conductance of MCJ about integer multiples of e^2/h as due to the configuration reorientation of the magnetization of the Mn-ions' clusters at the surface of the devices. This switching can be understood in terms of the exchange of angular momentum between the spin-polarized current and magnetic moments of the cluster situated between the electrodes or on their surfaces. Since the electron transmission through the barrier varies exponentially with thickness, most of the tunnel current flows through the thinnest part of the nanoconstruction.

P-2-22

Current-induced conductance jumps in mechanically controllable junctions of $La_{0.7}Sr_{0.3}MnO_3$ manganese

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The magnetic switching processes in mechanically controllable junctions (*MCJ*), made of high-quality ceramic of $La_{0.7}Sr_{0.3}MnO_3$, are studied as a function of the DC current (up to 10^9 A/cm^2) passing through the nanoconstriction. The relative displacement of the two electrodes is controlled by the piezodevice with a resolution of a few picometers. The current-voltage ($I-V$) curves of the *MCJ* are typical of an electron tunnelling process. By fitting the $I-V$ curves to the Simmons model the barrier width (0.8-1.6) nm and height (0.7-1.7) eV of the junctions and their effective tunnel area (1-10) $\times 10^{-12}$ cm^2 were estimated. Due to the close relation between transport properties and the magnetization in manganese compounds, the resistivity measurements provide an excellent indirect method to characterize the magnetic switching observed in atomic scale constrictions. Based on this, we interpret the jumps in conductance of *MCJ* about integer multiples of e^2/h as due to the configuration reorientation of the magnetization of the Mn-ions' clusters at the constriction surfaces. Our data suggest a quantum origin of the current-induced switching of the point contact prepared from half-metallic oxide ferromagnets.

P-2-23

Direct-current induced magnetic switching in Au- Fe/Si multilayers point contact

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The magnetic switching processes in point contacts (PC), made from Au tip - Fe/Si multilayers involving no lithography, are studied at RT as a function of the DC current passing through these nanoconstrictions. The nanocontacts were obtained by pressing Au wires (0.05 mm in diameter) into Fe/Si multilayers. The antiferromagnetically coupled $[Fe(3nm)/Si(1.1nm)]_{15}$ multilayers were deposited in UHV by magnetron sputtering at RT onto oxidized Si wafers. The crystalline structure of our samples and their multilayer periodicity were examined using the high- and small-angle X-ray diffraction, respectively. The $I-V$ characteristics of these nanocontacts at RT exhibit a non-linear variation. By fitting of the $I-V$ curves to the Simmons theory the barrier width (0.3-0.8) nm and height (0.4-0.7) eV of the junctions and their effective area (1-100)$\times 10^{-12}$ cm^2 were estimated. In the high intensity of the DC current (above 10^6 A/cm^2) passing through PC, a hysteretic jump in the resistivity was observed - a clear evidence for a current induced magnetization reversal of one of the magnetic multilayers. The present results are likely to raise interesting fundamental questions. At the same time, the observation of a high magnetoresistance effect at zero external fields is exciting from the viewpoint of the technological applications.

P-2-24

STRUCTURE, TRANSPORT AND MAGNETIC CHARACTERIZATION OF $La_{0.89}Sr_{0.11}MnO_3/YBa_2Cu_3O_7$ SUPERLATTICES

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We report on structural, transport and magnetic studies of $La_{0.89}Sr_{0.11}MnO_3/YBa_2Cu_3O_7$ (LSMO/YBCO) superlattices. For this doping level (x=0.11) the LSMO system is a ferromagnetic insulator (FMI). Proximity effect between a ferromagnetic insulator and YBCO system is very interesting problem , both for fundamental research and application. A series of LSMO/YBCO superlattices have been fabricated using a high pressure sputtering, with fixed LSMO layer thickness at 8 unit cells (u.c.) and varying YBCO layer thickness from 1 to 8 u.c. $c-axis$ layer thickness. An onset of superconducting transition is observed beginning from the samples with 2 u.c. YBCO layer thickness. Magnetization hysteresis curves measured close to superconducting transition show interplay between Meissner currents in YBCO layers and magnetic field present in LSMO layers.

P-2-25

Orbital Kondo effect and spin polarized transport through quantum dots

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The coherent spin dependent transport through a set of two capacitively coupled quantum dots placed in a magnetic field and coupled to ferromagnetic electrodes is considered within the equation of motion method. The magnetic field breaks the spin degeneracy. For special choices of gate voltages the dot levels are tuned to resonance and the orbital Kondo effect results either for the single or for both spin channels. Apart from the Kondo peak, also the satellite many-body peaks are found in the densities of states in the positions determined by the magnetic field. The peaks are characterized by different spin polarization. We discuss the spin polarization of conductance showing that for the case of orbital degeneracy in the one spin channel the system can operate as an effective spin filter.

P-2-26

Non-collinear magnetic states in Ni-Fe/Au/Co/Au multilayers investigated by magnetoresistance measurements

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Sputtered $Ni_{80}Fe_{20}$/Au/Co/Au multilayers exhibit perpendicular anisotropy of Co layers and easy-plane anisotropy of Permalloy layers [1]. In these samples the changes of relative orientation of magnetization between Co and Ni-Fe layers, with magnetic field, can be determined by magnetoresistance measurements. It is possible because the magnetoresistance effect is of the GMR-type and the resistance changes corresponding to the transition from parallel to perpendicular magnetization configuration are relatively large ($\Delta R/R$ up to 10% at RT). As in other spin-valves, the magnetization reversal and the resulting magnetoresistance effect depend on magnetic anisotropy of ferromagnetic layers and on the coupling between them. The effective anisotropy of cobalt layers was varied by changing their thickness and the anisotropy of Ni-Fe layers by introducing a thin Co layer at each of Ni-Fe/Au interface. The changes of interlayer coupling were controlled by Au spacer thickness. We will discuss the influence of the effective anisotropy of ferromagnetic layers and the important role of domain wall coupling on magnetic states in $Ni_{80}Fe_{20}$/Au/Co/Au multilayers.

[1] F. Stobiecki, B. Szymański, T. Luciński, J. Dubowik, M. Urbaniak, K. Röll, J. Magn. Magn. Mater. **282** (2004) 32

P-2-27

MAGNETIC PROPERTIES OF NI-RH NANOSTRUCTURES

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We have studied the magnetic properties of different Ni and Rh nanostructures. A tight binding hamiltonian in the unrestricted Hartree-Fock approximation was used to study bimetallic clusters and monolayers. By ab-initio methods we have calculated the local magnetic moments of several configurations of monolayers, slabs and nanowires. The general trend for Ni rich systems is that even when there is a great enhancement of the Rh magnetic moments, we found a lowering of the total magnetic moment of the alloyed structures with respect to the corresponding pure Ni ones as a consecuence of the decreased magnetic moment of the Ni atoms. We believe that a strong effect of hybridization between Rh and Ni atoms is responsable for this behaviour as can be seen from the modification of their partial density of states with respect to the pure metals.

P-2-28

SPIN-POLARIZED SURFACE STATES IN SEMICONDUCTOR SUPERLATTICES

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Electronic surface states in $Al_{0.1}Ga_{0.9}As|GaAs$ superlattice are calculated for a system with a $ZnMnSe$ barrier in a surface cell. In the absence of applied magnetic field the $ZnMnSe$ barrier has the same height as the $Al_{0.1}Ga_{0.9}As$ barriers in the bulk cells. When a magnetic field is applied perpendicularly to the superlattice layers, the surface cell magnetic barrier height is found to vary with spin orientation. Hence, each spin polarization involves different conditions of surface state existence. Our computations show a split of Shockley states into two levels (corresponding to different spin polarizations) and appearance of Tamm states (with specific spin polarization), induced by sufficiently strong magnetic fields.

P-2-29

DIODE EFFECT IN TRANSPORT THROUGH A QUANTUM DOT COUPLED TO NON-COLLINEARLY POLARIZED FERROMAGNETIC LEADS

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Electron tunneling through a spin-split discrete level of an interacting quantum dot coupled to two ferromagnetic electrodes with non-collinear magnetizations is investigated theoretically by means of the nonequilibrium Green-function approach. It is shown that the spin splitting of the dot level leads to a number of new effects. Asymmetry in the tunnel magnetoresistance (TMR) with respect to the bias reversal and non-monotonous angular variation of the spin-polarized current are found for symmetrical tunnel junctions. Numerical results also show that negative differential conductance and diode effect may occur in symmetrical junctions with non-collinear magnetizations and for large enough magnetic polarization of the leads. It is also found that in asymmetrical junctions with one electrode being half-metallic, the spin splitting gives rise to an enhancement of the diode-like behavior. The latter feature is accompanied by a splitting of the TMR peak in the bias range for which the sequential tunneling is exponentially suppressed.

P-2-30

The Influence of Fe Layer Thickness on Electronic and Magnetic Properties of Antiferromagnetically Coupled Fe/Si Multilayers

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The main goal of our study was to examine whether the existence of the antiferromagnetic (AF) exchange coupling in Fe/Si multilayers Mls is related to the appearance of the interfacial Fe silicide phases and how it is influenced by Fe layer thickness. The $[Fe(d_{Fe})/Si(1.1nm)]_{15}$ Mls were deposited in UHV by magnetron sputtering onto oxidized Si wafers for different Fe layer thicknesses $0.3<d_{Fe}<4$nm. The crystalline structure of our Mls and their multilayer periodicity were examined using the high- and small-angle X-ray diffraction, respectively. The transmission electron microscopy of the cross-section was used to examine the morphologies of selected samples. The temperature dependences of the Hall effect and the resistance supplemented with magnetic moment measurements showed that both magnetic and electronic properties of the AF coupled Fe/Si Mls are influenced by interfacial mixing between Fe and Si layers. The current-voltage characteristics measured perpendicularly to the Ml planes allowed us to show the semiconducting character of nominally pure Si spacer layers. The associated minimal tunneling barrier height evaluated for Fe(3nm)/Si(1.1nm) by the Simmons fit was found to be 1eV. We showed that the application of interfacial Co (or Au) thin layers prevent the mutual interlayer diffusion terminating the existing AF interlayer coupling.

P-2-31

^{59}Co NMR STUDY OF Co/CoO MULTILAYERS: AN EXCHANGE BIAS SYSTEM

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It is generally accepted that the exchange bias created at the interface between a ferromagnetic (FM) and an antiferromagnetic (AFM) material strongly depends on the spin structure at the FM/AFM interface. To achieve a better understanding of the interface phenomena we have used ^{59}Co NMR to monitor the structural and magnetic properties of the Co/CoO exchange bias system. A ^{59}Co NMR study has been performed on a series of sputtered polycrystalline Co(t)/CoO (t = 10 - 18 nm) bilayers and $[Co(t)/CoO]_{10}$ (t = 5 - 10 nm) multilayers deposited on Si/SiO_2 wafers. The microstructure of a metallic Co layer covered with CoO was found to be essentially the same as that of a non-oxidized Co single layer. It consists of predominantly hcp Co stacking order. However, the presence of the oxidized Co layer results in a significant drop of the ^{59}Co NMR signal intensity. This suggests that the electronic state of Co at the interface is not metallic but similar to the Co^{2+} state of CoO. Despite the fact that the bilayers were in the unbiased state, i.e. the characteristic shift of the magnetization hysteresis loop is not present, a strong anisotropic exchange coupling between Co grains and the underlying AFM CoO grains can be inferred from an increase, by an order of magnitude, of the NMR restoring field.

P-2-32

GMR EFFECT IN QUANTUM ATOMIC-SCALE CONTACT

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We study the transport properties of an atomic-scale contact connected to ferromagnetic semi-infinite electrodes in the ballistic regime. Systems with different geometries were considered. Our method is based on non-equilibrium Green's function (NEGF) theory. We fully deal with atomistic structure of the whole system, treating both the contact and the electrodes on the same footing. The results includes the transmission and electron densities vs. energy with parallel and antiparallel magnetization in the electrodes. Calculated GMR ratio is about 70% with 50% polarization of magnetization in the leads. In case of applying additional gate voltage the values up to 90% may be obtained. The influence of the magnetic polarization, coupling between leads and electrodes, and geometry of the device on transport properties is discussed. In addition to evolution from conductance quantization to resonant tunneling conductance peaks upon changing the hopping parameter, it has been found that with increasing polarization other features appear due to decreasing overlap between surface density of states in the leads for each transmission mode.

P-2-33

AB INITIO STUDY OF INTERLAYER EXCHANGE COUPLING IN Fe/Si MULTILAYERS

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Interlayer exchange coupling has been studied from first principles in Fe/Si multilayers. The calculations have been performed in the framework of spin-polarized linear-muffin-tin method within supercell approach. Different structures with the spacer layer of thickness up to 15 atomic layers have been modeled from pure Si to $Fe_{50}Si_{50}$ alloy and including structures with isolated Fe impurities in the Si layer. Antiferromagnetic exchange coupling has been found for $Fe_{50}Si_{50}$ alloy spacer as well as for Fe-doped Si layer. The results of the modeling have been compared with the experimental data for Fe/Fe_xSi_{1-x} multilayers prepared by magnetron sputtering for x=1, 0.66 and 0.5. The dependence of antiferromagnetic exchange coupling on the spacer layer thickness up to 3 nm has been determined from the magnetization and Kerr effect measurements. The experimental results for the nominally pure Si spacer layer (x=1) can be explained assuming the Fe-doped Si model structure of the spacer layer. The magnetic moments and partial density of states for the model structures have been calculated and discussed.

P-2-34

THE TEMPERATURE DEPENDENCE OF THE MAGNETIC AND MAGNETO-OPTICAL PROPERTIES IN Fe/Au LAYERED STRUCTURES

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In the small bilayer thickness range the Fe/Au multilayers (MLS) can be prepared in the state with perpendicular anisotropy. The characteristic properties of Fe/Au superlattices is appearance of the oscillatory interlayer exchange coupling as a function of Au spacer layer thickness. We report studies of the temperature dependence of magnetic and magneto-optical properties for the series of Fe/Au MLS prepared by dc-sputtering on GaAs(001) substrates. The x-ray diffraction analysis shows that the Fe/Au films studied exhibit well defined layered structure with pronounced (111) fcc texture. The magnetization processes were measured by magneto-optical technique in polar and longitudinal geometry in the temperature range 8-300K. The remanence rotation and the saturation and coercivity fields as a function of the temperature were measured for the series of Fe/Au MlS with different Au sublayer thickness, and the relation of the properties with interface structure has been studied. The Fe/Au MLS under study show strong dependence of the Curie temperature on the Au spacer layer thickness. The exponential temperature dependence of the coercivity field observed experimentally has been explained within the model of thermal activation. The out of plane anisotropy in low temperature range was observed in the Fe/Au systems studied.

P-2-35

MAGNETIC PROPERTIES OF Fe/Tb MULTILAYERS

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Magnetic and magneto-optical properties have been studied for a series of sputter deposited Fe/Tb multilayers (MLS) on Si(111) substrates. The process of magnetization reversal of the system was studied experimentally by the magneto-optical techniques in both polar and longitudinal geometry. The hysteresis loops of the Fe/Tb MLS measured show complex structures connected with structural and magnetic heterogeneity of the system. To interpret the complex magneto-optical hysteresis loops measured in the Fe/Tb MLS, the method based on strong photon energy dependence of the magneto-optical effects on the system composition has been proposed. The contributions to the hysteresis loops, coming from interface Tb-Fe alloy region with perpendicular anisotropy and coupled to a modified Fe volume with in plane anisotropy, were evaluated. The analysis of the magneto-optical data leads to the conclusion that the change of Fe magnetic moments orientation with respect to the applied magnetic field direction takes place for the studied systems when the Fe sublayer thickness in the Fe/Tb MLS is above 2 nm.

P-2-36

CURRENT-INDUCED SPIN DYNAMICS IN SPIN-VALVE STRUCTURES

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Spin polarized electrons traversing a ferromagnet can transfer spin-angular momentum from the system of conduction electrons to the local magnetization. This offers new possibility of manipulating magnetization without applying an external magnetic field. Recently, it has been demonstrated experimentally that the dynamical phase diagram contains several distinguishable steady-state precessional modes and static magnetic states. In this paper we use Landau-Lifshitz-Gilbert equation for magnetization dynamics, extended by including the torque due to spin-transfer. The torque is described within a macroscopic model based on the classical spin diffusion theory. Solution of the Landau-Lifshitz-Gilbert equation for spin-valve structures allows us to describe stable magnetic states, magnetization switching between different states, and also precessional modes.

P-2-37

CURRENT INDUCED SWITCHING DUE TO SPIN-TRANSFER IN SPIN VALVES: MACROSCOPIC MODEL

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We develop a macroscopic description of current-induced torque due to spin transfer in layered systems consisting of ferromagnetic films separated by a nonmagnetic layer. The description is based on the classical spin diffusion equations for the distribution functions inside the films used in the theory of CPP-GMR, and macroscopic boundary conditions for the longitudinal and transverse components of the spin current. Due to strong exchange field in ferromagnetic films, we assume that the perpendicular component of spin current is totally absorbed within the narrow interface region giving rise to the torque. Our model can be used to describe normal and inverse switching phenomena studied in recent experiments. We also present conditions, at which the steady precession states above certain critical current should occur.

P-2-38

ELECTRONIC AND TRANSPORT PROPERTIES OF THIN $GdCo_4B$ ALLOY FILMS

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$GdCo_4B$ thin films were prepared onto liquid nitrogen (LN) cooled or heated glass substrates by an UHV flesh evaporation technique. Structural studies have shown that the samples deposited onto the LN cooled or non-cooled glass substrates are amorphous and crystallize after an UHV annealing at 770 K. The resistance of the amorphous thin films increases with temperature decreasing from RT down to 0.3 K. The crystallization process was observed by resistivity measurements in the temperature range varied from RT to 863 K at a rate of 10 K/min. Results of the XPS studies reveal that the surface composition of the $GdCo_4B$ thin films is practically the same as the average volume composition determined by XRF method. On the other hand, we have observed a systematic change in the shape and peaks position of the XPS valence band after *in-situ* annealing of the 'as-prepared' amorphous $GdCo_4B$ thin films. The above behavior could be explained by a structural transition and/or relaxation of the flesh-evaporated thin films after UHV annealing. XPS spectra measured for the thin films will be compared with those determined for the bulk polycrystalline $GdCo_4B$ compound.

P-2-39

SPIN-DEPENDENT TRANSPORT IN FERROMAGNETIC SINGLE-ELECTRON TRANSISTORS WITH NONCOLLINEAR MAGNETIZATIONS

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Spin-polarized electron transport through a ferromagnetic single-electron transistor (FM SET) is studied theoretically in the sequential tunneling regime. Two external electrodes and the central part (island) of the device are assumed to be ferromagnetic, with the corresponding magnetizations being generally non-collinear. Transport properties of the device are analyzed using the master equation approach, and the respective transition rates are determined from the Fermi golden rule. Basic transport characteristics, like tunneling current, differential conductance and the tunnel magnetoresistance, are calculated for an arbitrary magnetic configuration of the system. All the characteristics are shown to be strongly dependent on the relative orientation of the magnetizations. We have also calculated torque due to spin transfer, which acts on the central part of the system. Such a torque may lead to magnetization switching on the island.

P-2-40

EXCHANGE BIAS COUPLING IN IrMn/Cu/CoFe TRILAYERS DEPOSITED ON DIFFERENT BUFFERS

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The exchange bias coupling between antiferromagnetic (AF) IrMn and ferromagnetic (F) CoFe through the different thickness of nonmagnetic spacer layer of Cu (S) has been investigated. The samples were deposited at room temperature by sputtering technique on thermally oxidized Si(100) wafers, on two different buffers: Cu(25nm) and Ta(5nm)/Cu(25nm). Samples with bottom (AF/S/F) and top (F/S/AF) configuration of AF layer, with reference to F layer, were investigated magnetically and structurally in as deposited and after field annealing. For all samples, exchange bias field decreases exponentially, with different decay length that depends on the system of buffer layers, as a function of Cu spacer thickness. The exchange bias field is four times higher for bottom than for top configuration, if the bottom configuration (IrMn/Cu/CoFe) is deposited onto Ta/Cu buffer. This fact can be attributed to the stronger texture of the IrMn layer, which is induced by the Ta/Cu buffer. In this work, influence of the two buffers on the texture of IrMn and exchange bias coupling will be discussed.

