10th Prague Colloquium on f-electron Systems

Prague, 21st – 24th August 2012

Program & Abstracts

The10th Prague Colloquium on f-Electron Systems takes place with the contribution of material and human potential of the Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague.

PROGRAM

Tuesday, 21 August 2012				

10.00 – 18.00		*Registration*		

Session I Regular rare earths		Chairperson	L. Havela	Charles University in Prague
14.20 – 14:30		Welcome address	Vladimir Sechovsky	Charles University Prague
14:30 – 15:00	o01	Magnetic properties of RFe_5Al_7 (R – Gd, Dy, Ho) single crystals	Denis Gorbunov	Institute of Physics, Prague
15.00 – 15.30	o02	Ferrimagnetic R_2T_{17} single crystals in high magnetic fields	Yurii Skourski	Dresden High Magnetic Field Laboratory

15.30 – 16.00		*Coffee Break*		

Session II Yb compounds		*Chairperson*	A.P. Goncalves	Instituto Tecnológico e Nuclear Lisbon
16.00 – 16:30	o03	Pressure induced valence fluctuation and heavy fermion state in $YbCu_2Si_2$	Atsushi Miyake	Osaka University
16.30 – 17.00	o04	Valence ordering and its pressure effect in YbPd	Akihiro Mitsuda	Kyushu University
17.00 – 17.30	o05	Magnetism and super-heavy fermion state of YbT_2Zn_{20} under high pressure and magnetic field	Fuminori Honda	Osaka University

18:00 – 21.00		*Welcome party*		

Wednesday, 22 August 2012				

Session III Ce compounds		*Chaiperson*	*F. Honda*	Osaka University
9.00-9.30	o06	Inhomogeneous magnetic ground state in CeAgGa and CeCoGa	Andrzej Slebarski	University of Silesia
9.30-10.00	o07	High pressure phase diagram of the heavy-fermion compound $CeCoGe_{2.2}Si_{0.8}$	Julio Larrea	Vienna University of Technology
10.00-10.30	o08	Development of specific heat in the Ce(Ni,Pd)In series	Milan Klicpera	Charles University Prague

10:30 – 11.00		*Coffee break*		

Session III Ce compounds-cont.		*Chairperson*	A. Slebarski	*University of Silesia*
11.00 – 11:30	o09	Investigation of the new heavy fermion compound Ce_2PtIn_8 : single crystal study	Marie Kratochvilova	Charles University Prague
11:30 – 12.00	o10	Structure transitions in CeRuSn	Jan Fikacek	Charles University Prague
12:00 – 12.30	o11	$CePd_3$: a strongly correlated system for low temperature thermoelectric applications	Antonio Pereira Goncalves	Instituto Tecnológico e Nuclear Lisbon

12:30 – 14:30		*Lunch break*		

Session IV Actinides		Chairperson	*A. Lacerda*	Los Alamos National Laboratory
14:30 – 15:00	o12	Uranium-iron-germanium intermetallic compounds	Margarida Henriques	IST-ITN/CFMC-UL Lisbon
15:00 – 15:30	o13	The increase of the Curie temperature in UGa_2 under pressure	Alexandre Kolomiets	Lviv Polytechnic National University
15:30 – 16.00	o14	Orbital specificity in the unoccupied states of UO_2 from resonant inverse photoelectron spectroscopy	James Tobin	Lawrence Livermore National Laboratory

15:30 – 16.00		*Coffee break*		

Session IV Actinides-cont.		Chairperson	Nhu Tarnawska H Kim Ngan	Pedagogical University Krakow
16.00 – 16.30	o15	Hydrogen absorption in f-electron compounds of 221-type	Silvie Maskova	Charles University Prague
16.30 – 17.00	o16	$NpPt_2In_7$ and Np_2PdIn_8: new Np-based intermetallic compounds	Tomasz Klimczuk	ITU Karlsruhe
17.00 – 17.30	o17	Evolution of ferromagnetism and quantum criticality in $UCo_{1-x}(Fe,Ru)_xGe$ compounds	Michal Valiska	Charles University Prague