P-2-41

CORRELATION BETWEEN GROWTH AND MAGNETIC PROPERTIES OF Fe/Ti MULTILAYERS

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Fe/Ti multilayers (MLs) were prepared onto glass and oxidised Si(111) substrates at 295 and 520K using UHV RF/DC magnetron sputtering. Planar growth of the Fe and Ti sublayers deposited at 295K was confirmed in-situ by X-ray photoelectron spectroscopy (XPS). We have observed exponential variation of the XPS Fe-2p and Ti-2p integral intensities with increasing sublayer thicknesses. On the other hand, quantitative XPS analysis and comparison with a model system revealed a significant interface alloying during the deposition process at 295 K. Furthermore, results showed that the deposition of the 0.18 nm - Fe / 0.22 nm -Ti ML at 520 K leads to the formation of an uniform nanocrystalline Fe-Ti alloy film due to interdiffusion process. Systematic structural and magnetic studies showed, that iron sublayers grow on Ti in the soft magnetic nanocrystalline phase up to a critical thickness $d_{crit} \sim 2.3$ nm. For a thickness greater than d_{crit}, the Fe sublayers undergo a structural transition to the polycrystalline phase with much higher coercivity.

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P-2-42

EXCHANGE COUPLING ACROSS QUASI-AMORPHOUS Zr-Fe SPACER

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Fe/Zr/Fe trilayers with wedge-shaped Zr interlayer were prepared using UHV (5×10^{-10} mbar) DC/RF magnetron sputtering. The planar growth and interface alloying of the Fe and Zr layers was confirmed in-situ by X-ray photoelectron spectroscopy. Furthermore, structural and magnetisation studies revealed spontaneous formation of an quasi-amorphous Fe-Zr alloy layer at the interfaces during the deposition process. Results on magnetic domains studies showed that the Fe sublayers are very weakly exchange coupled or decoupled for nominal Zr sublayer thickness greater than 3 nm. For Zr layer thickness 0.5 – 3 nm we have observed patch domains characteristic for AFM interlayer exchange coupling. The rapid decrease of the interlayer exchange coupling could be explained by its strong damping due to formation of a non-magnetic quasi-amorphous Zr-Fe alloy layer at the interfaces.

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P-2-43

Kondo effect in spin-polarized transport through a quantum dot: limit of a finite correlation parameter U

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Kondo effect in electronic transport through a quantum dot is investigated theoretically with the use of non-equilibrium Green function formalism. The system is described by the Anderson model with a finite correlation parameter U. Renormalization of the dot energy level and correlation parameter U is taken into account. It leads to some shift of the electron and hole energy levels and to a splitting of the Kondo peak in DOS in the presence of ferromagnetic electrodes. The approach gives results similar to those obtained in the approach in which the exchange interaction with ferromagnetic electrodes is described by an effective molecular field. Both approaches give very similar results also for a dot attached to non-magnetic electrodes, but in an external magnetic field. The splitting of the Kondo anomaly in the differential conductance occurs for magnetic field exceeding a certain value and is slightly lower than the doubled Zeeman splitting. A reduction of the splitting is a result of the effective field induced in the system by an external magnetic field.

P-2-44

The influence of different magnetic configurations on tunneling current in double tunnel junctions with ferromagnetic electrodes

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Tunnelling current in double-barrier junctions with ferromagnetic electrodes depends on relative orientation of the magnetic moments of all the three electrodes. When four different current densities for a specific value of the bias voltage can be obtained, the junctions may be used in MRAM devices as 2-bits memory cells. In this paper we present and discuss results of numerical calculations of I-V characteristics, tunnel conductance, and TMR in such two-barrier junctions. The calculations are performed in the free-electron model, assuming a trapezoidal shape of the barriers and neglecting tunnelling with simultaneous reversal of electron spin. The influence of various parameters, like for instance of the spin splitting of the electron bands on the TMR effects is analyzed. Generally, one can obtain four different values of the tunnelling current density for a fixed bias voltage. The corresponding four values of the junction resistance can be particularly well separated when the electrodes are made from materials with different spin polarizations.

P-2-45

Changes in magnetic and magnetoresistive characteristics of Ni-Fe/Au/Co/Au multilayers induced by annealing

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Magnetic layered structures characterized by alternating in-plane and out-of-plane magnetization configuration at remanence are interesting for different applications, particularly as magnetoresistive sensors (GMR-type) with a linear $R(H)$ dependence. We have demonstrated that for a proper choice of the deposition conditions and thickness of constituent layers, sputter-deposited ($Ni_{80}Fe_{20}$/Au/Co/Au) multilayers exhibit such a behavior for magnetic field applied perpendicularly to the surface ($H_\perp$). In this contribution the influence of annealing on magnetization reversal and magnetoresistance was studied. Measurements performed for as-deposited samples and after subsequent isothermal annealing ($150^oC<T_a<250^oC$) show that the GMR effect is stable under annealing below 200^oC. It even slightly increases, for T_a above 200^oC, what opens a path for the GMR value control and therefore is important for applications. The most pronounced changes were observed in the central part of the $M(H_\perp)$ and $R(H_\perp)$ curves, influenced by both the nucleation H_N and the saturation H_S fields. They are related to the appearance and disappearance of stripe domain structure in Co layers. The influence of T_a on values of H_N and H_S will be discussed.

P-2-46

ON THE RANGE OF INTERACTIONS FROM FINITE SIZE SCALING IN MAGNETIC Ni NANOWIRES

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A recent experiment [PRB 61 (2000) R6463] which reports a dependence of magnetic properties of Ni nanowires on their size has been reinterpreted in terms of localized spin model with spin-spin interactions ranging beyond nearest neighbors. Two possible mechanisms of variation of magnetic properties have been considered. Firstly, a simple finite size scaling with a shift of *pseudocritical* temperature with the size of the system. Secondly, a crossover to classical critical behavior [PRE 59 (1999) 4997] as a function of the range of interactions R between spins – with R treated as a parameter. Finally, the value of $R \approx 1nm$ of the exchange interactions has been found by a fit to a literature experiment on Ni nanowires.

P-2-47

MAGNETIZATION AND FMR STUDIES OF $[Fe/Cr]_n$ STRUCTURES WITH ULTRATHIN IRON LAYERS

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A set of magnetic multilayer structures $[Fe(t_{Fe})/Cr(t_{Cr})]_n$ with ultrathin ($t_{Fe} < 5$ Å) iron layers was studied using SQUID-magnetometry and ferromagnetic resonance (FMR) technique. The samples were prepared on MgO substrates by means of molecular beam epitaxy method. Two different types of multilayers were investigated: with ferromagnetic ($t_{Cr} \approx 20$ Å) and antiferromagnetic ($t_{Cr} \approx 10$ Å) interlayer coupling. For the samples with $t_{Fe} \geq 5$ Å, magnetization curves and FMR spectra at room temperature show a behaviour typical for magnetic superlattices. On the contrary, the samples with $t_{Fe} \leq 5$ Å demonstrate superparamagnetic-like properties. Nevertheless, magnetization curves measured in $4 - 300$ K temperature range do not obey a superposition rule for superparamagnets. In addition, a four-fold in-plain anisotropy of the FMR spectra was detected in samples with $t_{Cr} \approx 10$ Å and $t_{Fe} \sim 3$ Å at low temperatures. This anisotropy vanished as the temperature grew. To explain the obtained results, we propose a theoretical model considering a cluster structure of iron layers. Magnetization curves and FMR spectra are calculated in the frame of a mean field approximation taking into account an interlayer interaction. The calculated dependencies show a qualitative agreement with the experimental data.

P-2-48

INFLUENCE OF SEED-BUFFER LAYERS ON BIAS AND TEMPERATURE DEPENDENCE OF DYNAMIC CONDUCTANCE OF IrMn SPIN VALVE MTJ

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The conductance and I-V characteristics two groups of spin valve magnetic tunnel junctions (SV-MTJs) are measured as a function of temperature and bias voltage. The junctions are characterized by low texture degree of group "a" and high texture degree of group "b". The strongly textured buffer layers grow in a columnar like fashion and induce interfacial roughness. The texture and roughness modified very strongly exchange bias and interlayer coupling effects in the SV-MTJs[1]. It has been observed also substantial influence texture and roughness on the resistance area product (R×A) of the junctions. The R×A of the group "a" junctions is almost two times higher than that of the group "b". While there is no significant difference between TMR at low and room temperature of the two groups. It has been observed, however, slightly decrease of TMR with increasing bias voltage for the "a" group. The thermal smearing of the electron energy distribution (via Fermi distribution function), proposed for the first time in[2] is used to evaluate zero bias anomaly of the junctions. These results imply that buffer layers composition and their sequence can be use to optimize tunneling properties of MTJs.

[1] T. Stobiecki et al., phys. stat. sol. a **201** (2004) 1621.

[2] J. J. Åkerman et al., Europhys. Lett. **63** (2003) 104.

P-2-49

Spin-dependent transport through double-island single-electron devices

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Spin-dependent electronic transport through a double-island device with Coulomb blockade is considered theoretically in the sequential tunneling regime. The analysis is based on the master equation method, with the corresponding tunneling rates calculated from the Fermi golden rule. Electric current and the resulting tunnel magnetoresistance are analyzed as a function of bias and gate voltages for different collinear magnetic configurations of the device. Furthermore, the nonequilibrium spin accumulation in the islands is calculated self-consistently from the appropriate spin balance conditions. It is shown that the interplay of spin accumulation and charging effects may lead to negative differential conductance. This is in agreement with recent experimental observations.

P-2-50

TORQUE INDUCED BY SPIN-POLARIZED CURRENT IN FERROMAGNETIC SINGLE-ELECTRON TRANSISTORS

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We present theoretical analysis of current-induced torque which is exerted on the central part (island) of a ferromagnetic single-electron transistor. The considerations are restricted to the regime of sequential tunneling. The island is assumed to be ferromagnetic and attached to two ferromagnetic leads (electrodes), whose magnetic moments are oriented arbitrarily. The torque is calculated from the net spin current absorbed by the island. In turn, spin currents are calculated within the master equation approach. The torque has been calculated as a function of gate voltage, spin polarization of the leads, and charging energy. It is also calculated as a function of the angle between magnetic moments of the leads. Two different situations are compared in detail; single-electron transistor with one electrode being ferromagnetic and one nonmagnetic, and single-electron transistor with both electrodes ferromagnetic. In both situations the central island is ferromagnetic. All calculations are carried out in the limit of fast spin relaxation processes, when no spin accumulation builds up on the island.

P-2-51

First-principles study of magnetization relaxation enhancement and spin-transfer in thin magnetic films

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The interface-induced magnetization damping of thin ferromagnetic films in contact with normal-metal layers is calculated from first principles for clean and disordered Fe/Au and Co/Cu interfaces. Interference effects arising from coherent scattering turn out to be very small, consistent with a very small magnetic coherence length. Because the mixing conductances which govern the spin transfer are to a good approximation real valued, the spin pumping can be described by an increased Gilbert damping factor but an unmodified gyromagnetic ratio. The results also confirm that the spin-current induced magnetization torque is an interface effect.

P-2-52

Resonant tunneling through a single level quantum dot attached to ferromagnetic leads with non-collinear magnetizations

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Resonant electronic transport through a non-interacting single-level quantum dot attached to ferromagnetic leads is analyzed theoretically. Magnetic moments of the leads are assumed to be noncollinear. Apart from this, an external magnetic field, noncollinear with the magnetizations, is applied to the system. However, magnetic moments of the leads and the external magnetic field are in a common plane. Basic transport characteristics, including current-voltage curves, linear and nonlinear conductance, and tunnel magnetoresistance associated with magnetization rotation are calculated using the nonequilibrium Green function technique, and the Green functions have been calculated via the equation of motion method. Dependence of the transport characteristics on the system parameters, like energy level position, spin polarization of the leads, asymmetry between right and left leads, has been calculated numerically and the results are discussed from the fundamental and application points of view.

P-2-53

Spin polarized resonant tunneling through coupled quantum dots

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Resonant electronic transport through two coupled non-interacting single-level quantum dots attached to ferromagnetic leads is analyzed theoretically. Magnetic moments of the leads are assumed to be collinear. Coupling of the dots to external leads as well as between the dots is assumed to be spin dependent. Basic transport characteristics, including current-voltage curves, linear and nonlinear conductance, and tunnel magnetoresistance associated with magnetization rotation are calculated using the Green function technique. The relevant Green functions have been calculated by the equation of motion method. Variation of the transport characteristics with such system parameters like energy level position, spin polarization of the leads, coupling between the dots, etc., has been calculated numerically. The results are also discussed from the point of view of possible applications in spintronics devices.

P-2-54

ROLE OF INTER–DOT COULOMB REPULSION AND EXCHANGE INTERACTIONS ON TRANSPORT IN DOUBLE QUANTUM DOT

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Effects of inter–dot many–body electronic correlations on the coherent transport through double quantum dots (2QD) connected in series are studied. Conductance as well as another physical quantity are calculated by means of Green's functions. The many–body electronic correlations are treated in the slave–boson (SB) mean field approach, developed by Kotliar and Ruckenstein. Results are obtained by solving of a set of self–consistent nonlinear equations. The conductance in the model is characterized by competition between the dot–dot tunnelling coupling and the level broadening (dot–lead coupling). An interesting behavior was found for a double occupation of the 2QD system. In the case, when the inter–dot coupling is weaker than the dot–lead coupling each dot accommodates one electron and forms the Kondo resonant state with conducting electrons in a lead. In the opposite limits, when the inter–dot coupling exceeds level broadening, the conductance vanishes for sufficiently low gate voltages, which means the Kondo effect disappeared. A generalization of the SB method allow us to show the role of inter–dot Coulomb repulsion and exchange interactions on the gate–voltage dependence of the differential conductance in both the limits as well as for the intermediate dot–dot couplings. The resonance region is broadened with increasing inter–dot Coulomb repulsion as well as with decreasing exchange interactions.

P-2-55

Magnetoconductance of Fano Systems

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We study the magnetotransport properties of a side attached Quantum Dot placed between ferromagnetic electrodes. The side-attached Q.D. has been previously used to probe coherent transport, as it is a simple way to obtain quantum interference and Fano line shapes in transmittance. We find that the magnetoconductance is a nonmonotonic function of the gate-voltage and it shows a maximum at the Fano resonance. For asymmetric coupling, the spin polarization of the dot can be reversed and also negative magnetoconductance may occur. Next we consider the magnetotransport through a quantum ring that is another Fano system and a classical tool for the study of Aharonov-Bohm oscillations.

P-2-55

Spin-valve effect in double-barrier systems with noncollinearly polarized magnetic barriers: linear response regime

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Electron tunneling through a double-barrier structure with ferromagnetic barriers and nonmagnetic external and central electrodes has been considered theoretically in the linear response regime. Magnetic moments of the barriers are assumed to be generally non-collinear, but oriented in the plane of the junction. Tunnel conductance and tunnel magnetoresistance are calculated theoretically as a function of the angle between magnetizations. Possible applications of such systems in spintronic spin-valve devices are also discussed.

O-3-01

ELECTRON-QUASIPARTICLE INTERACTION IN VAN HEUSLER ALLOY Cu_2MnAl

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The van Heusler alloy Cu_2MnAl is a ternary intermetallic compound with a unit cell composed of four interpenetrating fcc sublattices. This so-called half metallic ferromagnet is ideal for applications in tunnelling magnetoresistance (TMR) or giant magnetoresistance (GMR) elements as well as electrodes for spin polarized current injection into semiconductors. We have investigated the point-contact and transport properties by measurements of point-contact (PC) spectra and the temperature dependence of the electrical resistivity, respectively. We have used the same sample as in the neutron optics of neutron beam guides in ILL, Grenoble. The temperature dependence of the electrical resistivity ρ(T) has shown the normal metallic behaviour with the shoulder at T $\sim$ 10 K. PC measurements were carried out in the temperature region from 1.5 K to 10 K (T_C = 630 K) and in the magnetic field up to 1 T. We have observed an asymmetric behaviour of $dV/dI(V)$ which has been probably due to spin polarization at the Fermi energy. Moreover, the observed $d^2V/dI^2(V)$ dependencies in spectroscopic regime show the characteristic energies of the electron-quasiparticle interaction in Cu_2MnAl.

O-3-02

Charge transport through ionic clusters of the magnetic oxides

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In order to interpret empirical data related to doped garnets,we analyze the spin-controlled charge transfer through a heterostructure consisting of site-coupled octahedral and tetrahedral iron-oxygen clusters. A number of charge carriers can be manipulated by valence-uncompensated doping, which indirectly tailors also the magnitude and orientation of permanent magnetic moments attached to the clusters. The electron-energy structure of both clusters, involved in the transfer, as well as that of the heterostructure are found within the framework of the Anderson model. Current-voltage characteristics, derived from the Landauer-like formula, turn out to be highly sensitive to the position of the Fermi level of the system. We also calculated the magnetoresistance, which is different for different orientations of the external magnetic field. The result confirmed the empirical data, indicating anisotropy of the magnetoresistance. In the microscopic mechanism of the spin-controlled charge transfer, the key role is played by the inter-band $p-d$ hybridisation. The charge carrier compensating holes tend to remain on the oxygen ions. In the presence of the compensating hole, the antiferrromagnetic order of the spins attached to the clusters, changes its sign. It is an orbital contribution to magnetic moments of the clusters that gives rise to the anisotropy of the magnetoresistance.

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O-3-03

IMPROVED SOFT MAGNETIC PROPERTIES IN HITPERM NANOCRYSTALLINE ALLOYS BY HEAT TREATMENT UNDER EXTERNAL MAGNETIC FIELD

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The nanocrystalline FeCo-based alloys prepared by devitrification of melt-spun amorphous precursors, called also HITPERM, belong to an important group of soft magnetic materials. In this work, the formation of a nanocrystalline structure and its influence on the magnetic properties was investigated in the series of $(Fe_{1-x}Co_x)_{81}Nb_7B_{12}$ (x=0, 0.25, 0.33, 0.5, 0.66, 0.75) alloys. We report on a beneficial effect of the external magnetic field applied during the heat treatment on the magnetic characteristics of these materials. Most remarkable improvement of soft magnetic properties after magnetic annealing is observed for equiatomic (x=0.5) and Co-rich compositions. As an example, the $(Fe_{0.5}Co_{0.5})_{81}Nb_7B_{12}$ alloy can exhibit after the amorphous/crystalline transformation under longitudinal field of 20 kA/m the values of coercive field less than 8 A/m. For the same sample annealed under transverse field of 640 kA/m, the induced anisotropy constant reaches the value $K_u \approx 1400$ J/m^3. These values are superior to those previously reported for HITPERM materials and they remain fairly stable also at elevated temperatures. The differences in the development of induced anisotropy versus Co-content are discussed in the frame of magnetic atoms pair ordering theory.

O-3-04

Magnetic Behaviour of $YCo_{4-x}M_xB$ Intermetallic Compounds with M=Al or Cu

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The $YCo_{4-x}M_xB$ compounds with M=Al or Cu crystallize in a hexagonal $CeCo_4B$ type structure, having P6/mmm space group for x$\leq$ 2. Magnetic measurements were performed in the temperature range, 5-900K and external fields up to 9T. Both saturation magnetizations, M_S, and Curie temperatures decrease dramatically when Cu and Al gradually substitute Co. As example, for M=Cu, the M_S values change from 2.65 $\mu_B/f.u.$(x=0) to 0.82 $\mu_B/f.u.$(x=1) and T_C from 385K to 205K, respectively. The alluminium compounds for $x > 1$ are paramagnetic and show a spin fluctuation behaviour. Band structure calculations were also performed. The composition dependence of Y4d band polarization was analysed considering the effect of short range exchange interactions with neighbouring Co atoms.

O-3-06

ON THE STRENGTH OF THE DOUBLE EXCHANGE AND SUPEREXCHANGE INTERACTIONS IN $La_{0.67}Ca_{0.33}Mn_{1-y}Fe_yO_3$ - AN NMR AND MÖSSBAUER STUDY

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A combined study of $La_{0.67}Ca_{0.33}Mn_{0.97}{}^{57}Fe_{0.03}O_3$ compound by means of zero field ^{55}Mn and ^{57}Fe NMR as well as ^{57}Fe Mössbauer spectroscopy (MS) is reported. The ^{55}Mn NMR spectra exhibit a single double exchange line up to the magnetic ordering temperature, 200 K, determined from magnetization measurements. The hyperfine field (HFF) remains finite at the magnetic ordering temperature, which reveals discontinuous character of the transition and the occurrence of a ferromagnetic - paramagnetic phase segregation. The Mössbauer ^{57}Fe HFF decreases much faster with increasing temperature than the Mn HFF, which indicates a much lower strength of magnetic interaction of the Fe moments. Application of a molecular field model to the temperature dependence of the Mn and Fe HFF provides values of the Mn-Mn and the Fe-Mn exchange integrals, which amount to 1.24(2) meV and -0.62 meV, respectively. In addition, the Curie temperatures $T_C{}^*$ of ferromagnetic metallic clusters were derived as 297(4) K for the Fe doped and 344(5) K for the undoped compounds. Such values are considerably higher than T_C originally obtained from magnetization measurements.

P-3-01

SPIN DIFFUSION AND RELAXATION IN DILUTED MAGNETIC ALLOYS.

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The theory of the nuclear spin relaxation in solids is formulated from general statistical-mechanical arguments. The generalized kinetic equations for a system weakly coupled to a thermal bath are used to describe the relaxation and diffusion of nuclear spins in solids. The aim was to develop a successive and coherent microscopic description of the nuclear magnetic relaxation and diffusion in solids. The nuclear spin-lattice relaxation is considered and the Gorter relation is derived. A detailed theory of spin diffusion of the nuclear magnetic moment in dilute alloys (like Cu-Mn) is developed. It is shown, that due to the dipolar interaction between host nuclear spins and impurity spins, a nonuniform distribution in the host nuclear spin system will occur and consequently the macroscopic relaxation time will be strongly determined by the spin diffusion. The explicit expressions for the relaxation time in certain physically relevant cases are given.

P-3-02

MAGNETIC PROPERTIES OF Fe_3Si/GaAs(001) HYBRID-STRUCTURES

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The magnetic properties of Fe_3Si/GaAs(001) hybrid structures are studied. These epitaxial ferromagnetic films of 33 and 39 nm thickness show a high crystalline and interfacial perfection [1]. Structural characterization and SQUID magnetometry has been done [2]. We present ferromagnetic resonance (FMR) studies determining the uniaxial and fourfold anisotropy fields. The easy axis of magnetization is the in-plane [010] direction. The full angular dependence of the resonance field reveals a small uniaxial in-plane anisotropy field of -6 to -34 Oe which increases with the Fe concentration. Thus, the $[1\bar{1}0]$ direction is not equivalent to the [110] direction, anymore. Moreover, these samples show an exceptional narrow linewidth ($\approx$5 Oe) confirming the high structural quality.
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[1] J. Herfort *et al.*, Appl. Phys. Lett. **83**, 3912 (2003).
[2] J. Herfort *et al.*, J. Vac. Sci. Technol. B **22**, 2073 (2004).

P-3-03

Magnetic studies of iron(III) – croslinked chitosan

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The extensive research of metallo-organic chelating compounds is inspired by perspectives of industrial, ecological and biomedical applications. One of this type of metallo-organic materials are transition metal - chitosan complexes. Recent investigations of Fe-chitosan complexes were mainly concentrated on the analysis of their chemical structure. It has been found that both amino [-NH_2] and hydroxyl [-OH] groups chelate Fe(III) ions and more than one polymer chain is involved in the formation of the complex. Moreover, it has been indicated that Fe(III) ions are either penta- or hexa-coordinated and that at low temperatures these systems exhibit magnetic ordering. The iron clustering has been suggested as a plausible explanation for the observed magnetic behaviour. The lack of the extended magnetic characterization as well as satisfactory description of the magnetic ordering in Fe-chitosan (related partly to the uncertainty of their structure) became the reason for the present investigations. In this work the low-temperature *dc* and *ac* magnetic measurements are reported. The results obtained indicate that the iron atoms do not segregate in the polymer matrix forming clusters, as was suggested formerly, but the magnetic behaviour of Fe-chitosan is typical of a spin-glass-like rather than a superparamagnet.

P-3-04

MAGNETIC PROPERTIES OF $Tb_{1-X}Zr_XFe_2$ COMPOUNDS

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The $Tb_{1-X}Zr_XFe_2$ compounds with $x \leq 0.5$ cristallize in a cubic C15 structure. Magnetic measurements were performed in the temperature range 4.2-1000K and external magnetic fields up to 9T. All the compounds are ferimagnetically ordered. The Curie temperatures and the spontaneous magnetization at 4.2K decrease when the zirconium content increase. Considering the terbium magnetic moment like that determined on $TbFe_2$ by neutron diffraction, the iron magnetic moments at 4.2K were determined. The iron magnetic moments are dependent on composition, decreasing from $1.67\mu_B$ to $0.69\mu_B$. The temperature dependences of the reciprocal susceptibilities are non-linear. The iron effective magnetic moments, determined from linear region in the high temperature range are little dependent on composition. The ratio $r = \frac{S_P}{S_0}$ between the number of spins determined in the paramagnetic region and the number of spins at 4.2K increase when the zirconium content increase, suggesting the increase of the ittinerancy. Finnaly, the magneetic behavior of iron in this compounds is analyzed.

P-3-05

EPR AND MAGNETIZATION STUDIES OF THE $LaMn_{0.46}Co_{0.54}O_3$ AND $HoMn_{0.49}Co_{0.51}O_3$ SINGLE CRYSTALS

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The electron paramagnetic resonance spectra of Mn^{4+} and Co^{2+} ions in the orthorhombic $LaMn_{0.46}Co_{0.54}O_3$ and $HoMn_{0.49}Co_{0.51}O_3$ single crystals grown by the electrodeposition method have been studied at 9.2 GHz. The observed fine structure was fitted using spin-Hamiltonian with S=3/2, confirming Mn^{4+} assignment. The temperature-induced spin reorientation accompanied with enhancing of Ho magnetic moment was found at T≈28K in $HoMn_{0.49}Co_{0.51}O_3$. The overall results of magnetization studies and EPR indicate on presence of both ferro- and antiferromagnetic interactions at low temperatures.

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P-3-06

A new class of MEMS LC-resonators for magnetic sensor

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A new class of LC-resonators for magnetic sensor was invented and fabricated using MEMS technique. The LC-resonator consists of a micro-inductor with ferromagnetic microwire cores and a capacitor connected in parallel to the micro inductor. The microwire was fabricated by a glass-coated melt spinning technique. The solenoid type micro-inductor is 1.5 mm in length with 10 turns. Since the permeability of ultra soft magnetic microwire is changing rapidly as a function of external magnetic field. The resonance frequency as well as the current through the circuit is changing drastically according to the external magnetic field. The measurement of impedance of the LC-resonator was carried out at high frequency range from 100 MHz up to 1 GHz with a network analyzer and an impedance analyzer along the microwire direction and at varying axial dc-magnetic field in range of ±300 Oe. The impedance vs. magnetic field curve was changing abruptly at near the resonance frequency. The change of phase angle as much as 180 degree evidenced the occurrence of resonance. The resonance frequency can be tuned from 100 MHz to 1 GHz by changing. Numerical simulations as well as theoretical investigation are also discussed.

P-3-07

INFLUENCE OF HYDROGEN BONDS ON MAGNETIC PROPERTIES OF Cu($dmen$)$_2$M(CN)$_4$, (M=Ni, Pt) - $S = 1/2$ LOW-DIMENSIONAL HEISENBERG ANTIFERROMAGNETS

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The magneto-structural correlations in materials Cu($dmen$)$_2$M(CN)$_4$, where M=Ni or Pt, and $dmen$ is N,N-dimethylethylenediamine, have been investigated. In previous work [M. Orendáč *et al.*, Solid State Commun. **94** (1995) 833] devoted to the study of Cu(en)$_2$Ni(CN)$_4$, where en is ethylenediamine, layered magnetic structure is created by weak exchange paths between magnetic Cu(II) ions. The ligand en was consequently replaced by larger $dmen$ with aim to weaken the exchange coupling through the ligands. Thermodynamic and magnetic properties of the studied systems suggest the presence of a weak antiferromagnetic exchange interaction. Observed λ-like anomaly in the temperature dependence of the specific heat of Cu($dmen$)$_2$Ni(CN)$_4$ at T=0.19 K might be attributed to the formation of long-range order due to the presence of exchange coupling between the planes but the entropy removed above the transition temperature represents 50% of the total magnetic entropy suggesting low-dimensional character of the system. The influence of hydrogen bonds connecting larger $dmen$ ligands on magnetic dimensionality of studied materials is discussed.

P-3-08

MAGNETIC PROPERTIES OF $TM_3[Cr(CN)_6]_2 \cdot nH_2O$

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Recently, Prussian blue analogues $TM_3^{II}[Cr^{III}(CN)_6]_2 \cdot nH_2O$, crystallizing in fcc crystal structure, have received increasing attention as molecule-based magnets. In these materials the effective exchange interactions between TM and Cr via the cyano ligand are strong, leading to high Curie temperature T_c ranging from $T_c = 16$ K for $Fe_3^{II}[Cr^{III}(CN)_6]_2 \cdot nH_2O$ to $T_c = 314$ K for $V_3^{II}[Cr^{III}(CN)_6]_2 \cdot nH_2O$. Magnetic ordering varies from ferrimagnetic to ferromagnetic in relation to $3d$ ions present in the structure. The Curie temperature decreases linearly from maximal value for V^{II}–compound reaching minimal value for Fe^{II}–compound and increases again linearly having the maximal value for Cu^{II}–compound. All compounds obey the Curie–Weiss law in the high temperature region. In our paper we report on detailed study of magnetic properties of Prussian blue analogues $TM_3^{II}[Cr^{III}(CN)_6]_2 \cdot nH_2O$, where TM = Mn, Fe, Co and Ni. In addition to already published results we have found hysteresis behavior in ZFC and FC magnetization curves for all compounds with temperature of bifurcation only slightly dependent on applied magnetic field. A detailed study of $M(B)$ curves and $M(T)$ dependencies suggests possible field induced re–arrangement of magnetically ordered state leading to increase of the Curie temperature of about 4 K for Fe- and Co-hexacyanochromates.

P-3-09

GIANT MAGNETOIMPEDANCE IN SOFT MAGNETS

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Magnetic field dependence of the electrical impedance in a magnetic material (magnetoimpedance) may be very strong in the case of soft magnetic conductors (in a form of thin wire, ribbon, film or various composite structures) at sufficiently high frequencies of an ac-current. The giant magnetoimpedance (GMI) effect, which is a manifestation of strong change of penetration depth of the ac current through a magnetic conductor (skin effect), is related to changes in the dynamics of magnetization process which affect the magnetic permeability. This effect attracts much attention because of its potential applications and as a tool for magnetic materials characterization. In the present work, GMI effect and its relation with magnetic anisotropy was studied in Co-based amorphous ribbons modified by thermal treatment (which leads to changes in magnetic and magneto-impedance characteristic of the ribbon because of alterations in local magnetic anisotropy). The samples with residual stress, stress relaxed and with intentionally induced anisotropy were studied. The magnetization characteristics and impedance dependence on magnetic field at various frequencies of an ac-current (up to 30 MHz) have been measured. The influence of various anisotropy contributions has been determined and a possibility of tailoring of magnetoimpedance effect has been demonstrated.

P-3-10

EFFECTIVE SPIN-ORBITAL MODEL FOR MANGANITES

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We study a two-dimensional (2D) effective orbital t-J model [1] derived for strongly correlated e_g electrons in doped manganites. At half doping, ferromagnetic (FM) and antiferromagnetic (AF) correlations closely compete, and a relatively small additional AF for the t_{2g} core spins can trigger either antiferromagnetism or ferromagnetism. In the ferromagnet, alternating orbital order develops, while predominantly, but not exclusively, the orbitals within the plane are occupied in the AF case. Because the FM and AF states have very similar energy, small changes in the concerning parameters can have a large impact and can switch the system from one scenario to the other. For the same reason, spin order is destroyed easily with rising temperature. Upon doping, the kinetic energy drives a transition to ferromagnetism in the AF case and enhances occupation of the more mobile in-plane orbitals for the FM plane. We investigate the 2D model for parameters relevant to monolayer manganites and also treat the case of two coupled layers, i.e., bilayer compounds. Finally, we discuss the cooperative character of the changes in magnetic correlations and orbital reordering found recently in monolayer manganites.

[1] M. Daghofer, A. M. Oleś and W. von der Linden, Phys. Rev. B **70**, 184430 (2004).

P-3-11

THE STRUCTURE AND PROPERTIES CHANGES OF DISPERGATED FILMS ON THE BASIC OF 3d-METAL

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Amorphous and crystalline Fe-Ge films (thickness on 50-200 nm) were prepared by thermal coevaporation on the dielectric substrate. The results obtained by means of a X-ray diffraction analysis method have shown the complete absence of diffraction peaks, corresponding to a crystalline state. Crystalline films were deposited on substrates at temperature above 500 T,K.

The subject of this paper is the effect of a single-layer film structural condition, its thickness and the grain size on a coercive force quantity (H_c). It was used padding exterior magnetic (H=3103 Oe) and electrical ($E = 10^5$ V/m) fields for regulation the grain size in films. A dominant role of an electrical field at decrease of 3d-metal clusters size, and increase of specific share of antimagnetic matrix interlayer were established. Decrease the concentration Ge in system to lead to increase the coercive force quantity (H_c).

The present results on the microstructure and physical properties of dispergated films on the basic of 3d-metal has allowed to implement conditions to produce of the high resistance materials. Coercive force quantity depend primarily on the crystalline grain size and Ge-concentration of the alloys.

P-3-12

Magnetic properties and ^{1}H NMR spectroscopy of $TM_2^{2+}[W^{IV}(CN)_8].nH_2O$

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Possible existence of photoinduced magnetically ordered state in octacyanowolframates with $3d$–ion attracts attention of physicist and chemists. In our paper we report on a detailed study of magnetic properties of bimetallic extended networks built from $W^{IV}(CN)_8{}^{4-}$ and M^{2+} = Cu^{2+}, Co^{2+}, Ni^{2+}, Mn^{2+}, Fe^{2+}. Prepared powders were characterized by means of thermogravimetry, UV–VIS, IR spectroscopy and X–ray diffraction. Mn and Fe containing compounds were found to crystallize in tetragonal, while Cu and Ni in orthorombic system. It is well known that W^{IV} is in non–magnetic state with $S = 0$ and therefore magnetic properties of octacyanowolframates are fully determined by weak antiferromagnetic exchange interaction between magnetic $3d$–ions via NC–W^{IV}–CN diamagnetic spacer. The weak exchange interaction is the reason for appearance of magnetically ordered state only at very low temperatures. We have found that susceptibility data follows the Curie Weiss law above $T = 20$ K. Deviations from Curie–Weiss law below 10 K indicate a short range magnetic ordering. In addition, when T decreases $\chi_m T$ value is roughly constant till $T = 10$ K and then decreases. This is another indication of very weak antiferromagnetic interactions at low temperatures. The ^{1}H NMR signals reflect the magnetic moment of the TM ions (μ_P). The decay rates of FID signals increase as μ_P and the applied static *rf* field increase.

P-3-13

Magnetic properties of $La(Co_{1-x}M_x)_{13}$ Intermetallic Compounds with M=Ni or Mn

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The $La(Co_{1-x}M_x)_{13}$ compounds with M=Ni or Mn crystallize in a $NaZn_{13}$ type structure, for x$\leq$ 0.2. Magnetic measurements were performed in the temperature range, 4.2-1300K and external fields up to 9T. The Curie temperatures decrease nearly linear from 1290K (x=0) up to 740K (x=0.2) for M=Mn and 760K (x=0.2) for M=Ni. The mean transition metal moments at 4.2K increase slowly from 1.6 $\mu_B/atom$ for x=0 to 1.7 $\mu_B/atom$ for x=0.05 (M=Mn) and x=0.08 for M=Ni and then decrease. Paramagnetic measurements were also performed for compounds with high substitutions at cobalt sites. The magnetic behaviour of transition metals were correlated with the varriation of the exchange interactions in the systems.

P-3-14

THE ORIGIN OF LOW-DIMENSIONAL MAGNETISM IN $Cu(en)_2Ni(CN)_4$ AND $Cu(en)_2Pt(CN)_4$.

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The comparative analysis of the structural and magnetic properties of the chain-like materials $Cu(en)_2Ni(CN)_4$ and $Cu(en)_2Pt(CN)_4$ ($en = C_2H_8N_2$) has been performed. The results suggest that the origin of the two-dimensional (2d) short-range correlations observed below 1 K cannot be unambiguously ascribed to a combined effect of intrachain covalent pathways and interchain coupling formed by hydrogen bonds, as previously proposed [1]. An EPR investigation of the symmetry of the local Cu(II) surroundings at 4 K, complemented by the studies of the hydrogen bond geometry, susceptibility, and magnetization, suggest the magnetic correlations between Cu(II) ions are mediated predominantly through a 2d net of hydrogen bonds.

[1] M. Orendáč, A. Orendáčová, J. Černák, A. Feher, Sol. St. Commun. 94 (1995) 833.

P-3-15

$[Ni(Pr^ixa)_2(pyr)]_n$ - LOW - DIMENSIONAL $S = 1$ HEISENBERG MAGNET.

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$[Ni(Pr^ixa)_2(pyr)]_n$ was previously identified as an $S = 1$ Heisenberg chain with intrachain interaction $J/k_B = -2.7$ K and subcritical single-ion anisotropy D [1]. Specific heat measurements conducted from 100 mK to 10 K in zero magnetic field revealed the presence of a λ-like anomaly, at $T_c = 2.2$ K, that can be associated with a phase transition to an ordered state. Magnetic entropy removed above T_c indicates a low-dimensional character of the magnetic system. Strong deviations between the specific heat data and the $S = 1$ Heisenberg chain model with various D/J ratios can be ascribed to the presence of a set of hydrogen bonds, mediating an additional exchange coupling J'. This interaction and the intrachain coupling J form a two-dimensional triangular $S = 1$ Heisenberg lattice that governs the magnetic behaviour above T_c.

[1] A. Orendáčová, M. Orendáč, Z. Trávníček, M.W. Meisel, phys. stat. sol. (a) 196 (2003) 278.

P-3-17

HYPERFINE INTERACTIONS AND MAGNETIC, TRANSPORT AND STRUCTURAL PROPERTIES OF $La_{0.67}Ca_{0.33}Mn_{0.94}{}^{57}Fe_{0.06}O_3$

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The $La_{0.67}Ca_{0.33}Mn_{0.94}{}^{57}Fe_{0.06}O_3$ compound was studied using powder X-ray diffraction (XRD), VSM magnetometry, four-probe resistance (R) measurements and Mössbauer spectroscopy. XRD measurements were performed between 4 and 500 K and precise values of the unit cell parameters *vs* temperature were obtained. The metal-insulator transition temperature T_{M-I}, defined as the maximum of the $R(T)$ curve, was found surprisingly low and equal to 62 K. The ^{57}Fe Mössbauer spectra were recorded between 15 K and 850 K. The Curie temperature ($T_C \cong 141$ K), determined from temperature dependence of the ^{57}Fe hyperfine field, was in good agreement with the magnetisation result (142 K). Our results on $La_{0.67}Ca_{0.33}Mn_{0.94}{}^{57}Fe_{0.06}O_3$ clearly reveal that substitution of Fe^{3+} for Mn^{3+} suppresses locally double exchange interactions and strongly affects the magnetic and transport properties of the parent compound. It causes the strong reduction of T_C, the huge difference between T_C and T_{M-I} temperatures and complete suppression of the thermal expansion anomaly at T_C.

P-3-18

MAGNETIC PROPERTIES OF Ni_2MnGa HEUSLER ALLOY FILMS

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Ni–Mn–Ga Heusler alloys have recently attracted a great attention since they reveal a magnetically driven shape memory effect. We report our results concerning structure and magnetic properties of off - stoichiometric Ni–Mn–Ga films prepared by magnetron sputtering or flash-evaporation. The aim of this contribution is to investigate the effect of ordering on the magnetic properties of Ni-Mn-Ga films. The films with composition $Ni_xMn_yGa_z$ ($x = 50 \pm 5, y = 25 \pm 5, z = 25 \pm 5$) were deposited on mica or glass substrates at room temperature. The films were annealed in a high vacuum at 770 - 780 K for 0.1 to 1 hr. XRD at room temperature reveals the presence of B2 (or $L2_1$) type of structure. Magnetic properties were studied by ferromagnetic resonance (FMR) at temperatures from 78 K to 500 K. It is shown that the magnetic properties of the films critically depend on structural ordering. The as-received films are practically nonmagnetic with no trace of a martensitic transformation while those annealed at the highest temperatures show the magnetization $M(78K) \approx 600$ G, the Curie temperature $T_C \approx 390$ K and the martensitic transformation at $T_M = 200$ - 300 K depending on composition. Results show that both the effective magnetization and FMR linewidth are useful for monitoring structural ordering in these films.