18:00 – 20.00		*Poster session and refreshment - **find the [List of Posters](#) in the end of the program***		

Thursday, 23 August 2012

Session V Thin films and actinides		Chairperson	J. Tobin	Lawrence Livermore National Laboratory
09:00 – 09:30	o18	The cubic gamma-phase in U-Mo alloys synthesized by splat-cooling	Nhu Tarnawska H Kim Ngan	Pedagogical University Krakow
09:30 – 10.00	o19	Superconductivity in the cubic gamma phase uranium molybdenum alloys synthesized by ultrafast cooling	Ilya Tkach	Charles University Prague
10:30 – 10.30	o20	Structure and magnetic properties of UO_2/Fe_3O_4 thin films	Evgeniya Tereshina	Institute of Physics, Prague

10:30 – 11.00		*Coffee break*		

11:00 – 11.30	o21	Thermodynamic constraints for magnetic systems approaching Quantum Criticality	Julian Sereni	CAB - CNEA, San Carlos de Bariloche
11. 30 – 12.00	o22	Synthesis of uranium sesquicarbide and rediscovery of its physical properties	Rachel Eloirdi	ITU Karlsruhe

12:00 – 14:00		*Lunch Break*		

Session VI Theory		**Chairpersons**	P. Oppeneer	Uppsala University
			A. Shick	Institute of Physics, Prague & ITU Karlsruhe
14.00 – 14.30	o23	The disordered-local-moment state in d- and f-electron itinerant magnets	Ilja Turek	Charles University Prague
14.30 – 15.00	o24	Antiferromagnetic ordering on frustrated fcc lattice in the intermetallic compound GdPtBi	Sergey Khmelevskyi	Technical University Vienna
15:00 – 15.30	o25	Electronic structure of compressed americium metal	Jindrich Kolorenc	Institute of Physics, Prague

15.30 – 16.00		*Coffee break*		

16.00 – 16.30	o26	Electronic structure theory of $PuCoGa_5$ and $PuCoIn_5$ unconventional superconductors	Alexander Shick	Institute of Physics, Prague & ITU Karlsruhe
16.30 – 17.00	o27	Strongly correlated 5f-electrons in actinides: Unusual ground states and electron spectroscopies	Gertrud Zwicknagl	Technical University Braunschweig
17.00 – 17.30	o28	Multipole state in 5d transition metal oxides	Hiroaki Onishi	Advanced Science Research Center, JAEA

17.30 – 22.00		*Grill party & wine tasting (depending on weather)*		

Friday, 24 August 2012

Session VII Theory		Chairperson	V. Janis (tbc)	Institute of Physics, Prague
09:00 – 09:30	o29	From magnetism to superconductivity: a unified approach to high Tc and heavy fermion systems	Jozef Spalek	Jagiellonian University, Cracow, Poland
09:30 – 10:00	o31	Unconventional superconductivity at the border with magnetic and Kondo insulating states	Olga Howczak	Jagiellonian University, Cracow, Poland

10:00 – 10.30		*Coffee break*		

10.30 – 11.00	o32	Magnetic field effect on the heavy-fermion state	Katsunori Kubo	Advanced Science Research Center, JAEA, Japan
11.00 – 11.30	o33	Aspects of the hidden order phase in URu_2Si_2: Remarkable nesting and spin-orbital hybridization	Peter Oppeneer	Uppsala University
11:30 – 12.00	o34	A novel phase transition in the underscreened Anderson lattice model: A candidate for the understanding of hidden order in URu_2Si_2	Peter Riseborough	*Temple University*