P-3-19

THE EFFECT OF Ge SUBSTITUTION IN $Ni_2MnGa_{1-x}Ge_x$ HEUSLER ALLOYS AND FILMS

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Structural instabilities typical of Ni-Mn-Ga Heusler alloys with ferromagnetic shape-memory effect have recently been predicted to exist in Ni_2MnGe [1]. We present the results on the effect of adding Ge on the magnetic properties of $Ni_2MnGa_{1-x}Ge_x$ ($0 < x < 0.4$) alloys and thin films. It is found that the alloys are single phase with $L2_1$ ordering (cubic lattice constant $a \simeq 0.581$ nm). The Ge addition causes a drastic decrease in the martensitic transformation temperature from $T_M = 200$ K ($x = 0$) to $T_M = 50$ K ($x = 0.4$) with almost no effect on the Curie temperature $T_C \simeq 390$ K and magnetization $M_S(0) \simeq 450-500$ G. The magnetic properties of thin films strongly depend on ordering. The ordered films deposited by flash-evaporation from the powdered alloys have similar $L2_1$ (or B2) ordering and exhibit the magnetic properties similar to the properties of corresponding bulk alloys. First principle calculations of site-projected density of states for Ga and Ge were carried out to trace differences in the spin-down electronic states close to the Fermi level.

[1]A. T. Zayak and P. Entel, J. Magn. Magn. Mater. (preprint)

P-3-20

THE INFLUENCE OF BALL MILLING ON CURIE TEMPERATURE OF AMORPHOUS CoFeSiB POWDER

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The amorphous ribbons with nominal composition $Co_{70.3}Fe_{4.7}Si_{10}B_{15}$ (at.%) were prepared by melt spinning technique. These ribbons were cut into small pieces (5×10 mm^2) and milled up to 12 hours using a RETSCH PM4000 planetary ball mill. The milling was done under argon atmosphere at ball to powder weight ratio 31:1 with a speed of 200 rpm. X-ray diffraction on powder samples revealed no significant change of structure and after 12 hours of milling powders remain amorphous. On the other hand, observed change in crystallization process by use of differential scanning calorimetry indicate quite strong influence of milling on microstructure of milled powders. Further, from the thermo-magnetic measurements it is evident that ball milling causes the Curie temperature of amorphous phase (T_C^{am}) to increase. After 12 hours of milling the powder sample exhibited 40 K higher T_C^{am} as compared to as quenched ribbon ($T_C^{am} = 627$K). The thermo-magnetic measurements on heat-treated ribbons suggest that such increase in T_C^{am} is not only due to temperature rises during the milling and may be attributed to the combination of mechanical and thermal effects connected with nature of milling.

P-3-21

A XAS STUDY OF Ru DOPED N=1,2 RUDDLESDEN POPPER MANGANITES AND $Ca_{2.5}Sr_{0.5}GaMn_2O_8$.

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We report on the results of XAS studies at the Mn:$L_{2,3}$, Ru:K and O:K edges of novel manganites, $Sr_2Mn_{0.5}Ru_{0.5}O_4$, Sr_3MnRuO_7 and $Ca_{2.5}Sr_{0.5}GaMn_2O_8$. Measurements were carried out on polycrystalline powder samples at room temperature. From the analysis, values of the mean Mn valence amounting to 3.42(5) for bilayer Sr_3MnRuO_7 and 3.08(5) for single layer $Sr_2Mn_{0.5}Ru_{0.5}O_4$ are obtained. The corresponding Ru valences are 4.58(5) and 4.92(5), respectively. This indicates that Ru doping gives rise to a decrease of Mn valence, whereas Ru valence increases, compared to Mn^{4+} and Ru^{4+} in undoped compounds. Measurements on $Ca_{2.5}Sr_{0.5}GaMn_2O_8$ show the Mn mean valence of 3.50(5), which agrees with stoichiometry and, consequently, no deviation from nominal oxygen stoichiometry is concluded. A relation of the results to bulk magnetic properties of the compounds is discussed.

P-3-22

ELECTRONIC STRUCTURE AND MAGNETISM OF $LaVO_3$ and $LaMnO_3$

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$LaVO_3$ and $LaMnO_3$ are a subject of large interest by almost of 30 years due to their anomalous magnetic properties. In this contribution we derive and discuss energy levels of the strongly-correlated d^2 configuration of the V^{3+} ion and of d^4 configuration of the Mn^{3+} ion in the octahedral surroundings in the presence of the spin-orbit coupling and the resulting magnetic properties. We take into account very strong correlations among the d electrons and work with strongly-correlated atomic-like electronic systems, ground term of which is, also in a solid, described by two Hund's rules quantum numbers. In a solid we take into account the influence of crystal-field interactions, predominantly of the cubic (octahedral) symmetry. We describe both paramagnetic state and the magnetically-ordered state getting a value of 1.4 u_B for the V^{3+}-ion magnetic moment in the ordered state at 0 K of $LaVO_3$ ($^3T_{1g}$) and of 3.7 u_B for $LaMnO_3$ (^5E_g). Both values well reproduce the experimental data. A remarkably consistent description of both zero-temperature properties and thermodynamic properties indicates on the high physical adequacy of the applied atomic approach, being somehow a continuation of Van Vleck's studies. The shown ground states have been confirmed recently by other researchers. We point out the necessity to unquench the orbital moment in 3d-ion compounds.

P-3-23

MAGNETIC EXCITATIONS IN FCC Mn (37%Fe, 3%Cu) ALLOY.

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The similarity of phase diagrams of Mn-Fe and Mn-Ni alloys was thougt to imply the similarity of the concentration dependence of the parameters of the magnetic excitations in these alloys. Our systematic studies demonstrated the essential differences between these two systems. Within this program the inelastic neutron scattering (INS) in the FCC Mn(37%Fe,3%Cu) alloy was measured at temperatures ranging from 1.7 K up to 600 K. Since our earlier study of the FCC Mn(38%Ni) demonstrated the pronounced uniaxial anisotropy both in the static and dynamical part of the generalised susceptibility one of the aims was the search for the similar feature in the FCC Mn-Fe system. The results of our present measurements did not confirm these expectations. The temperature dependence of spin wave parameters was another aim of our investigations. The spin wave dispersion relation for higher temperatures becomes stronger than the linear one observed at low temperature. The spin wave damping increases with temperature slower for lower energies than for higher energies. This is in contrast with the data for the fct Mn(10%Fe, 3%Cu) where the damping parameter was found to be temperature independent excepting the region close to the Neel temperature.

P-3-24

Density functional calculations of Au_3Co

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The investigation of magnetic properties and the electronic structure of cobalt atom in different chemical and structural environment is a fascinating field of research. In the present work, we modelled the hypothetical Au_3Co theoretical compound, where the Co atom is surrounded by three gold atoms as a model for high Co concentration in gold. The magnetic properties of the Co atom in this structure have been calculated in the framework of local spin density approximation (LSDA) using the relativistic version of the full-potential local orbital minimum basis code. We also compare the two different approaches to calculate the magnetocrystalline anisotropy energy called the total energy approach and the force theorem approach.

P-3-25

A microscopic model of the oxygen vacancies in Ca-doped YIG

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Annealing experiments carried out on calcium doped yttrium iron garnet ($Ca : YIG$) in a reducing atmosphere, show decreases in the magnetisation over the entire temperature range. The electrical resistivity and the electric activation energy, however, increase. Charge carriers in $Ca : YIG$ are positive compensating holes. We compare with each other two situations, in which a compensating hole can be found. The first is the localization at an oxygen site which means the occupation of a hybridized eigen-energy level of an iron-oxygen cluster. The other is the localization of the hole in an attractive trap center. The latter is regarded as a result of a missing oxygen ion between the tetrahedral and octahedral iron-oxygen ionic clusters. For a sufficiently shallow trap, localized energy levels of the vacancy are considered to be eigen-energies of the hydrogen-like "atom". Assuming the Bohr radius equal to the calcium - oxygen distance, we can estimate the ground-state energy varying both the dielectric constant and the hole's effective mass. Communication between the tetrahedral and octahedral iron-oxygen clusters is maintained due to the $s-d$ hybridization. We find the energy-level structure of the pair of the clusters with either the ferro- or antiferromagnetic order of the spins. A difference in the respective ground states energies of the pair is equal to a superexchange parameter between the clusters' spins. Moreover, we find the current-voltage characteristics of the pair on the basis of the Landauer-like formula for the charge transfer.

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P-3-26

FINE HEXAFERRITE PARTICLE POWDERS AS MAGNETIC RECORDING MEDIA, PREPARED BY COPRECIPITATION-SELFCOMBUSTION

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In order to obtain Sr and Ba hexaferrite powders with submicron crystallites, we used a new method, self combustion, and heat treatments. By combustion it was obtained magnetic powders having a nanometer granular structure and characterized by the followings: M = 44.7 emu/g and H_c= 520 Oe for $SrFe_{12}O_{19}$ and M = 31 emu/g and H_c= 350 Oe for $BaFe_{12}O_{19}$ and nanosized crystallites (about 50 nm). It was investigated the effect of the annealing time on the grain size and several magnetic properties (magnetization and coercivity). After a short annealing time (5 – 10 minutes) at 1000^0C the coercivity achieved an important increase, to about 5000 Oe for Ba hexaferrite and to about 3400 Oe for Sr hexaferrite, whereas the grain size does not exceed 300 nm. By doping with 1 mol CaO, it was obtained a spectacular increase of coercivity of $SrFe_{12}O_{19}$, to about 6000 Oe by annealing at 800^0C for 5 – 10 minutes. Smaller magnetization for Ca-doped samples than that of the undoped samples can be explained by rearranging Fe ions in the distorsioned structure.

P-3-27

ON THE MAGNETIC GLASS-CERAMIC CONTAINING Li AND Ba FERRITE CRYSTALS

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In this paper we present some results for the oxide composites containing Li or Ba-M ferrite fine particles randomly dispersed in a glassy matrix. The samples were obtained by glass crystallisation method which permits a gradual control of particle size. It was investigated the evolution of the microstructure and the magnetic properties in terms of heat treatment temperature of the glass ceramics containing $LiFe_5O_8$ and $BaFe_{12}O_{19}$ fine magnetic crystals. The average crystal block size, D_m, was determined by X-ray diffraction using Scherrer's formula. Crystals of ferrite with sizes ranging from 3.5 to 50 nm for Li ferrite and from 50 to 320 nm for Ba-M ferrite, depending on the annealing temperature, were observed. Correspondingly, it was obtained that the crystalline fraction in the glassy mass increases with increasing annealing temperature. The magnetic behaviour (specific magnetization σ and coercivity H_c) is discussed in terms of the evolution with thermal annealing of the size of $LiFe_5O_8$ and $BaFe_{12}O_{19}$ crystals, dispersed in the glassy matrix.

P-3-28

The NMR ^{55}Mn study of the $La_{0.75}Sr_{0.25}MnO_3$ nanoparticles

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We report on a ^{55}Mn NMR study of the $La_{0.75}Sr_{0.25}MnO_3$ nanoparticles with the average grain size of 33nm and 114nm at 4.2K and at the applied field 0, 0.2 and 0.5T. A dominant signal from the double exchange (DE) controlled metallic ferromagnetic interior of the grains as well as a small signal from insulating ferromagnetic surface regions of the grains are observed. The DE resonant line shows a frequency shift in the applied field according to a full gyromagnetic ratio and a value of the demagnetizing field much smaller than 0.2T is obtained. In both samples studied a two-exponential nuclear spin-spin (T_2) relaxation is observed at zero field, whereas a single-exponential relaxation is observed at the applied field of 0.5T. For the sample with larger grains a higher NMR enhancement is observed, which indicates a higher magnetic susceptibility of the sample at the NMR frequencies. A comparison to the NMR data obtained on a bulk material is made. The results are discussed in terms of the influence of the grain size and on the presence of domain walls or other magnetic inhomogeneities and on the magnetic anisotropy.

P-3-29

MAGNETIC AND THERMODYNAMIC PROPERTIES OF $Cu(NH_3)_2Ag_2(CN)_4$ AN $S = 1/2$ QUASI - TWO DIMENSIONAL MAGNET.

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The crystal structure, thermodynamic properties and ESR spectra of $Cu(NH_3)_2Ag_2(CN)_4$ have been studied. The material consists of 2d sheets in which octahedrally coordinated Cu(II) ions are linked by diamagnetic $[Ag(CN)_2]^{2-}$ units forming a square lattice. Although the susceptibility and specific heat data reveal the existence of short - range order at about 2 K, quantitative analysis of the experimental data confirmed that the magnetic behaviour differs from that expected for 2d Heisenberg magnet on the square lattice. Structural features responsible for the observed difference are discussed. In addition, it is suggested that additional degrees of freedom represented by rotational states of NH_3 units contribute to thermodynamic equilibrium properties in the milikelvin temperature range.

P-3-30

Structure and magnetic anisotropy of $Co\backslash Au(111)$ films

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Numerical calculations combined with the theoretical analysis,concerning $Co\backslash Au(111)$ and $Ag\backslash Co\backslash Au(111)$ thin films, aim at a microscopic interpretation of empirical data obtained by A. Maziewski and his group. The data show rather striking properties of surface and interface magnetism in these materials, and indicate their strong magnetic anisotropy. The structural and magnetic properties of thin Co films epitaxially grown on $Au(111)$ substrates, are investigated using ab-initio local density calculations. It is shown that there is a large lattice intermismatch between Co and $Au(111)$, which causes a growth mode of the polygonal Co islands of two atomic layers with a hcp structure. The lattice mismatch at the $Co - Au$ interface leads to a buildup of the lattice strain. An enhancement of the magnetic moment on the free surface as well as at the $hcp\backslash fcc$ interface is found. The influence of the capping Ag layers on the film's relaxation and on its magnetic moment has been also considered. In order to obtain energy of the magnetic anisotropy for the cobalt films, we perform relativistic spin-polarized local spin density calculations.We analyze an influence of Ag , which plays a prominent role as a substantial effect of the shape anisotropy in $Co\backslash Au(111)$ films. It is also proved that magnetic anisotropy of $Co/Au(111)$ and that of $Ag\backslash Co\backslash Au(111)$ films essentially differ from each other.

O-4-01

MAGNETIC STRUCTURES IN CUBIC RCu_5 (R=Tb, Dy, Ho) COMPOUNDS

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The magnetic and structural properties of melt spun RCu_5 (R=Tb, Dy, Ho) with the cubic $AuBe_5$ type structure have been investigated with the neutron diffraction and magnetic measurements. Samples consisting of small polycrystalline plates of RCu_5 have been measured in a magnetic field up to $5T$ and a temperature range of $1.7 - 50K$. By magnetisation measurements it has been found that $TbCu_5$ and $DyCu_5$ behave antiferromagnetically below a temperature of $15K$ and $7K$, respectively. In zero magnetic field the magnetisation of $HoCu_5$ shows a sharp maximum at $3K$ characteristic for antiferromagnetic ordering, but below $3K$ its dependence of the magnetisation on an applied magnetic field is typical for ferromagnetic materials. For R=Tb an antiferromagnetic G-type structure in the fcc lattice was determined by neutron diffraction experiments at $4.2K$ [1]. Our measurements confirm these results. The $HoCu_5$ sample did not show long range magnetic order zero field. At $2K$ and at magnetic fields greater than $0.5T$ ferromagnetic peaks were found.

[1] T. Kaneko et al., J. Magn. Magn. Mater. 54-57 (1986) 469

O-4-02

Electronic structure of RAg_2Ge_2 ($R = Pr$, Nd) compounds

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The electronic structure of ternary RAg_2Ge_2 ($R = Pr$, Nd) compounds, which crystallize in the tetragonal $ThCr_2Si_2$ - type structure, were studied by X-ray photoemission spectroscopy. The magnetic data indicate that $PrAg_2Ge_2$ remains paramagnetic down to 1.9 K, whereas $NdAg_2Ge_2$ orders antiferromagnetically at about 2 K. The XPS results clearly show that the valence bands in both germanides consist mainly of the Ag $4d$ band. The XPS spectra of Pr and Nd $3d_{5/2}$ and $3d_{3/2}$ core levels were analyzed in the framework of the Gunnarsson-Schönhammer model [1] in order to derive information on the hybridization of $4f$ orbital with the conduction band. Separation of the XPS peaks, based on the Doniach-Šunjić theory [2], yielded the ratio $r = I(f^{n+1})/[I(f^n) + I(f^{n+1})]$ being equal to 0.09 for $PrAg_2Ge_2$ and 0.17 for $NdAg_2Ge_2$, which corresponds to the hybridization energy of 58.1 and 84.4 eV, respectively. The obtained values indicate a stability of the $4f$ shell in these two compounds, in good agreement with the magnetic data.

[1] O. Gunnarson, K. Schönhammer, Phys. Rev. B, **28** (1983) 4315.

[2] S. Doniach, M. Šunjić, J. Phys. C, **3** (1970) 285.

O-4-04

MAGNETIC AND TRANSPORT PROPERTIES OF Cu-FLUX-GROWN UCu_2Si_2

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In the literature a serious controversy exists as to the magnetic properties of the silicide UCu_2Si_2, crystallizing in the tetragonal $ThCr_2Si_2$ type crystal structure. Various authors reported either ferro- or antiferro-ferro transitions at temperatures below about 100 K. To solve this problem we have grown single crystals of UCu_2Si_2 from Cu flux and performed a detailed study carrying out measurements of ac and dc susceptibility, electrical resistivity, magnetoresistivity and thermoelectric power. UCu_2Si_2 orders presumably antiferromagnetically with $T_N = 106$ K, i.e. about 2-3 K above the ferromagnetic transition at $T_c = 103$ K, as demonstrated by the temperature variation of the ac-susceptibility. In contrast to previous single-crystalline report on UCu_2Si_2, no sign of the transition into antiferromagnetic behaviour has been observed below 50 K. The magnetic properties are highly anisotropic, with an easy axis [001], as one can expect from the crystal structure. The saturation moment has been determined at 4.2 K is 1.55 μ_B. The electrical resistivity in the ferromagnetic region may be described assuming an energy gap Δ in the spin wave energy spectrum. In the paramagnetic region, where the effective moments are about 3.0 μ_B, the electrical resistivity is determined by an interplay of Kondo scattering and crystal field effects. The magnetoresistivity below T_C for both tetragonal axes is negative, as one expects for a ferromagnet. The thermopower is negative at low temperatures and positive at higher temperatures.

O-4-05

Unusual negative magnetisation effect in antiferromagnetic $YbFe_4Al_8$ compound

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The nowadays-published experimental reports on the magnetic and transport properties of rare earth RFe_4Al_8 systems are not numerous and still controversial. One of the most intriguing is the possibility of superconductivity in the Lu- or Yb systems [1]. To clarify this point we performed investigations of the magnetic and transport properties of $YbFe_4Al_8$ intermetallic compound by the methods of DC magnetisation, microwave absorption, Mössbauer effect and four-point resistivity measurements. The Mössbauer effect measurements reveal a broad antiferromagnetic phase transition which begins at $T_N = 160$ K and is completed at the temperature of 100 K. This compound exhibits also a negative magnetisation below 34 K. We explain this effect in terms of antiferromagnetic interactions between the moment of Yb and the effective moment of canted Fe spins.

[1] H. Drulis et al., Solid State Commun. 123 (2002) 391.

P-4-01

MAGNETIC PROPERTIES AND ELECTRONIC STRUCTURES OF $Gd_3Cu_4X_4$ (X = Ge, Sn)

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Polycrystalline samples of $Gd_3Cu_4X_4$ (X = Ge, Sn) were investigated by means of magnetometry and XPS. Additionally, calculations of the electronic structures with the TB-LMTO method were performed for both compounds. They were found to be antiferromagnets; the stannide - below 13 K and the germanide - below 11 K. The electronic structures determined from the photoemission spectra agree well with the results of the calculations. Analysis of the core levels indicates presence of the Cu^{+1} ions in both compounds. Besides, charge transfers from the Cu and Ge atoms, the latter only in $Gd_3Cu_4Ge_4$, were detected.

P-4-02

Is $LaNi_2$ corresponding reference material for $La_xHo_{1-x}Ni_2$ solid solutions ?

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The heat capacity measurements have been performed on $La_xHo_{1-x}Ni_2$ solid solutions with x values of 0.2 and 0.4 for temperatures between 2 and 295 K in zero and 0.42 T magnetic fields. To isolate conduction electron and phonon contributions from the total heat capacity the measurements of heat capacity of isostructural $LaNi_2$ and $LuNi_2$ compounds were performed. The magnetic susceptibility measurements of $LaNi_2$ and $LuNi_2$ compounds exhibits a very weak temperature dependence above 50 K. The results obtained suggest that in case $La_xHo_{1-x}Ni_2$ solid solutions $LaNi_2$ should be not employed as reference material and only $LuNi_2$ may be consider as reliable one.

P-4-03

Thermal expansion on some $REIn_3$ (RE=La,Pr,Gd)

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Results of the linear thermal expansion coefficient α measurements are reported for $PrIn_3$, $GdIn_3$ and $LuIn_3$. Those systems belong to the large family of the $REIn_3$ (RE = Rare Earth) compounds which crystallize in the $AuCu_3$-type of crystal structure.
The measurements were carried out on monocrystaline samples in temperature range 5K $\div$ 200K. Compounds under investigation differ to their magnetic properties. $PrIn_3$ is a typical example of the singlet ground-state paramagnet in which the interionic interactions may be neglected while the $GdIn_3$ is the crystal-field free antiferromagnet in which the RKKY interactions play essential role. Therefore, apart from the results for α, also magnetic contributions to α have been estimated and compared with those calculated from theoretical predictions. Results obtained for the nonmagnetic $LaIn_3$ stand here as a phonon reference.

P-4-04

Electrical properties of carbon dopped EuB_6

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EuB_6 is ferromagnetic below 16 K and its low-temperature properties show remarkable similarities to those of manganese oxides, exhibiting the phenomenon of colossal magnetoresistance [1]. Substitution of boron by carbon brings electrons into the conduction band of EuB_6, thus $EuB_{6-x}C_x$ carbide borides behave as degenerate semiconductors in which both carrier concentration and antiferromagnetic interaction increase with increasing of carbon content. Our former results of electrical resistivity measurements of the sample (with x close to 0.05) show the high (residual) resistivity at lowest temperatures while measurements of the magnetic field dependence of electrical resistivity at 4.2 K indicate a giant magnetoresistance, as the ratio between the resistivity in zero magnetic field and in the field of 3 T has been 3.7 [2]. In this work, we present careful measurements of the electrical resistivity and the electron tunneling spectroscopy studies. On the basis of obtained results, conclusions on the nature of the magnetic scattering of charge carriers in the vicinity of the magnetic phase transition and conclusions on the density of electronic states of the studied system have been done.

1. H.R.Ott et al., Physica B **281**&**282** (2000) 423-427
2. I. Baťko et al., Solid State Commun. **98** (1996) 895

P-4-05

CRYSTAL STRUCTURE AND ELECTRICAL RESISTIVITY OF $GdNi_{5-x}Cu_x$COMPOUNDS

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The effect of substitution of Cu for Ni on the lattice parameters and electrical resistivity of the polycrystalline $GdNi_{5-x}Cu_x$ compounds has been studied. All investigated compounds crystallize in the hexagonal $CaCu_5$ type of crystal structure (space group P6/mmm). The compound $GdNi_5$ is a ferromagnet with T_C=32K where we have observed small negative *Ni 3d* band polarization and a small nickel moment is induced by exchange interactions with magnetic Gd. The compound $GdCu_5$ is considered as an antiferromagnet with T_N=26K. The influence of Cu substitution for Ni is reflected in both lattice parameters a and c as well as in the volume unit cell V. Quite peculiar behavior is observed in the temperature variation of the resistivity for Cu - rich compounds. At low temperatures especially below 30K the variation is quite unusual and is probably related to the incommensurate magnetic structure which arises from the weakly negative interaction between Gd nearest neighbours.

P-4-06

MAGNETIC, ELECTRIC PROPERTIES AND ELECTRONIC STRUCTURE OF $GdNi_{3-x}Fe_x$

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We report results of measurements of the magnetic susceptibility, the electrical resistivity, the crystal and electronic structure of the polycrystalline intermetallic $GdNi_{3-x}Fe_x$ compounds. The partial substitution Ni by Fe is reflected in the linear increase of the lattice parameters in the whole range of x. The Curie temperature depends on Fe concentration. The value of T_C increases at first, reaches a maximum around x=0.4 and then decreases. For higher concentration of Fe we have observed the compensation temperature T_{comp} . The changes in the magnetic properties are interpreted in correlation with the electronic structure of the investigated system, which have been studied by using X-ray Photoelectron Spectroscopy (XPS). The valence band spectra at the Fermi level *(E_F)* exhibit the domination of the hybridized *Ni/Fe (3d)* and *Gd (5d)* states. We have observed a remarkable decrease of the density of states near E_F and the shift of $4f$ Gd peaks in the energy scale for the Fe-rich compounds.

P-4-07

Electronic structure of RCo_xGe_2 ($R = Ce$, Pr, Gd) compounds

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Electronic structure of $CeCo_{0.89}Ge_2$, $PrCo_{0.85}Ge_2$ and $GdCo_{0.64}Ge_2$ which crystallize in the orthorhombic $CeNiSi_2$-type structure was studied by X-ray photoemission spectroscopy.

The valence bands of $CeCo_{0.89}Ge_2$ and $PrCo_{0.85}Ge_2$ have similar character. The two maxima at 0.9 and 2.0 eV for the Ce-compound and at 0.9 and 3.0 eV for the Pr-compound are observed. In the case of $GdCo_{0.64}Ge_2$, the strong intensity peak at 8.7 eV corresponding to Gd $4f$ states except the broad peak with the maximum at 1.4 eV was found. The analysis of the XPS spectra of Ce and Nd $3d_{5/2}$ and $3d_{3/2}$ in the Gunnarson-Schönhammer model [1] give the information on the hybridization of the f orbital with the conduction band. The separation of the peaks based on the Doniach-Šunjić theory [2] gives the ratio: $r = I(f^{n+1})/[I(f^n) + I(f^{n+1})]$. The r values are equal 0.12 for $CeCo_{0.89}Ge_2$ and 0.22 for $PrCo_{0.85}Ge_2$ which correspond to the hybridization energy 58.1 eV and 106.6 eV respectively. These values indicate stability of the f shell in these compounds.

[1] O. Gunnarson, K. Schönhammer, Phys. Rev. B, **28** (1983) 4315.

[2] S. Doniach, M. Šunjić, J. Phys. C, **3** (1970) 285.

P-4-08

THERMAL PROPERTIES OF $U_3Al_2Si_3$ SINGLE CRYSTAL

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We report on a detailed study of heat capacity performed on the $U_3Al_2Si_3$ single crystal in the temperature range from $T = 0.15$ K up to $T = 300$ K in magnetic fields up to $\mu_0 H = 5$ T applied along the easy axis of magnetization. Recently $U_3Al_2Si_3$ was reported as ferrimagnet or non–collinear ferromagnet with the Curie temperature $T_c = 38$ K. Magnetic structure is not completely understood at present. Heat capacity measurements performed on polycrystalline and textured samples revealed an enhanced value of the electronic coefficient of specific heat $\gamma = 250$ mJ/mol K^2. The transition to the magnetically ordered state was accompanied by a broad maximum and the heat capacity data below magnetic transition could be fit very well within the model introducing the energy gap Δ in the dispersion relation of magnons. The applied magnetic field shifted the anomaly to higher temperatures and smeared it out. Our results obtained on the single crystal resemble the earlier results obtained on polycrystalline and textured samples. In addition, an upturn of $C/T(T)$ curve, found below $T = 2$ K, can not be fully attributed to nuclear contribution. For the full description of the phonon part of the specific heat we used the harmonic approximation of the phonon spectrum including both the Einstein and Debye models and the correction for an anharmonicity. We made an attempt to separate the contribution of CEF–splitting to the heat capacity.

P-4-09

ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $Fe_2V_{1-x}Ti_xAl$

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Recent transport, specific heat and magnetic susceptibility measurements indicated that the Heusler-type Fe_2VAl compound is a candidate for a 3d heavy-fermion system [1]. Experimental investigations have shown the large (compared to the normal metal) value of the low-temperature electronic specific heat coefficient γ and the semiconductor-like behavior of the resistivity in the paramagnetic state. Therefore, Fe_2VAl has been classified to the non-magnetic narrow-gap semiconductors (Kondo insulators) having similar properties as FeSi [2]. Another compound, Fe_2TiAl is weakly ferromagnetic [3], $T_C \cong 120$ K in agreement to the Slater-Pauling behavior [4], however, its magnetic moment at $T = 0$ is much smaller than expected.
In this presentation we discuss the results of our electronic structure investigations (XPS experimental results and LMTO calculations of the valence bands) for $FeV_{1-x}Ti_xAl$ series of alloys. We also present the magnetic susceptibility measurements of $FeV_{1-x}Ti_xAl$. We try to understand the ground state properties of these alloys basing on the atomic disorder, which leads to the formation of the magnetic clusters.

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P-4-10

MAGNETIC PROPERTIES OF NON–STOICHIOMETRIC $U_{1+x}Ni_{1+y}Al$ COMPOUNDS

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UNiAl (hexagonal ZrNiAl crystal structure) is antiferromagnetic (AF) below T_N =19 K. In magnetic fields above the metamagnetic transition (B_c = 11.25 T at T = 4.2 K) the AF coupling is destroyed yielding magnetization μ = 0.8 μ_B/f.u.. However it is well known that the crystallographic as well as electronic structure of all UTX compounds are sensitive to external perturbations such as temperature, pressure, magnetic field and very important is also the influence of the local surroundings of U atoms. The deviation from the stoichiometry can also be gainfully employed to probe the structural and magnetic instabilities of the U–based intermetallic compounds. The purpose of this work is, therefore, to investigate accurately the effect of variations in stoichiometry on the basic magnetic properties of $U_{1+x}Ni_{1+y}Al$, where x $\leq$ 0.04 and y $\leq$ 0.06. The samples were prepared by arc–melting in protective Ar–atmosphere. Phase purity, crystal structure and lattice constants were checked by standard X–ray diffraction methods. Metallographic examination showed the presence of small amount (less then 3 %) of a parasitic phase in the form of intergranular networks. Magnetization measurements were carried out by VSM magnetometer in the temperature range 4.2 K $\leq T \leq$ 300 K in applied magnetic field up to μ_0H = 6 T. Obtained results have shown that the transition temperature T_N of investigated compounds is directly proportional to x and y.

P-4-11

STRUCTURE AND MAGNETIC PROPERTIES OF Sm-Ni-Cu COMPOUNDS AFTER MECHANICAL TREATMENT

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We have investigated the influence of mechanical alloying on structural changes and magnetic properties of the $SmNi_4Cu$ compound. This compound crystallizes in the hexagonal structure of $CaCu_5$, space group P6/mmm. $SmNi_4Cu$ is ferromagnetic with the Curie temperature of 36 K and the saturation magnetic moment of 0.36 μ_B at 4.2 K. The decrease of intensity and broadening of the diffraction lines have been detected after milling as a consequence of the grains' size reduction. The analysis of the as-prepared sample using EDAX has revealed a stable composition without a presence of any additional phases and elements. The obtained results show that the magnetic properties significantly depend on the milling time. The temperature and magnetic field dependences of the magnetization exhibit a presence of antiferromagnetic behavior of the milled samples. The transition temperature does not vary as a function of the milling time. This antiferromagnetism has been ascribed to a creation of the orthorombic $SmCu_2$ phase with $T_N = 23$ K.

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P-4-12

Magnetic phase transitions in $TmNi_4Al$ studied by magnetometry and neutron diffraction

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Tm and its alloys are known to create the numerous non-collinear magnetic phases, therefore this same can be expected in the case of $TmNi_4Al$. Indeed, we have observed that this compound, contrary to the other RNi_4Al members, exhibits a double phase transition in the ac magnetic susceptibility with $T_{C1} = 5.8$ K and $T_{C2} = 2.8$ K. We have performed the magnetization curve measurements and the neutron diffraction experiments above the higher temperature transition, between the two transitions and below the lower temperature peak of the ac susceptibility. However, magnetization curves as well as the neutron diffraction patterns do not provide any evidence of the antiferromagnetic ordering. There is only an increase of the intensities observed between 4.2 K and 1.8 K. Therefore, the two peaks in the ac magnetic susceptibility have been ascribed to a switch between two various slightly non-collinear orders of the magnetic moments.

P-4-13

Electronic structure studies of $DyNi_4Cu$

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Electronic structure of the $DyNi_4Cu$ compound, crystallizing in the hexagonal $CaCu_5$-type of structure has been studied using the XPS method with monochromatized Al K_α radiation as well as the self-consistent spin-polarized TB-LMTO (tigh-binding linear muffin-tin orbital) method. The self-consistent band calculations were performed for the experimental lattice parameters (a=4.918 Å, c=3.991 Å), which were determined by X-ray diffraction. Our calculations show that $DyNi_4Cu$ is ferromagnetically ordered at 0 K. The analysis of the valence band shape in vicinity of the Fermi level shows that this part of the spectrum comes mainly from 3d electrons of Ni and Cu atoms (peaks at -1 eV and -4 eV). The features of the experimental XPS valence band spectra near the Fermi level are reproduced in our calculations. Peaks below -7.5 eV are connected with the contribution of the f-electrons of Dy. The obtained peaks positions in the valence band are in good agreement with the binding energies of metallic dysprosium, copper and nickel.
Core levels of Dy, Cu nd Ni are also investigated.
This research was supported by the Polish State Committee for Scientific Research (KBN grant No1 PB03 077 28).

P-4-14

Exchange splitting of the photoemission core levels in Eu and its compounds

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The intra-atomic exchange interaction leads to the known effect of splitting of the photoemission core s levels and to the complex multiplet structures of the p and d levels. The divalent Eu with its 4f7 configuration and maximal spin value of 7/2 shows in photoemission well resolved structures similar to those found in Gd. The trivalent Eu ion has the 4f6 configuration and due to the Hunds rules the total momentum J=L-S=0. As a consequence EuF3, where Eu is trivalent, exhibits a weak van Vleck like paramagnetism. However, our investigations showed that both Eu 4s and 5s levels in EuF3 (crystal, amorphous thin film, ultrathin MBE grown layers) exhibit in photoemission doublets characteristic for exchange splitting. At the same time the emission from the 4d level do not show any visible splitting. The same situation was found for Eu doped LiYF4 where Eu ions are nominally trivalent. Our studies aim to find how coupling between spins of a photo-hole and 4f level depends on the spin-orbit interactions within the 4f shell and photo-excited level. Moreover, preliminary results of magnetic circular dichroism in photoemission have shown for EuF3 ultrathin layers a clear dichroic effect in valence band.

P-4-15

ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES $Gd_{1-x}Tb_xNi_3$ COMPOUNDS

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The magnetic susceptibility, the crystal and electronic structure of the polycrystalline intermetallic $Gd_{1-x}Tb_xNi_3$ compounds has been investigated. All investigated compounds crystallize in the rombohedral $PuNi_3$type of crystal structure (space group R-3m). The effect of partial substitution Gd by Tb is reflected in the linear decrease of the lattice parameters in the whole range of x, whereas the Curie temperature determined from AC susceptibility measurements decreases from 114 K for $GdNi_3$ to 100 K when x=0.5 and is unchanged until full concentration of Tb (x=1). Additionally the presence of the helimagnetic phase when Gd is substituted by Tb was observed. The electronic structure was studied by using X-ray Photoelectron Spectroscopy (XPS). Both valence band and core level spectra are analyzed. The valence band spectra close to the Fermi level are dominated by the *Ni 3d* and *Gd/Tb* states.

P-4-16

Electronic structure of rare-earth compounds $TmGa_3$, $ErGa_3$, and $CeIn_3$ studied by positrons[1]

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The isostructural systems $TmGa_3$, $ErGa_3$, and $CeIn_3$ constitute an interesting subject for their magnetic properties and, in the case of $CeIn_3$, for the fascinating interplay of antiferromagnetism, heavy-fermion behaviour and superconductivity under application of pressure[3]. The electronic structure of these compounds has recently been investigated by measurements of the two-dimensional angular correlations of positron annihilation radiation (2D ACAR), providing line projections of the electron-positron momentum density $\rho(\mathbf{p})$[4]. Whereas for all systems the *f*-electrons are mostly localized in the paramagnetic phase, the exact shape of their Fermi surfaces (FS) is slightly different. Indeed, $TmGa_3$ and $ErGa_3$ show a FS *nesting*, consistent with the observed magnetic structure, which does not occur in $CeIn_3$ having a different magnetic structure. Since the FS geometry is decisive to draw these conclusions, we present how various tomographic methods can influence 3D momentum densities and FS of the compounds[5].

P-4-17

THERMAL HYSTERESIS OF THE PHASE TRANSITION TEMPERATURE OF SINGLE CRYSTALLINE GdB_6

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The intermetallic compounds $RE B_6$ type crystallize in the cubic CaB_6 structure. They display a great diversity of magnetic phenomena. Among them GdB_6 is interesting because of two magnetic transition at low temperatures. Recently, a detailed X-ray scattering study of the phase transition showed 2 new wave vectors at low temperatures [1]. We have studied the phase transition on the single crystalline sample of GdB_6, oriented along $< 111 >$ axis using the temperature dependence of electrical resistivity, heat capacity and susceptibility under an applied magnetic field. The temperature dependence of the electrical resistivity $\varrho(T)$ has shown 2 anomalies - a sharp drop at $T_N = 15$ K and a small maximum at $T_2 = 9$ K (when cooling down), as previously reported. However, the clear thermal hysteresis occurred at transition temperature T_2. When heating up the transition is shifted to $T_2 = 8.5$ K. Heat capacity $C(T)$ shows a sharp peak at T_N which was practically unaffected by an applied magnetic field up to 9 T. At the second transition temperature T_2 the heat capacity shows a small maximum which postion shows the thermal hysteresis behaviour. Moreover, this maximum is shifting its position to lower temperatures and vanishing with increasing magnetic field. Our measurements confirm the variety and complexity of magnetic phase diagram of GdB_6.

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P-4-18

3D Modeling of Nd-Fe-B Magnets for Magnetic Resonance Imaging Systems – Models and Reality

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A 3D modeling method of Nd-Fe-B magnets for Magnetic Resonance Imaging (MRI) Systems using FEMLAB computer program is reported. The magnetic field map produced by this method was compared with the measurements taken from the 0.09 T MRI magnet within a 15 cm Diameter Spherical Volume (DSV). The magnet was constructed for the Institute of Physics, Jagellonian University, Krakow as a part of the MRI system. Whereas the actual magnetic flux density varies less than a few percent from the calculations, the discrepancy between the actual and calculated field homogeneity within DSV is much higher. This discrepancy is mainly due to the technological errors and differences in the actual material parameters and these assumed in the model. Some of technological errors were introduced into the model. The model was then used to design a 0.2 T magnet with 30 cm DSV MRI system for Institute of Biodiagnostics of National Research Council Canada. At present the magnet, located at the Life Sciences Research Station in Calgary, is ready for final shimming with the target homogeneity of 30 ppm.

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P-4-19

ELECTRONIC STRUCTURE CALCULATIONS AND ELECTRICAL RESISTIVITY OF $Dy(Co_{1-x}M_x)_2$ (M=Ni, Cu)

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$R(Co_{1-x}M_x)_2$ (R=rare earth; M=transition metal) alloys exhibit interesting magnetic properties because of the differing nature of magnetism (localized and band) of their constituents. Results of measurements of the magnetic susceptibility, electrical resistivity of intermetallic compounds $Dy(Co_{1-x}M_x)_2$ (M=Ni, Cu) are presented. The dependence of the Curie temperature and lattice parameters versus concentration x of the M element are established. The effect of partial substitution of Co by M is reflected in a change of T_C, in the temperature dependence of electrical resistivity and in the magnetization as a function of externally applied magnetic field. The experimental results are compared with theoretical calculations based on the $ab-initio$ tight-binding linear muffin-tin orbitals method. The Ni and Cu impurities reduce magnetic moments on Co atoms from 1.21 μ_B/atom for the $DyCo_2$ compound to 1.17 and 1.07 μ_B/atomfor Ni and Cu impurities, respectively. The densities of states at the Fermi level are reduced about two times.

P-4-20

EFFECT OF PRESSURE AND MAGNETIC FIELD ON CONDUCTIVITY AND MAGNETORESISTANCE IN La-Ca MANGANITES WITH EXCESS MANGANESE

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The pressure, magnetic field and excess manganese effects on transport and magnetoresistance effect (MRE) have been studied in both the epitaxial films and bulk ceramics of manganites $(La_{0.7}Ca_{0.3})_{1-x}Mn_{1+x}O_{3-\delta}$ (x = 0 - 0.2). The pressure and magnetic field effects are shown to increase with increasing manganese content. Experimental data show that the pressure and magnetic field effects on temperatures of both metal-insulator transition (T_{MD}) and MRE peak (T_{MR}) are considerably stronger in the films than in ceramics. The hydrostatic pressure increases T_{MD} and T_{MR}. MRE for both types of samples was shown to be favored by the pressure and magnetic field in an opposite way. A direct correlation is established between T_{MD} and conductivity bandwidth as well as between MRE and concentration of charge carriers at applied pressure. The origin of pressure-magnetic field effects is analyzed in the frame of double exchange interaction and small polaron hopping and variable range hopping models.