12:00 – 14:00		*Lunch Break*		

14:00 – 18.00		Non-structured discussion & *farewell party*		

List of Posters:

p01	^{119}Sn Mössbauer spectroscopy of 3d-, 4f-, and U-intermetallic compounds	Vasily Krylov
p02	Magnetic states of $UCuGe_{1-x}Sn_x$ compounds studied by ^{119}Sn Mössbauer spectroscopy	Vasily Krylov
p02	An investigation concerning the corrosion and recrystallization characteristics of laser beam welded gadolinium	Camilla Stitt
p03	An investigation concerning the corrosion and recrystallization characteristics of laser beam welded gadolinium	Camilla Stitt
p04	Effect of hydrogenation on structural properties of multilayered Ti-TiO_2 thin films	Zbigniew Tarnawski
p05	Effect of La doping on the thermoelectric properties of Kondo lattice compound $CeFe_2Al_{10}$	Yung Kang Kuo
p06	Experimental study of alloys close to $Co_{11}Zr_2$ stoichiometry and modeling of electronic and crystal structure	Tetiana Kosorukova
p07	Fermi surface and magnetic order in UPt_2Si_2	Zubeyir Cakir
p08	Heat capacity and electrical resistivity of hexagonal Ce-Ni-Ge system	Mariana Zapotokova
p09	High field hall measurements on UPt_2Si_2 at very low temperatures	Dirk Schulze Grachtrup
p10	Hydrogenation-mediated structure transformations in UPtSn	Khrystyna Miliyanchuk
p11	Magnetic, magnetocaloric and magnetoacoustic properties of $Er_2Fe_{14}B$	Irina Tereshina
p12	Magnetism study in $NdMn_{1-x}Fe_xO_3$ doped system.	Matus Mihalik
p13	Metamagnetic behavior in cubic heavy fermion compounds YbT_2Zn_{20} and UT_2Zn_{20} (T : transition metal)	Tetsuya Takeuchi
p14	Metamagnetic behavior of YbT_2Zn_{20} (T : Co, Rh, Ir) and UT_2Zn_{20} (T : Co, Ir)	Yusuke Hirose
p15	NMR study of the possible charge-density-wave transition in $Ce_3Co_4Sn_{13}$	Chin Shan Lue
p16	Properties of the two novel polar intermetallics $Yb_3Pd_2Sn_2$ and $Eu_3Pd_2Sn_2$	Marian Reifers
p17	Role of structural state of Gd in the formation of its magnetocaloric effect value	Galina Politova
p18	Specific heat of the $CeCu_4Mn_yAl_{1-y}$ compounds	Karol Synoradzki
p19	Structure transformation of $EuNi_5In$ under hydrogenation	Inna Bigun
p20	Uranium magnetic materials - is it possible?	Alexander Andreev
p21	Epitaxial growth and exchange bias in Th-diluted $U_{1-x}Th_xO_2/Fe_3O_4$ thin film bilayers	Zhaohui Bao
p22	Optical Spectroscopy on Heusler compounds	Jaroslav Hamrle
p23	Phonon spectrum, thermal expansion and heat capacity of UO_2 from first-principles	Dominik Legut

Orals

Magnetic properties of RFe_5Al_7 (R – Gd, Dy, Ho) single crystals

Denis I. Gorbunov[1,2], Alexander V. Andreev[1]

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RFe_5Al_7 (R – Sm-Lu, Y) intermetallics crystallizing in the tetragonal $ThMn_{12}$-type structure (space group $I4/mmm$) display peculiar magnetic properties. As found on polycrystalline samples, RFe_5Al_7 exhibit strong thermal and magnetic hysteresis. It is also suggested that RFe_5Al_7 display high magnetic anisotropy. Detailed studies of their magnetic properties require single crystals. In this work results of magnetic studies of RFe_5Al_7 single crystals with R = Gd, Dy and Ho are presented.

The $GdFe_5Al_7$ compound orders ferrimagnetically at the Curie temperature T_C = 262 K. The compound does not exhibit compensation point since in the whole temperature range up to T_C the Fe sublattice magnetization exceeds that of the Gd sublattice. $GdFe_5Al_7$ displays easy-plane anisotropy. Anisotropy is also found within the basal plane between the [100] and [110] axes, the in-plane anisotropy field is H_a = 2 T at 2 K. The easy-magnetization direction (EMD) is the [110] axis with the spontaneous magnetic moment M_s = 0.58 μ_B/f.u. at 2 K. The presence of the in-plane anisotropy is quite remarkable since contributions to the anisotropy from both magnetic sublattices should be rather low, especially in case of Gd. However, the rather high in-plane anisotropy field, H_a = K_{eff}/M_s (K_{eff} is an effective in-plane anisotropy constant) is provided by the near-compensation state at low temperatures, the low M_s value clearly corresponds to this situation.