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P-4-21

PECULIARITIES OF ACOUSTOELECTRON INTERACTION IN MANGANITES IN STRONG MAGNETIC FIELD

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Recently an anomalous (even in the wave vector of sound) acoustoelectric (AE) effect produced by surface acoustic waves (SAW) in manganite $La_{0.67}Ca_{0.33}MnO_3$ (LCMO) films was discovered. The anomalous effect was shown to coexist with the ordinary odd acoustoelectric effect. The anomalous AE effect appeared to result from strong modulation of the film conductivity produced by the SAW elastic deformations.

In the present paper we report on investigations of the influence of the magnetic field H on the magnitude of acoustoelectric current I_{AE} in LCMO films grown on piezoelectric $LiNbO_3$ substrate. We have found that the total AE current substantially increases with H applied parallel to the SAW wave vector, but this increase is limited to the anomalous component of I_{AE}, while the ordinary AE current is left essentially unchanged. The behavior of the ordinary AE component can be explained by the opposing effects of increased film conductivity and reduced SAW attenuation. With regard to the comportment of the anomalous component of AE current in magnetic field, we speculate that it is determined by magnetic field induced changes in the dependence of the film conductivity on pressure.

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P-4-22

ACOUSTOELECTRIC STUDIES OF MANGANITE FILMS

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We report on the observation and investigations of transversal and longitudinal acoustoelectric (AE) effects produced by surface acoustic wave (SAW) in a layered structure composed of manganite $La_{0.67}Ca_{0.33}MnO_3$ (LCMO) film and piezoelectric $LiNbO_3$ (LNO) substrate. The investigated LCMO films were pressed with a gap of 0.5 μm to the LNO substrate where the acoustic wave is generated. In such a structure the AE effect arises only due to the penetration of the electric field accompanying the SAW into manganite film and its interaction with free charge carriers which results in a dc acoustoelectric voltage. Our investigations have shown that both transversal and longitudinal AE voltage display nonmonotonic temperature dependencies and approach their maximum values in the vicinity of metal-insulator transition in LCMO. The sign of the AE voltage corresponds to the hole-like conductivity in the films. The transversal effect was revealed to be even with respect to the SAW wave vector. The longitudinal AE effect was shown to be odd in the wave vector. Experimental results on the investigation of AE effects as a function of the conductivity of manganite films, intensity of sound, and SAW pulse duration are presented. The data obtained are discussed in the frame of the theory of acoustoelectric effect in layered structures.

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O-5-01

GIANT MAGNETOCALORIC EFFECT IN $Mn_{1-x}T_xAs$

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The MnAs ferromagnet belongs to intermetallic compounds with the largest magnetocaloric effect (MCE), which is governed by strong first order magnetostructural transition from hexagonal (NiAs type) to orthorhombic (MnP type) structures. We have studied the MCE amplitude in $Mn_{1-x}T_xAs$ (T = V, Cr, Fe, Co with x=0.01) series of compounds. Magnetisation measurements in d.c. magnetic field were carried out (B = 10 T, T = 4.2-400 K) and magnetic field induced phase transitions were investigated. Based on the isothermal M_T(H) magnetisation curves, the entropy change ΔS was deduced. In order to elucidate the MCE mechanism electronic structure of $Mn_{1-x}T_xAs$ was calculated by KKR-CPA method. It was found that all T atoms diluted in MnAs possess magnetic moments which are coupled either ferromagnetically i.e. V (1.3 μ_B), Cr (2.6 μ_B) and Fe (2.3 μ_B) or antiferromagnetically Co (-1 μ_B) with respect to Mn (3.03 μ_B). The magnetic entropy change is discussed in view of total energy KKR-CPA results. We conclude that all samples should be classified as giant magneto-caloric effect compounds, since the magnetic entropy change was found as 2-3 times higher than in pure MnAs (e.g. for T= Cr, $\Delta S \approx 25$ J/kgK).

P-5-01

PHASE DIAGRAMS AND MULTICRITICAL POINTS IN THE TERNARY MIXED-SPIN ALLOY WITH A SINGLE-ION ANISOTROPY

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The phase diagram of the AB_pC_{1-p} ternary alloy consisting of different Ising spins S^A=3/2, S^B=2, and S^C=5/2 in the presence of a single-ion anisotropy is investigated by the use of a mean-field theory based on the Bogoliubov inequality for the Gibbs free energy. The structure and spin values correspond to the Prussian blue analog of the type $(Fe_p^{II}Mn_{1-p}^{II})_{1.5}[Cr^{III}(CN)_6].zH_2O$ [1] and the couplings between the A and X ($X = B$ or C) ions include both ferromagnetic ($J_{AB} > 0$) and antiferromagnetic ($J_{AC} < 0$) interactions. Depending on the values of the parameters in the model Hamiltonian, the phase diagram exhibits a quite rich structure, with several multicritical points such as tricritical point, critical end point and isolated critical point. The calculated phase diagrams are conveniently controlled in the limit $T \to 0$ K where, for the ground state, the exact results have been obtained.

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P-5-02

PECULIARITIES OF MAGNETIC HYSTERESES IN THE MAGNETOELECTRIC $LiCoPO_4$

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Recently, it has been found an ultra-weak ferromagnetism in antiferromagnetic $LiCoPO_4$ single crystals. Origin of this effect remains unexplained until now. The features of hysteretic behavior of magnetic and magnetooptical properties of such crystal are presented here. Studies of the magnetic linear birefringence have shown the hysteretic behavior of a global character. Magnetization processes have revealed the shifted rectangular hysteresis loops. The shift direction depends on a thermo-magnetic history of the sample. According to our opinion this shift is not trivial. The observable behavior of the loops indicates on a non-uniform spin ordering in $LiCoPO_4$. Most likely, a magnetic structure of this antiferromagnet is the incommensurate modulated one and is represented by alternated stripes of antiferromagnetic and weak-ferromagnetic character. The shift of the magnetic hysteresis loop could be explained in this case by the exchange bias, the value of which is defined by: an exchange interaction between AFM and WFM layers, a stiffness of the spin wall formed between them, a value of spontaneous magnetization and by a or volume of WFM stripes. The expected parameters of or proposed modulated structures are discussed.

P-5-03

ELECTRONIC PHASE TRANSITIONS IN THE TWO DIMENSIONAL SPIN-ONE-HALF FALICOV-KIMBALL MODEL

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The extrapolation of finite cluster calculations is used to study the ground-state properties of the spin-one-half Falicov-Kimball model in two dimensions. Particular attention is paid on the description of the ground state phase diagram and the corresponding picture of valence and metal-insulator transitions. A number of remarkable results are found. (i) The phase separation in the spin-one-half Falicov-Kimball model takes place for a wide range of f-electron concentrations n_f and d-f interactions U, including U large. (ii) For weak and intermediate interactions ($U = 1$ and $U = 2$) the model exhibits an inhomogeneous charge ordering (the axial charge stripes). (iii) In the strong coupling limit the model exhibits a pressure induced discontinuous insulator-metal transition from an integer-valence state ($n_f = 1$) into another integer-valence state ($n_f = 0$). (iv) For small and intermediate values of U the model undergoes a few consecutive discontinuous and continuous intermediate-valence transitions.

P-5-04

GROUND-STATE PROPERTIES OF THE THREE-DIMENSIONAL FALICOV-KIMBALL MODEL

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The ground-state properties of the three-dimensional spinless Falicov-Kimball model are studied by a well-controlled numerical method. The results obtained are used to categorize the ground-state configurations according to common features for weak, intermediate and strong interactions. It is shown that only a few configuration types form the basic structure of the phase diagram. In particular, the largest regions of stability correspond to phase segregated configurations, striped configurations and configurations in which electrons are distributed in diagonal planes with incomplete chessboard structure. Near half-filling, mixtures of two phases with complete and incomplete chessboard structure are determined. In addition, the picture of valence and metal-insulator transitions is presented. The relevance of these results for a description of real material is discussed.

P-5-06

The study of Heisenberg magnetic systems using Creutz cellular automaton

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There is a lot of methods devoted to the simulation of thermodynamical properties of magnetic systems. Most of them use the temperature as an input value. In the beginning of eightieth Creutz proposed the model in which temperature is the output value and the spin change possibility is connected to some additional entity responsible for energy accumulation. In the nineties such a model has been successfully used to reproduce the critical properties of Ising model for wide range of dimensionalities. In spite of some limitations concerning the temperature scale in the region of phase transition the results were characterized by very good accuracy.
In this work we present the attempt to study the Heisenberg magnetic model using the approach based on the Creutz cellular automaton. The change of possible spin values spectrum from discrete one to continuous required the different meaning of some basic simulational operations like spin flip or temperature calculation procedure. As a result there are presented the critical properties of Heisenberg model obtained using presented model. The discussion of as well some technical as physical features concerning this way of simulation is included.

P-5-07

THE STUDY OF STRUCTURAL TRANSITIONS IN LIQUID CRYSTAL DROPLETS DOPPED BY MAGNETIC PARTICLES.

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Ferronematics are colloidal suspensions of fine magnetic particles in nematic liquid crystals. Their response to external magnetic field sufficiently exceeds that of pure nematics, what encourages investigators in the study of their properties and of the possibilities of their application. The presence of magnetic admixture shifts, compared with pure nematics, the threshold fields of structural transitions invoked by external magnetic or electric fields. The investigation of the changes of these threshold fields is useful for the estimation of the type of anchoring of nematic molecules on magnetic particles surfaces in studied ferronematic. In our present work we study the structural transitions and estimate the type of anchoring and anchoring energy value in MBBA-based ferronematic and in ferronematic droplets, formed in solutions of nematogenic 6CHBT with fine magnetic particles dissolved in phenyl isocyanate. The size of the prepared ferronematic droplets,which are magnetically active, can be easily controlled by the change of temperature and of the molar fraction of dissolved liquid crystal. The magneto-dielectric measurements of various structural transitions in this new system enabled us to estimate the type of anchoring and to find the anchoring energy of nematic molecules on magnetic particles surfaces in droplets.

P-5-08

THE DC AND AC INSULTING PROPERTIES OF MAGNETIC FLUIDS BASED ON TRANSFORMER OIL.

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Insulating and thermal properties of insulating media limited lowest sizes and largest currents in transformers. Large current densities may leads in sites with high strength field to form bridge between sites with large potential difference. The bridge consists with clusters of particles of fluid. Magnetic fluids (MFs) based on transformer oils with fine magnetite particles of nanometer scale improve thermal behaviors and in some cases insulating behaviors of transformer oils too. The improvement of the insulating properties is connected with sufficiently diluted MFs with low particle volume concentration bellow 1 what is very surprised phenomenon. In our previous work we have studied DC insulating properties and we found that critical concentration for crossover from worse to better insulating properties has the value of volume concentration as to be 0.25%. In this contribution we will present the results concerning to AC insulating properties in magnetic fluids based on transformer oil ITO 100. The results confirmed improvement of AC insulating properties our magnetic fluid in comparison with pure transformer oil too.

P-5-09

The transfer-matrix study of the critical properties of the Ising model following from the MFRG.

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Using a transfer matrix technique [1] and the Ising model, the predictions of the MFRG concept [2] for clusters with linear size up to 18 have been tested for the three-cluster MFRG approach [3], which corrected the deficiency of the earlier approach. Even for small sizes of the clusters the three-cluster estimates of critical couplings give the accuracy level equal to that of two-cluster renormalization for much greater sizes. Performing the asymptotic analysis, the convergence of the finite-size critical couplings and the critical exponents towards the exact values is illustrated. Our improved method has enabled us to obtain the results for clusters with substantially greater sizes, to accelerate the calculations and also to confirm the reliability of the MFRG method for the Ising model.

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[2] J.O. Indekeu, A. Maritan, A. Stella, Phys. Rev. B**35**, 305 (1987)
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P-5-10

Interplay between diagonal and off-diagonal disorder in a hard-core boson system: A mean-field approach

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We study the interplay between diagonal and site-dependent Mattis-type off-diagonal disorder in a hard-core boson system within the mean-field approach. The ground state phase diagrams are presented. We analyze effects of various types of diagonal disorder. We have found differences with respect to the previously reported results. We comment on the possible existence of the bose glass phase in this system.

P-5-11

MULTIPHASE STRUCTURE OF FINITE-TEMPERATURE PHASE DIAGRAM OF BLUME-CAPEL MODEL. WANG-LANDAU SAMPLING METHOD.

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We investigate the density of states (DOS) in antiferromagnetic spin-system on a square lattice described by Blume-Capel (BC) model. We use new, very efficient simulation method, proposed by Wang and Landau [1], in which we estimating very precisely DOS by sampling in the space of energy. Then we calculate the thermodynamical averages like the internal energy, the free energy, the specific heat and the entropy.
The BC model exhibits multicritical behaviour such as first- or second-order transitions and tricritical points. It is known that in the ground state of the BC model we observe two kinds of staggered antiferromagnetic phases: AF_1 (two interpenetrating lattices with $S = -1$ and $S = 1$) or AF_2 ($S = -1$ and $S = 0$ for $H < 0$; $S = 1$ and $S = 0$ for $H > 0$). We analyze the coexistence of such phases in finite temperatures and determine border lines between them. To understanding the microscopic nature of such boundaries we present also some results using standard Monte Carlo method.

[1] F. Wang and D.P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).

P-5-12

MULTI-STEP RADIAL MELTING IN SMALL TWO-DIMENSIONAL CLASSICAL CLUSTERS.

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We report a molecular dynamics study of small classical two-dimensional clusters with ring-like configurations [1-3]. We present a detailed investigation of the particles motion of small clusters as a function of temperature before any jumps between shells occur and thus before the radial melting sets in. Our results were compared with the previous ones, done with the use of Monte Carlo simulation method [1]. In this work we found that the melting process of two-dimensional classical cluster is much richer than presented till now. It is shown that in magic number configurations a local radial melting of sub-shells occur, which is related to the intershell rotation.

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P-5-13

HIGH-FIELD MAGNETIZATION OF SINGLE-CRYSTAL $LiCoPO_4$

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The results of the differential magnetic susceptibility measurements of the single-crystal $LiCoPO_4$ in a pulse magnetic field up to 270 kOe are reported. This crystal is a magnetoelectric antiferromagnet with the Neel temperature T_N = 21.8 K. According to neutron-diffracted data, the magnetic structure of $LiCoPO_4$ is collinear, and its properties at low temperatures can be described by the Ising model. But some magnetic and magnetoelectric properties of this antiferromagnetic crystal have anomalies, which are unexplained till now. Thus, in $LiCoPO_4$ recently has been found out an ultra-weak ferromagnetism, origin of which remains uncertain. Moreover, the properties of the magneto-optical hysteretic specify an opportunity of a weak incommensurable magnetic structure.

The pulsed-field measurements were carried out in two temperature intervals: 1.6 - 4.2 K (in liquid helium) and 14 - 20.8 K (in liquid hydrogen). The magnetic field strength was directed along the antiferromagnetic ordering axis **H**||**b**. At helium temperatures, the magnetic phase transformations at 122 kOe and 210 kOe were observed. The complex structure of peaks of the magnetic differential susceptibility at these transformations had been revealed. These complications specify that transitions to saturated paramagnetic state in LiCoPO4 are more complex, than in the Ising antiferromagnetic model with two competitive interactions between the nearest and next nearest neighbors.

P-5-14

On the possibility of nonuniversal behavior in 3D Ashkin-Teller model

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The Monte Carlo simulations in 3D Ashkin-Teller model on a cubic lattice are performed. The study is undertaken in the region where the universality class of the phase transitions has not been unambigously resolved yet [1, 2]. Using the finite-size scaling relation between the magnetization, the temperature and the size of the system, the method of calculation of the critical exponent y_h is proposed. The results obtained for y_h suggest such a nonuniversal behavior, because its value seems to change continuously in some interval approaching the Ising value near the tricritical points, similarly as it was observed in the 2D case [1].

P-5-15

A Monte Carlo study of the Falicov-Kimball model in the perturbative regime: preliminary results

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Finite-temperature properties of the Falicov-Kimball model on the square lattice have been studied in the perturbative regime, i.e. in the case: $t/U \ll 1$, where t is the hopping constant and U denotes the Coulomb interaction strength. For such a range of t and U parameters, it is possible to develop perturbation theory in the parameter t/U. As a result, the Ising-like model emerges. In the second order of the perturbation theory it is the antiferromagnetic Ising model in the magnetic field, whereas in the fourth order it constitutes the Ising model with more complicated frustrated antiferromagnetic interactions. The main observables examined were order parameters and their temperature (T) dependences for different values of the magnetic field (h). In our study, we have determined the phase diagram of the model in the second-order of the perturbation theory and partially in the fourth-order. We have employed the Monte Carlo method, that proved its accuracy in analysis of other spin models like Ashkin-Teller model, which we have recently investigated. To determine the type of ordering and phase boundaries, we have analysed the behavior of Binder cumulants based on the order parameters under consideration.

P-5-16

CRITICAL SOUND ATTENUATION IN MnF_2

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We analyse the critical sound attenuation in the antiferromagnet MnF_2 above its Neel temperature. A general formula for the acoustic self-energy, derived in the model in which a sound mode is coupled to both the order-parameter fluctuations as well as to the energy mode, is applied to interpret the experimental data in MnF_2. It has been shown that very interesting competition between three asymptotic singularities is responsible for the behaviour of the sound attenuation coefficient in the high-temperature phase. The relative strength of these terms depends also on the ultrasonic frequency. For high frequency also a background attenuation starts playing an important role.

P-5-17

EFFECTIVE SOUND ATTENUATION EXPONENTS IN MAGNETS

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In this paper we try to explain how some magnets belonging to the Heisenberg universality class can be characterised by positive sound attenuation exponents near the critical point. In magnets which are also insulators the sound attenuation exponent should be equal to 2α [1,2] where α is the usual specific-heat exponent. This exponent is however negative in the Heisenberg universality class. In this paper we interpret the positive attenuation exponents measured in isotropic magnets as $RbMnF_3$, $Y_3Fe_5O_{12}$ and $Gd_3Fe_5O_{12}$ in terms of the effective critical exponents. The large value of sound attenuation exponent in anisotropic FeF_2 can also be interpreted in this way.

[1] Kawasaki K., *Phys. Lett. A* **29**, 406 (1968)
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P-5-18

STRUCTURE, THERMAL STABILITY AND MAGNETIC PROPERTIES OF $Fe_{80-x}Co_xP_{14}B_6$ METALLIC GLASSES

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Structure, thermal stability, and magnetic properties of $Fe_{80-x}Co_xP_{14}B_6$ ($20 \leq x \leq 40$) metallic glasses have been studied by means of X-ray diffraction (XRD), vibrating-sample magnetometry (VSM), non-isothermal differential scanning calorimetry (DSC) and thermomagnetic (TMG) measurements. All studied FeCo-based glasses crystallize into eutectic mixture of α-Fe and bc-tetragonal Fe_3P-like phases at temperatures in the range 730-745 K. Structural (sizes of the coherently scattered domains), thermal (the glass transition and crystallization temperatures, the heats and apparent activation energies of transformation) and magnetic (the saturation magnetization and the Curie temperatures) characteristics of the amorphous alloys have non-monotonic compositional dependencies. From the DSC and TMG data it follows that crystallization of the Co-rich glasses occurs at temperatures below its Curie points. The as-quenched amorphous $Fe_{80-x}Co_xP_{14}B_6$ alloys have improved magnetic properties and essentially enhanced thermal stability of the structure in comparison with the commercial $Fe_{80-x}Ni_xP_{14}B_6$ (MG2826) glasses.

O-6-01

ON THE SYMMETRY OF A PREISACH MAP

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After the FORC diagrams were introduced as a tool to characterize hysteretic samples, it quickly turned out, that they are not the same as the Preisach maps. The source of confusion are two observations:

- the Preisach maps have mirror symmetry with respect to the axis $H_{\mathrm{up}} = -H_{\mathrm{down}}$ while FORC diagrams are often asymmetric, and
- the FORC diagrams' amplitudes are sometimes negative, beyond any experimental uncertainties, while the amplitudes on the Preisach maps are expected to be non-negative, since they are the probability density amplitudes.

A simple and convincing example is presented, showing that the mirror symmetry of the Preisach map is in reality an exception rather than the rule. This paper is a first step towards the unification of both, FORC and Preisach, models of hysteresis. After this is done, the framework of a reworked/reinterpreted Preisach model should gain the capacity to accurately describe, in a unique way, the exchange biased static hysteresis loops, as well as those exhibiting unusual effect of negative remanence. Such a generalized model of hysteresis should be equally applicable to other classes of materials, like superconductors, (multi)layered structures, nanocrystalline materials, patterned media, etc.

O-6-02

MAGNETIC PROPERTIES OF CORRELATED ELECTRONS

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We analyze a system composed of itinerant electrons and localized magnetic moments with on-site interactions representing Coulomb repulsion, Hund's first rule and the external magnetic field. Properties of the system are studied rigorously but in a configurational space restricted to low-period phases only. Using exact expressions for the ground state energy an evolution of the phase diagram with the magnetic field is determined and a series of metamagnetic phase transitions is detected. Field-dependent characteristics of magnetically ordered phases, such as magnetization and susceptibility, are calculated and compared to those experimentally observed in mixed valence materials.

O-6-03

SPECIFIC HEAT AND MAGNETIZATION FOR THE SEMIMETALLIC Yb_4As_3

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The $S = 1/2$ antiferromagnetic Heisenberg model with the transverse staggered field and uniform magnetic field perpendicular to the staggered field is applied to a semimetallic compound Yb_4As_3. The field - dependent specific heat for infinite and finite chains as well as the magnetization for infinite chains are calculated by the numerical quantum transfer-matrix method. Specific heat data for polydomain samples Yb_4As_3 and $(Yb_{0.99}Lu_{0.01})_4As_3$ at $B = 12$T are presented and compared with numerical results obtained for microscopic parameters taken from theoretical predictions. Magnetization experimental data for a single domain and polydomain sample Yb_4As_3 are also compared with our simulation results.

P-6-01

TWO-FERMION DYNAMIC SUSCEPTIBILITIES OF SPIN-1/2 XX CHAINS

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One-dimensional quantum spin-1/2 models are known to undergo a spin-Peierls transition (see, for example, Refs. [1,2]). In our study we consider the spin-1/2 XX chains to examine rigorously a relation between the spin-Peierls dimerization and the dynamic properties of the model. For this purpose we calculate the dynamic susceptibilities

$$\chi_{AB}(\kappa,\omega) = \sum_n \exp\left(\mathrm{i}\kappa n\right) \int_0^\infty \mathrm{d}t \exp\left(\mathrm{i}\left(\omega + \mathrm{i}\epsilon\right) t\right) \frac{1}{\mathrm{i}} \left\langle [A_j(t), B_{j+n}] \right\rangle , \quad \epsilon \to +0$$

with the local spin operators $\{A_m, B_m\} = \{s_m^z, D_m\}$ where s_m^z is the transverse spin operator and $D_m = s_m^x s_{m+1}^x + s_m^y s_{m+1}^y$ is the dimer operator. These dynamic quantities for the considered models can be calculated analytically employing the Jordan-Wigner transformation. All of them are determined entirely by two-fermion excitations and can be analyzed in detail. The obtained results for the special case which corresponds the a free fermion point should be valuable as a guide for attacking the general case of spin-1/2 XXZ chains.

[1] P. Pincus, Solid State Commun. **9,** 1971 (1971).

[2] M. C. Cross and D. S. Fisher, Phys. Rev. B **19,** 402 (1979).

P-6-02

EXTENSION OF THE METHOD OF LINEAR EQUATIONS BY NONZERO TEMPERATURES ON THE EXAMPLE OF ONE-DIMENSIONAL ISING MODELS

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The method of linear equations has been applied to nonzero temperatures. Two models have been considered. The first is the disordered model of random ferromagnetic and antiferromagnetic integrals whose transition matrix meets the condition of invariance of the sum of terms in each line. Although the other model (one-dimensional Ising model in an external field) is devoid of disorder it does not require any assumptions on the form of the transition matrix.

P-6-03

RKKY INTERACTION IN THE PRESENCE OF AN EXTERNAL MAGNETIC FIELD

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The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction has been extended for the case when the external magnetic field is taken into account. It has been shown that the RKKY hamiltonian should contain the Zeeman-like term in which the effective giromagnetic factor, g^{eff}, occurs. This g^{eff} factor contains, in addition to the usual giromagnetic factor connected with the localized spins, g_S, the correction term, which is linearly dependent on the contact potential, A, of the localized spin with the conduction electrons. The origin of this additional correction has been explained by the polarizing effect exerted by the external magnetic field on the electronic gas. Depending on the strength and sign of the contact potential A, the g^{eff} factor can be increased or decreased with respect to g_S, which gives a possibility for experimental study of the sign of the contact potential with the help of external field. As we know, in the conventional RKKY exchange interaction without the field, the information about the sign of the contact potential is hidden due to the quadratic relationship, $J^{\mathrm{RKKY}} \propto A^2$, and hence this sign remains unknown. The numerical estimations indicate that the correction term in g^{eff} can be recognizable in some materials, for instance for Co embeded in Cu.

P-6-04

PHASE TRANSITIONS AND COMPENSATION TEMPERATURE IN THE MIXED SPIN-1/2 AND SPIN-1 ANISOTROPIC HEISENBERG FERRIMAGNET

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The effects of the single-ion anisotropy and the anisotropy exchange parameter on the phase transitions in the mixed spin-1/2 and spin-1 anisotropic Heisenberg ferrimagnet have been investigated by the use of an Oguchi pair approximation. Although the theory is developed for lattices with general coordination number z, the numerical calculation has been made for the system in the simple cubic ($z = 6$) and body-centered cubic ($z = 8$) lattices. In particular, we have found that the anisotropic exchange interaction has a remarkable influence on the phase diagram at low temperature. A possibility of the existence of a compensation temperature in the system at which the resultant magnetization vanishes below its transition temperature is also discussed.
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P-6-05

DYNAMICS OF SPIN-$\frac{1}{2}$ XY CHAIN WITH SYMMETRIC AND ANTISYMMETRIC ANISOTROPIES

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The quantum spin-$\frac{1}{2}$ XY chain can be mapped onto the noninteracting spinless fermions and as a result its thermodynamic and dynamic spin correlation functions can be examined rigorously. We consider the model with the (antisymmetric) Dzyaloshinskii-Moriya interaction which is present in many low-dimensional magnetic compounds. In the case of anisotropic XY chain this interaction cannot be eliminated by a unitary transformation in contrast to the case of isotropic XY chain and therefore some peculiarities in the dynamic properties may be expected. We study the effects of the Dzyaloshinskii-Moriya interaction on the two-fermion excitations which entirely determine the zz-dynamic structure factor. Moreover, we obtain the closed-form expression for the zz-dynamic structure factor analytically. We also study the xx- and yy-dynamic structure factors numerically for chains of up to 400 spins and analyze the changes caused by the Dzyaloshinskii-Moriya interaction. We compare and contrast different dynamic structure factors. We discuss how the Dzyaloshinskii-Moriya interaction manifests itself in scattering and resonance experiments.

P-6-06

MAGNONIC CRYSTAL THEORY OF THE SPIN-WAVE FREQUENCY GAP IN LOW-DOPED $La_{1-x}Ca_xMnO_3$ MANGANITES

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This study is devoted to an investigation of the spin wave spectrum in 3D periodic macrostructure composed of two ferromagnetic materials: spherical ferromagnetic grains disposed in the nodes of a bcc crystal lattice are embedded in a matrix with different ferromagnetic properties. Frequency ranges forbidden to spin wave propagation are found to exist in the calculated magnonic spectrum, with both the position and the width of the gaps depending on the magnetic (exchange and magnetization) contrasts in the composite material, as well as on its structural parameters (filling fraction). This theoretical study refers to the recent finding of a spin-wave gap in low-doped $La_{1-x}Ca_xMnO_3$ manganites (in neutron scattering experiments [1]); this experimental study contained a suggestion that the magnetic ground state in the studied samples could be inhomogeneous, with ferromagnetic droplets embedded in a canted antiferromagnetic matrix. Therefore, we model the respective manganite sample as a magnonic crystal, in which droplets are disposed in a *regular* bcc lattice; the respective magnetic contrast values are estimated on the basis of the available experimental data. A very reasonable estimation of the droplets mean size and spacing is obtained by fitting the magnonic frequency gap resulting from our theoretical study to that found experimentally.
[1] P. Kober-Lehouelleur *et al.*, Phys. Rev. B **70**, 144409 (2004).

P-6-07

SIMULATIONS OF THE THERMODYNAMIC PROPERTIES OF A DODECANUCLEAR NICKEL RING

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The numerical exact diagonalization technique exploiting the point-group symmetry is worked out for the anisotropic Heisenberg spin Hamiltonian with the ring geometry. It is applied to the supramolecule $Ni_{12}(O_2CMe)_{12}(chp)_{12}(H_2O)_6(THF)_6$, in large-scale simulations, yielding the low-level energy spectra as a function of the single-ion anisotropy D and the thermodynamic functions. The constant D is analysed and estimated at $D/k_B = 1.5$ K. The results for the zero-field susceptibility and the field-dependent magnetization are presented and compared with experimental data.

P-6-08

Generalized theoretical approach to quasi-one-dimensional molecular magnets

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Two quasi-one-dimensional compounds $[Ln^{III}(terpy)(DMF)_4][W^V(CN)_8]\cdot 6H_2O$, where Ln stands for Gd or Sm, were synthesized and the measurements of their magnetic features were carried out. Magnetization was measured at 2 K in the field range 0–5 T. To extract physical information from the experimental data a generalization of the theoretical approach given by Verdaguer *et al.* [Phys. Rev. B 29, 5144 (1984)] is put forward. That theoretical model is found to fit the data well. It allows for the determination not only of the coupling constant but also of the zero-field splitting parameter.

P-6-09

ORBITAL POLARIZATION IN DOPED MANGANITES

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Using finite-temperature diagonalization we investigate the optical conductivity, the resistivity and the spin-orbital dynamics in the colossal magnetoresistance (CMR) regime of manganites. Our study is based on an orbital degenerate Kondo lattice model including orbital polarization effects due to Coulomb interaction and the coupling of carriers to breathing phonons. The characteristic activated behavior of resisitivity in the paramagnetic phase, and its dramatic decrease in the ferromagnetic phase, follows in a natural way as a combined effect of orbital polaron formation and spin disorder. The activated behavior of resistivity is reflected by the evolution of a pseudogap in the optical conductivity. At low temperature the spin dynamics is characterized by ferromagnetic spin waves with strong damping induced by temporal fluctuation of exchange interactions due to the orbital dynamics.

Although currently phase separation scenarios seem to dominate the CMR literature, we argue here in favour of an intrinsic explanation of CMR. To our knowledge our study is the first numerical simulation of the dynamics and thermodynamics of a realistic model for manganites, i.e., including spin-, orbital-, charge-, and to some extent also the lattice degrees of freedom.

P-6-10

COLLECTIVE SPIN FLUCTUATIONS IN NONCOLLINEAR FERROMAGNET

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In Mn based III-V and II-VI diluted magnetic semiconductors the impurity spins,in a ferromagnetic phase, are noncollinear [1,2]. They constitute the noncollinear ferromagnet (NF). In NF the problem of coexistance of a noncollinear spin's alignment with an effective ferromagnetic long range order arises. Because of the spin's noncollinearity NF is not invariant with respect to the local rotations about an axis directed along a spontaneous moment, unlike in a ferromagnet. The change of the ground state symmetry of NF, compare to a ferromagnet, results in essential changes in NF dynamics and requires new methods of descriptions. The relevant 'order parameter' for NF is a rotation matrix that describes a rotation of spin space.
We propose a phenomenological description of NF, which respects a symmetry of that phase. A dynamically induced magnetic moment, anisotropies(nonuniform also) and an external magnetic field as well as dissipative processes are included in the presented description. We shall derive a phenomenological Hamiltonian of NF. The dissipative processes are described by a dissipative function. The spin dynamics of NF is studied by means of equations of motion in Liouville's form. The well defined three branches of spin waves(ferrimagnetic like) are found. The dynamical susceptibility and correlation functions of magnetic moment components are evaluated.
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P-6-11

CRYSTAL FIELD STATES IN CONDUCTING MAGNETIC MATERIALS: $NdAl_2$, UPd_2Al_3 and $YbRh_2Si_2$

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There is still a hot debate on the formation and a role of localized crystal-field states in conducting magnetic materials. By years we have pointed out that in metallic compounds localized crystal-field states coexist with conduction electrons. The former are predominantly responsible for magnetic and low-energy spectroscopic properties, the latter for the conduction. In our atomic-start approach to 3d-/4f-/5f-atom containing compounds, being somehow a continuation of Van Vleck's studies, we take into account crystal field and spin-orbit interactions as well as very strong electron correlations. These electron correlations, predominantly of the intra-atomic origin, involving local orbital moment form physical conditions for realization of an anisotropic spin liquid ground state, that, however, in case of atomic-like configuration with an odd number of electrons, is unstable with respect to spin fluctuations for T–>0 K. We take the experimental observation of localized states of UPd_2Al_3 (Prof. Steglich's group in 1996) and recently of a localized Electron-Spin-Resonance signal in $YbRh_2Si_2$ as nice confirmation of our crystal-field-based approach not only to conventional conducting magnetic materials but also to those exhibiting anomalous low-temperature properties, known as heavy-fermion behavior. Influence of CEF states on the magnetism of $NdAl_2$, UPd_2Al_3 and $YbRh_2Si_2$ will be discussed.

P-6-12

THE GROUND STATE OF QUANTUM SPIN HALF HEISENBERG ANTIFERROMAGNETS

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The ground state properties of the spin half Heisenberg antiferromagnets (HAFM) on the 11 two-dimensional uniform Archimedean lattices have been investigated. These lattices are the prototypes of 2D arrangements of spins and vary in their geometrical and topological properties. Ground states of HAFMs on bipartite and frustrated lattices have been found in a short-range Resonating Valence Bond (SRRVB) basis to answer the question whether such states and low-temperature physics in such systems may be properly described in this basis. The SRRVB states have two important properties: they are not linearly independent and not orthogonal. The SRRVB basis is also overcomplete. The numerical calculations have been made for clusters up to 42 sites with boundary periodic conditions. Exact diagonalization method (LAPACK) has been used.

P-6-13

DYNAMIC PROBES OF QUANTUM SPIN CHAINS: MULTI-FERMION EXCITATION CONTINUA

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We calculate analytically the dynamic dimer and trimer structure factors of the one-dimensional spin-1/2 XX model in a transverse magnetic field at any temperature. In the framework of the Jordan-Wigner approach the accessible spectrum of the dimer (trimer) fluctuation operator is limited to two-fermion (two- and four-fermion) excitations. We examine some features of the four-fermion excitation continuum and compare them with the well known properties of the two-fermion continuum. Finally, we discuss the experimental relevance of the calculated structure factors. Our calculations extend the list of exact results for dynamic properties of quantum spin chains.
Further details can be found in Ref. 1.
This study was performed within the framework of the STCU project #1673.

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P-6-14

The quantum spin-1/2 Heisenberg antiferromagnet on a triangular lattice with some bonds removed in a translationally invariant manner - ground state and lowest excitations.

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This work is aimed at demonstrating the ground state and lowest-excitation states properties of the quantum spin-1/2 Heisenberg antiferromagnet on a 2D triangular lattice with some bonds removed in a translationally invariant manner which results in 2 non-equivalent types of sites with 4 or 6 nearest neighbours (n.n). The calculations were performed using an exact diagonalization (ED) approach in the complete RVB and non-complete short-range RVB (SRRVB) basis. The main question was whether the reduced basis leads to reasonable ground state and low temperature properties. Mean singlet length is slightly above 1 and almost insensitive with respect to the size of the system, which indicates that the ground state can in principle be described properly by SRRVB. The ground state energy was calculated both in the SRRVB and in the RVB basis. For 16-spin system the former is -7,598058 (-0,474879 per spin) and the latter -7,654240 (-0,478390 per spin) (the SRRVB value is 99,3% of the exact value). For 32-spin system the values are -15,031844 (-0,469745 per spin) and ...[IN CALC.], respectively. To give an answer whether the lowest excitations of the system can be described properly in the n.n. basis, specific heat was calculated, which showed that the lower part of the excitation spectrum seems to be well described in the SRRVB basis.

P-6-15

EQUATION OF MOTION FOR SPIN IN ELECTROMAGNETIC FIELD

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The equation of motion for spin $\boldsymbol{s}$ in continuum in absence of the electromagnetic field has been considered. In the present paper the equation for $\boldsymbol{s}$ in presence of the electromagnetic field is derived on the basis of the conservation law of the total angular momentum (orbital and spin) of the continuum and electromagnetic field .This equation has the form

$$\rho \dot{s} + \mathbf{R}_{n,n} = \mathbf{N}^P + \mathbf{N}^D + \mathbf{N}^A + \mathbf{N}^G,$$

where ρ is the continuum mass density, $\mathbf{R}_n$ is the surface torque, $\mathbf{N}^P=\mathbf{e}_i e_{irk} P_{nk}$ is the volume torque due to nonsymmetrical stress tensor $\mathbf{P}_n$, e_{irk} is the unit antisymmetric tensor, $\mathbf{e}_i$ is the base vector, $\mathbf{N}^D=[\mathbf{PE}]+[\mathbf{MB}]$ is the electromagnetic torque, $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic fields, $\mathbf{P}$ and $\mathbf{M}$ are the polarization and magnetization, $\mathbf{N}^A=c^{-1}[\mathbf{J}^{eff}\mathbf{A}]$ is the torque due to vector potential $\mathbf{A}$, $\mathbf{J}^{eff}=\mathbf{J}+\mathbf{P}_{,t}+c\mathrm{rot}\mathbf{M}$ is the effective current, $\mathbf{N}^G=\mathbf{N}^L+\mathbf{N}^{AD}$ is the torque existing without Lorenz gauge, $\mathbf{N}^L=z^A\mathbf{B}-c^{-1}[\mathbf{J}^A\mathbf{E}]$ and $\mathbf{N}^{AD}=(4\pi)^{-1}A_n\nabla B_n$ are the torques in a form similar to Lorenz force and electromagnetodipole force, $z^A=\mathrm{div}\mathbf{A}/4\pi$, $\mathbf{J}^A=(c/4\pi)\nabla\varphi$, φ is the scalar potential. The parameters z^A and $\mathbf{J}^A$ are related by the equation of continuity $z^A{}_{,t}+J^A{}_{n,n}=-c(z-P_{n,n})$, where z is the electric charge. Therefore J^A is the flux of z^A.

P-6-16

BIPARTITE AND TRIPARTITE ENTANGLEMENT IN 2D SPIN-$\frac{1}{2}$ HEISENBERG ANTIFERROMAGNETS

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Quantum entanglement was lately investigated mainly in the context of quantum information processing. Recently, however, the quantum entangled quantum states are being recognized to play an important role in many quantum phenomena (BCS, Hall effect, quantum phase transitions) and were used in the description of many-body strongly correlated systems. Here, we consider bipartite and tripartite entanglement present in the ground state ($S = 0$) of Heisenberg spin-half antiferromagnets attached to some 2D Archimedean lattices. Additionally we discuss a relation of the von Neumann entropy (which is a measure of entanglement) to the ground state degeneracy.

P-6-17

Quasi-one-dimensional S=1/2 magnet Pb[Cu(SO_4)$(OH)_2$]: frustration due to competing inchain exchange

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Zero-field susceptibility and specific heat of Pb[Cu(SO_4)$(OH)_2$] single crystal were studied. Magnetic measurements were performed using a commercial SQUID magnetometer in the temperature range 2-300 K and the temperature dependence of magnetic susceptibility were found along the symmetry axes. Heat capacity measurements were carried out for $T < 20$ K, using the adiabatic heat pulse method, showing a sharp anomaly at $T = 2.8$ K. In order to verify that linarite is a quasi-one-dimensional system with competing nearest-neighbour and next-nearest-neighbour inchain exchange interaction, theoretical results based on electronic structure calculations within the LDA and a phenomenological analysis using the finite-temperature transfer-matrix method are presented. Depending on the value of the screened onsite repulsion $U \approx 3$ to 5 eV the possibility of a variety of ground states is discussed: ordinary commensurate Néel or spin-Peierls phases versus incommensurate spiral states with acute or obtuse pitch angles. We compare linearite with other related edge-shared cuprate chain materials.