The $DyFe_5Al_7$ and $HoFe_5Al_7$ compounds order at T_C = 231 and 220 K, respectively, and display high easy-plane anisotropy. Strong anisotropy is found in the basal plane as well, the EMD is along [100] in $DyFe_5Al_7$ and along [110] in $HoFe_5Al_7$. Upon approaching the compensation point, 93 K for $DyFe_5Al_7$ and 65 K for $HoFe_5Al_7$, from above and below, both compounds display field-induced magnetic transitions along the EMD. The temperature dependencies of the transition fields are very sharp. At low temperatures strong thermal and magnetic hysteresis is observed.

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Ferrimagnetic R_2T_{17} single crystals in high magnetic fields

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Rare-earth intermetallic compounds R_2Co_{17} and R_2Fe_{17} form an important group of magnetic materials and their properties have been extensively studied in the last decades. In these compounds, as generally in R-T transition-metal compounds, the strongest interaction is the $3d$-$3d$ interaction which primarily determines the Curie temperature. The $4f$-$3d$ interaction, although much weaker than the $3d$-$3d$ interaction, is of special importance since by this interaction the strongly anisotropic R-sublattice magnetization is coupled to the much less anisotropic T-sublattice magnetization. R_2Co_{17} and R_2Fe_{17} compounds in which R is a heavy rare-earth element are ferrimagnetic. The exchange interaction between the $4f$ and $3d$ electrons is usually represented by the molecular field by which the R- and T-sublattice moments are coupled. For Fe- or Co-rich R-T compounds, the values for the molecular field are typically of the order of 100 T, so that large magnetic fields are needed to induce changes in the magnetic configurations of the two magnetic sublattices in these compounds.

The R_2Co_{17} and R_2Fe_{17} compounds in which R is one of the heavy-rare-earth elements Gd, Tb, Dy, Ho, Er, or Tm crystallize in the hexagonal Th_2Ni_{17} type of structure. For the majority of these ferrimagnetic compounds (Er_2Fe_{17} and all R_2T_{17} compounds with R = Gd, Tb, Dy, Ho), the preferred moment direction is located in the basal plane. If a sufficiently large magnetic field is applied along one of the main crystallographic directions in the basal plane, field induced transitions will occur before the forced-ferromagnetic state is reached.

There is a small group of R_2T_{17} compounds consisting of only 3 representatives, i.e., Er_2Co_{17}, Tm_2Co_{17} and Tm_2Fe_{17}, in which the hexagonal c axis is the easy moment direction and only one transition can be expected before the forced ferromagnetic state is reached. The real behaviour of the easy-axis ferrimagnets is sometimes more peculiar.

In the present work we report on high-field (typically up to 60 T, in some cases up to 85 T) magnetization studies performed on single crystals of Ho_2Fe_{17}, Er_2Fe_{17}, Tb_2Fe_{17}, Er_2Co_{17}, Tm_2Co_{17} and Tm_2Fe_{17}. Magnetization of these compounds exhibits a set of field-induced transitions. We show that in many cases we can use high-field magnetization data for determining molecular field acting on R ion without any prior knowledge of crystal electric fields. As we need relevant magnetization data measured along high symmetry crystallographic directions, high quality single crystals are essential.

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Pressure Induced Valence Fluctuation and Heavy Fermion State in $YbCu_2Ge_2$