O-7-01

Calculation of structural, electronic and magnetic properties of MnSi and $Co_2MnSi(001)$ thin films

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We investigate thin films of Mn intermetallic compounds using density-functional calculations and the FP-LAPW or APW+lo method, with the goal to identify materials systems of possible use as spin injectors on Si(001). We find that the surface electronic structure of the ferromagnetic half-metal Co_2MnSi is strongly affected by the type of surface termination. In particular, an ad-layer of Mn atoms preserves the half-metallic gap, whereas surface states occur for other terminations. From calculated surface energies for $Co_2MnSi(001)$ we conclude that terminations either by a layer of only Mn atoms, only Si atoms, or a mixture of both are thermodynamically stable, depending on chemical environment. Next, we investigate the properties of ultra-thin films (1-3 monolayers) on Si(001), focussing on MnSi and Co_2MnSi. From our total-energy calculations, we conclude that a novel, CsCl-like crystalline phase of MnSi should be producible as a metastable epitaxial structure on Si(001). Thin films with CsCl-like sandwich structure of alternating Mn and Si layers have sizeable magnetic moments of 1–2 μ_B at Mn, and show a layered magnetic ground state, with pronounced ferromagnetic coupling between the Mn spins within the layers, and weak interlayer coupling. For ultrathin Co_2MnSi films on Si(001), we find Mn magnetic moments of 2.7–3.5 μ_B, and strong ferromagnetic coupling both within the same layer and between layers.
Both for the MnSi and the Co_2MnSi films, our calculations predict values of 20% to 50% for the spin polarization at the Fermi level.

O-7-02

Cluster perturbation theory for transition metal oxides

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We propose a many-body method for band-structure calculations for strongly correlated electron systems and apply it to transition metal oxides with NiO as an example. The method may be viewed as an application of cluster perturbation theory to a realistic model of a transition metal oxide whereby the Coulomb interaction within the transition metal d-shells is treated by exact diagonalization and the hopping between different atoms (as described by an LCAO-parameterization of an LDA bandstructure) is treated by cluster perturbation theory. We find good agreement between the calculated single-particle spectrum and angle resolved photoemission experiments in NiO.

P-7-01

Competition of ferromagnetism and superconductivity in Sc_3InB_x

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Recent discovery of superconductivity in the intermetallic perovskite $MgCNi_3$ was a great surprise due to large Ni contents and this compound was rather expected to be near ferromagnetic critical point. We present results of electronic structure calculations with Full–Potential KKR-LDA method for similar perovskite material – Sc_3InB – which is very promising candidate for a new superconductor. Interestingly, this compound may be regarded as a boron–inserted cubic Sc_3In, which is a high–pressure allotropic form of the well-known hexagonal weak ferromagnet Sc_3In. KKR calculations showed that scandium atoms keep magnetic moment (of about 0.25 μ_B) in both phases of Sc_3In, while Sc_3InB exhibits non–magnetic state with large DOS in the vicinity of E_F. Estimation of the electron–phonon coupling constant λ from McMillan–Hopfield formulas and calculated phonon DOS gave $\lambda \sim 1$ for Sc_3InB. The effect of vacancy in Sc_3InB_{1-x} and In/B disorder in Sc_3(In-B) on critical parameters were also discussed in view of KKR–CPA method. All theoretical results supported possibility of the superconductivity onset in Sc_3InB. A sample was prepared by arc melting technique and preliminary experimental data were collected using AC susceptometer equipped with a parallel resistivity measurement. The transition temperature was established close to 4.5 K, with a very abrupt change in susceptibility and a correlated drop of the resistivity when cooling down.

P-7-02

STRUCTURAL, MAGNETIC AND HYPERFINE PROPERTIES OF B2–TYPE FeAl DOPED WITH TRANSITION METAL IMPURITIES

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The structural, electronic and magnetic properties of the transition metal (TM=Ti, V, Cr, Mn, Co, Ni, Cu, Zn) impurities in $Fe_{50}Al_{50}$ matrix with B2-type structure have been investigated applying the the super-cell approach and using the tight-binding linear muffin-tin orbital (TB-LMTO) method of electronic structure calculations. The location of the TM impurity at Fe and Al sites was tested. For each investigated composition $Fe_{44}TM_6Al_{50}$ and $Fe_{50}TM_6Al_{44}$ the volume optimization was performed and the formation energy was estimated. Both magnetically ordered and non magnetic solutions were analysed. Based on the calculated results the following conclusions can be drawn: a) In all investigated cases the magnetic solutions are stable against the non-magnetic one. b) The site preference established shows that the elements of the periodic table on the left of iron (Ti, V, Cr, Mn) prefer to occupy Al sublattice while the heavier atoms (Co, Ni, Cu, Zn) locate at the Fe sites. c) The site preference strictly correlates with the alignment of the impurity local moment. The local moment of the impurities located at the preferred site always show the antiferromagnetic alignment with respect to the bulk magnetization. d) The calculated (optimized) volume and the average ^{57}Fe isomer shift show the similar dependence on the impurity atomic number (Z). The calculated structural and electronic properties follow qualitatively the tendency observed experimentally for the TM impurities in FeAl host and the dilute Fe-TM alloys.

P-7-03

Density functional investigation of electronic structure, magnetic and structural properties of several Heusler alloys

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The lattice parameters,electronic structure, and magnetic moments of several Heusler alloys with cubic and tetragonal structures are studied by scalar relativistic full-potential local-orbital minimum basis band structure calculations. The influence of hydrostatic pressure on these properties is investigated. The calculation reveals that the cubic structure of one of the compounds is unstable at zero temperature, and the tetragonal structure has a lower energy. The predicted martensitic phase transformation from the higher temperature cubic phase to the lower temperature tetragonal phases can be understood as a band Jahn-Teller effect. The tetragonal distortions can lower the energy by splitting a peak of the density of states which is situated at the Fermi level in the cubic structure.

P-7-04

Spin and orbital magnetic moment on cobalt in Co/Ti multilayers: $ab-initio$ calculations

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The influence of local environment on the electronic and magnetic properties of Co-Ti multilayers is studied by ab-initio spin polarized tight binding LMTO [1] and FPLO [2] methods. In this work we present the electronic structure and the magnetic moments (spin and orbital) of Co calculated for the different structural models. Ab-initio calculations are performed for Co atom located on the surface of titanium. The band structure is also calculated for the chain of (3-5) cobalt atoms surrounded by the titanium layers.

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P-7-05

Influence of impurities on the electronic and magnetic properties of Fe_2TiSn

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The influence of Fe, Co and V on the magnetic and electronic properties of Fe_2TiSn Heusler type alloy was studied recently [1-2]. The transition elements strongly modified the electronic structure of Fe_2TiSn ,particularly near the Fermi level. In this work we present the electronic structure of $Fe_2Ti_{1-x}V_xSn$ and $Fe_{2-x}M_xTiSn$, where M=Ni and Co. The electronic structure, magnetic moments and the theoretical XPS spectra were calculated by SPR-KKR-CPA method [3]. The band structure of ordered Fe_2TiSn alloy was calculated by fully relativistic full potential FPLO [4-5] and full potential LMTO [6] methods.

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P-7-06

Influence of local atomic disorder on the electronic and magnetic properties of Ni_2MnGa Heusler alloy

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The electronic and magnetic properties of Ni_2MnGa Heusler alloy depend strongly on the atomic disorder in the fcc sublattices of $L2_1$ type structure and the tetragonal distortion. In this work we present the electronic structure of Ni_2MnGa obtained by ab-initio methods, SIESTA [1-2] and LMTO [3]. We study the influence of the atomic disorder on the shape of the density of states near the Fermi level as well the effect of the tetragonal distortion. Using the SIESTA code we have shown that the shape of the density of states depends on the form of the pseudopotentials and the parametrization of the exchange-correlation potentials.

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P-7-07

Magnetic properties and band structure of $Ni_2(Ti_xMn_{1-x})Sn$ Heusler type alloys

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We study the influence of Mn on the band structure and magnetic properties of $Ni_2Ti_xMn_{1-x}Sn$ Heusler type alloy. The calculations were performed by TB LMTO-ASA method [1] for the experimental [2] and the theoretical lattice parameter. The theoretical lattice parameters were obtained from the minimum of the total energy. The theoretical dependence of the magnetic moment on the concentration of Mn was similar to the experimental data [2]. We present also the total density of states convoluted with Lorentzians of half with 0.4 eV and multiplied by cross sections for bands with different l symmetry [3]

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P-7-08

Orbital moments in uranium compounds- *ab-intio* calculations

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The electronic structure and magnetic properties of the tetragonal $U_2T_2In_2$ (T=Ni,Rh,Pt) compounds were studied recently [1]. In this work we present the electronic structure and the magnetic moments (spin and orbital) of U_2Rh_2In and U_2Pt_2In compounds. The electronic structure and magnetic properties were calculated by the fully relativistic full potential local orbital minimum basic band structure scheme (FPLO-5 code) [2]. We used the Perdew-Wang [3] parametrization of the exchange-correlation potential.

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P-7-09

Band Structure of ternary antimonides YbPdSb compounds by ab-initio methods

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The physical properties of the ternary equiatomic antimonides YbPdSb and $YbPd_2Sb$ have been investigated in the recent years [1]. The structural analysis [1] has shown that YbPdSb has two type of structure: low temperature (LT) (MgAgAs type) F43m No.216) and high temperature (HT) (TiNiSi-type) Pnma No.62). In this work we present the electronic structure of YbPdSb. The ab-initio calculations are performed for two types of crystallographic structures. We applied fully relativistic full potential FPLO method [2]. The calculations the 4f states of Yb are treated as valence as well as semicore states. The band structure is also calculated by ASW method [3].

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P-7-10

ELECTRONIC SPECTRA AND MAGNETIC PROPERTIES OF $R\mathrm{B}_6$, $R\mathrm{B}_{12}$ AND $R\mathrm{B}_2\mathrm{C}_2$ BORIDES

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The electronic structures of $R\mathrm{B}_6$, $R\mathrm{B}_{12}$ and $R\mathrm{B}_2\mathrm{C}_2$ borides (where R is a rare-earth, alkaline-earth, or early transition metal atom) are studied *ab initio* by using the full-potential linear muffin-tin orbital method to shed light on the intriguing magnetic properties of these compounds. This includes the promising materials for spin electronics with reported high temperature ferromagnetism, namely, doped divalent hexaborides CaB_6, SrB_6, BaB_6, and the CaB_2C_2 compound, as well as Kondo semiconductors, SmB_6 and YbB_{12}. For CaB_6 and SrB_6 a semiconducting band structure has been obtained, in agreement with the recent experimental data, whereas a semimetallic ground state is expected for CaB_2C_2 and doped hexaborides. For CaB_2C_2 and the semimetallic $Ba_{1-x}La_xB_6$ alloys we have performed spin-polarized calculations in an external field to evaluate the induced spin and orbital magnetic moments. The calculations indicate a possibility of the field-induced weak ferromagnetic phase in CaB_2C_2 and the La doped hexaborides. The LSDA and GGA calculations for different spin configurations of YbB_{12} point to a predominantly antiferromagnetic coupling between Yb^{+3} ions. For SmB_6 and YbB_{12} our LSDA, GGA, and LSDA+U calculations have not revealed the hybridization gap for configurations with trivalent Sm^{+3} and Yb^{+3}.

P-7-11

Electronic Structure and Tunneling Magnetoresistance of M/GaAs/M (001) (M=Fe, Co and Ni) Junctions

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The electronic structure of M/GaAs/M (001) (M=Fe, Co and Ni) heterostructures have been studied by means of a first principle Green's function tecnique. The conductances and the tunneling magnetoresistance ratio (TMR), in the current perpendicular-to-the plane geommetry, were calculated by means of the transmission matrix formulation of the Kubo-Landauer formalism. For all systems, the M magnetic moments at the M/GaAs interfaces as well as the magnetic coupling between the magnetic slabs are sensitive at the value of the lattice constant. Thus, for calculated equilibrium lattice constant, The M magnetic moments decrease compared with the corresponding bulk value while for the experimental value of the lattice constant, they increase in the of iron systems and remain almost unchanged for the cobalt ones. The different magnetic behavior of M atoms corresponding to the two values of the lattice spacing is a consequence of the competition between two effects named the low coordination number and the hybridization between M and sp (GaAs) states at the interfaces. Small values of the TMR ratio are obtained for all systems. The TMR ratio depends on the termination of the GaAs spacer that may be related with the electronic structure at the M/GaAs interfaces.

P-7-12

ELECTRONIC STRUCTURE OF $URuGa_5$ AND $UIrGa_5$

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As a part of a systematic study of the uranium isomorphic ternaries $UTGa_5$ with transition metals results of calculations of the electronic structure for T = Ru and Ir are presented. The compounds crystallize in the $HoCoGa_5$-type structure, space group P4/mmm, and (except for T = Ni, Pd and Pt) are not magnetically ordered [1]. The electronic structure was calculated by the full-potential LMTO method [2]. General features of the calculated densities of states show similarities to the ones for $UCoGa_5$ [3].

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THE ELECTRONIC AND MAGNETIC PROPERTIES OF $Pr_3Co_{13}B_2$ AND $Pr_5Co_{19}B_6$ COMPOUNDS

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The $Pr_3Co_{13}B_2$ and $Pr_5Co_{19}B_6$ compounds were manufactured as promising systems suitable for fabrication of permanent magnets. They belong to the $R_{m+n}Co_{5m+3n}B_{2n}$ family with (m=2n, n=1), (m=2, n=3), and (m=3, n=2), respectively [1]. The band structure calculations are performed by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (TB-LMTO ASA) [2]. The calculated magnetic moments on Co atoms depend on their local environment and vary in the range of 0.22 to 1.70 $\mu_B/atom$. The calculated values of the total magnetic moments are equal to: 23.56 (20 [3]) and 29.62 (23.7[4]) $\mu_B/f.u.$ for $Pr_3Co_{13}B_2$ and $Pr_5Co_{19}B_6$ compounds, respectively, where the experimental values are given in the parenthesis. The main contributions to the total densities of electronic states at the Fermi level are provided by 3d electrons of the Co atoms.

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ELECTRONIC AND MAGNETIC PROPERTIES OF $UCoAs_2$ COMPOUND

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The $UCoAs_2$ compound crystallizes in the tetragonal $HfCuSi_2$ - type structure with space group $P4/nmm$ [1]. The compound orders ferromagnetically at $150K$ with spontaneous magnetic moment of about $1.8\mu_B$. The magnetic behaviour in $UCoAs_2$ exhibits a giant anisotropy in both ordered and paramagnetic region, which was interpreted as being caused predominantly by strong $f-d$ hybridization and pronounced crystal field effect [1]. In this paper we present results of $ab-initio$ band structure calculations based on the Full-Potential Local-Orbital Minimum-Basis Scheme (FPLO) [2].

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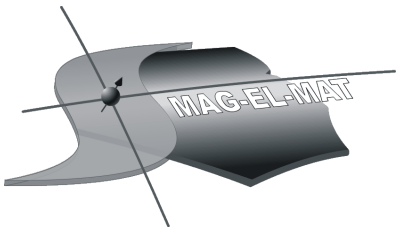

Scientific Network „New materials for magnetoelectronics - MAG-EL-MAT": subjects, tasks and the people

The recent progress and development of spin electronics has emphasised the need for the bringing together the leading domestic research groups operating in the similar scientific network for the exchange and dissemination of the latest accomplishments and achievements in the field in order to enable adequate and efficient scientific know-how exchange. The Scientific Network "New materials for magnetoelectronics - **MAG-EL-MAT**" established in the first months of 2003 received financial support from the State Committee for Scientific Research (KBN). The key objective of the Network is to focus on the theoretical and experimental search for modern magnetic materials and to provide explanation of some related physical phenomena.

The main tasks of MAG-EL-MAT include studies into the electronic and magnetic properties of a vast class of nanoscopic materials, such as thin films, multilayers, composites, molecular systems (including carbon nanotubes) and quantum dots. Particular attention is given to the magnetic phenomena in micro-junctions which contain ferromagnetic additions, or which are placed in a magnetic field. Among others, the studies cover GMR (giant magnetoresistance), TMR (tunnel magnetoresistance), spin accumulation, spin injection and current-induced switching of magnetization. The underlying physical mechanisms responsible for those phenomena are related to the electronic band structure of the components forming the microjunction, electron-electron interactions (Coulomb blockade, Kondo effect), and interactions of electrons with elementary excitations (*e.g.* spin waves, phonons *etc.*). The research activity is also oriented towards the magnetic and nanostructured materials for the applications in novel electronics. Efforts are being made towards the building of a scientific capacity of the Network, which is to serve as a potential research partner for the leading research groups.

Investigations are currently being carried out by 49 research groups (about 300 members), and are particularly focused on the use of the spin degree of freedom as well as the electric charge of the electrons. This is of great importance because of the cognitive purpose of the research as well as from the practical point of view as the conventional silicon-based electronics is now facing barriers of fundamental nature, which hinder further miniaturisation.

A wide range of topics in the following areas are in the current interests of the **MAG-EL-MAT** members:

(i) *Magnetic thin films and layered metallic structures.* The GMR is attractive owing to its application ability as a magnetic field sensor and a recording head. The present aim is to obtain layered structures exhibiting large GMR values accompanied by low magnetic saturation or switching fields. The issues include the influence of sublayer topology, morphology and thermal treatment on the amplitude and the field sensitivity of the GMR effect. One of the goals is the understanding of the magnetic behaviour and spin dependent electronic transport in thin films and multilayers which, being nanopattern elements, are capable of serving as magnetic sensors, M-RAMs (Magnetic Random Access Memory) and magnetic recording devices (*e.g.* heads, HDD-discs and magneooptical discs). Magnetic heterostructures show a relationship between the microstructure and the magnetic properties, including low-dimensional magnetic nanostructures. Hence, complex studies of artificial nanostructures such as magnetic heterostructures (granular films or layered granular structures), soft magnetic nanocrystalline multilayers, low-dimensional magnetic nanostructures (emphasizing the relationship between microstructure and magnetic properties) are being conduced.

(ii) *Surface effects in novel magnetic materials.* Keen interest is given to „photonic crystals". These are periodic structures composed of two types of transparent dielectric materials forming a „macrocrystal", with lattice constant ranging from 0.1 μm to 1 cm, showing a „photonic" energy gap, in which light propagation is forbidden. The promising prospects in this field allow taking up a theoretical research of systems analogue to the photonic structures, but composed of magnetic materials - the „magnonic crystals". They, too, can be expected to find applications.

(iii) *Magnetic nanostructures.* They involve electric and magnetic mesoscopic systems of peculiar geometry, e.g. carbon nanotubes, ring-shaped systems as well as single and coupled

quantum dots. Some of them have already found applications (flat displays, portable field-effect based Roentgen apparatus, current rectifiers, chemical and magnetic-field sensors, single electron transistor etc.). In particular, issues of the electron transport through nanostructures, depending on their internal structure, the type of electrodes used and the interface conditions, are being dealt with. In the case of ferromagnetic electrodes, special attention is put on the GMR and spin polarization of the electrical current. Other issues studied involve the response of the nanostructures to the external magnetic field, the proximity effects in nano-structure/superconductor systems, and the influence of the structural disorder, the spin-orbit interaction and the electron spin relaxation on the electron transport.

(iv) *Electron and hole transport in the doped transition metal oxides.* Recent experiments have shown a sharp drop of anisotropic magnetoresistance in calcium-doped yttrium-iron garnet thin films. An explanation is proposed concerning the spin dependent charge transfer in the yttrium-iron garnets doped with valence-uncompensated ions. The influence of the external magnetic field, both on the superexchange coupling between the spins attached to the orbital ground eigen-states of the iron-oxygen clusters as well as on the spin-conditioned charge transfer between those of a different and the same symmetry, are analyzed.

(v) *First principles computations.* Investigations of physical properties of solids are carried out by ab initio methods. In particular, the spin-polarized LMTO method is used to calculate the band structures, partial densities of states, spin and orbital magnetic moments, total energy, and the optical and magneto-optical properties. It is possible to find anisotropy of spin- and orbital-moments as well as the magnetocrystalline anisotropy. Extended advanced calculations of complex systems (up to 100 atoms per unit cell) with the use of supercell technique enable one to model the microstructure of the interface layers and of the short and long range chemical disorder of the alloys.

(vi) *Intermetallic compounds and 4f- and 5f- metal based alloys.* The current interest is the electronic structure and magnetic properties of strongly correlated electron systems which exhibit Kondo-lattice, heavy-fermions, non-Fermi liquid and unconventional superconductivity, as well as giant magnetocrystalline anisotropy *etc*. Currently, efforts are being made to find the mechanism behind these abnormal phenomena and the prospective applications of the compounds and alloys studied. For instance, thermoelectric materials can be used for power

generation or refrigeration using the direct conversion of heat and electricity. The determination of magnetic properties (including their magnetic structure) and the electronic structure of ternary rare-earth based compounds enables one to find correlations between the electronic and magnetic structures.

Several new activities and contacts established *via* the **MAG-EL-MAT** Network are already functional, ranging from bilateral contacts and preparations of joint research projects to larger scale programmes, conducted predominantly within the framework of the European scientific agencies.

Bogdan Idzikowski
Coordinator of **MAG-EL-MAT**