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Recently, the interplay of the valence instability and the novel electronic states in Yb-based compounds, such as very heavy electrons, non Fermi liquid and unconventional superconductivity, have been attracted much attention. $YbCu_2Si_2$ is well known as a typical valence fluctuating paramagnetic heavy fermion system with $Yb^{2.8+}$ configuration and a relatively large electronic specific heat coefficient g = 150 mJ/(K^2 mol). Pressure-induced ferromagnetic ordering has been confirmed above ~8 GPa. In contrast to $YbCu_2Si_2$, the isostructural compound $YbCu_2Ge_2$ having the ~10% larger unit cell than that of $YbCu_2Si_2$ seems to have nearly divalent configuration, e.g. typical metallic resistivity, small effective mass g = 10 mJ/(K^2 mol), and Pauli paramagnetic susceptibility. For Yb-compounds, pressure often changes Yb-valence to be more trivalent configuration, and thus magnetic ground state. Here, we have investigated the interplay of heavy electrons and valence fluctuation in $YbCu_2Ge_2$ with tuning the Yb-valence widely by the external pressure. The electrical resistivity (r) and the Yb L_2-edge XANES experiments have been performed under very high pressures up to 30 GPa. Temperature dependence of the resistivity r (T) shows a typical metallic behavior at low pressures, which is expected for the non-magnetic compound. With increasing pressure, the r is strongly enhanced, and a broad shoulder-like anomaly in the r (T) curve appears and becomes distinct, which is reminiscent of the valence fluctuating systems. The effective mass, which is deduced from the A value of the Fermi liquid relation r (T) = r_0 +AT^2, is strongly enhanced, indicating that $YbCu_2Ge_2$ changes to the heavy fermion system, i.e. the effective mass at 24 GPa roughly 40 times larger than that at 0.6 GPa. In addition, the strong enhancement of the residual resistivity is observed above 10 GPa, and correspondingly the mass also starts to increase drastically. With increasing pressure, the Yb-valence determined by the XANES experiments at room temperature increases strongly from ~2.4+ at ambient pressure to ~2.8+ at 10 GPa, and gradually on further pressure. The heavy fermion state is found to be correlated with a valence change. The present experimental results are compared with the results of $YbCu_2Si_2$ under pressure.

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Valence ordering and its pressure effect in YbPd

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The valence fluctuating compound YbPd, which crystallizes in the cubic CsCl type structure, exhibits four phase transitions at T_1=125K, T_2=105K, T_3=1.9K, and T_4=0.5K[1]. The one at T_3 is due to antiferromagnetic order, but the mechanisms of the other transitions remain unknown. ^{170}Yb Mossbauer effect spectra imply coexistence of magnetic and nonmagnetic Yb ions in the ratio of 1:1 at $T<T_3$[2]. This strongly suggests valence ordering of a magnetic Yb^{3+} ion and a nonmagnetic Yb^{2+} or valence fluctuating Yb ion, but there was no direct evidence of the valence ordering. Since most of systems showing valence (charge) ordering have poor electrical conductivity, the valence ordering of YbPd with metallic electrical conductivity is intriguing. We have speculated that the transitions at T_1 and/or T_2 should be associated with the valence ordering and examined X-ray diffraction and electron diffraction using a single crystal. These results indicates a structural phase transition from cubic symmetry to tetragonal or orthorhombic one at T_1 and superlattice reflections of (1/2 0 0) and (1/2 1/2 0) at $T<T_2$. The latter is possibly ascribed to the valence ordering. We have also investigated pressure effects on the transitions at T_1, T_2 and T_3. The application of external pressure suppresses T_1 and T_2 at a rate of dT_1/dp=-35K/GPa and dT_2/dp=-78K/GPa, respectively. After vanishment of T_1 and T_2 at around 3GPa, the antiferromagnetic transition at T_3 seems to disappear[3], which is novel behavior since applying pressure stabilizes magnetic ordering in most of Yb-based compounds. In YbPd, the valence ordering is destabilized and eliminated by pressure. In this stage, the high-temperature phase above T_1, which is characterized by the uniform valence fluctuating Yb ion, is stabilized down to zero temperature. Consequently, the antiferromagnetic ordering disappears.

[1] R. Pott et al., Phys. Rev. Lett. 54 (1985) 481. [2] P. Bonville et al., Phys. Rev. Lett. 57 (1986) 2733.

[3] M. Sugishima et al. J. Phys. Condens. Matter 22 (2010) 375601.

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Magnetism and Super-Heavy Fermion State of YbT_2Zn_{20} under High Pressure and Magnetic Field

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Novel electronic properties of heavy fermion compounds YbT_2Zn_{20} (T: Co. Rh. Ir) under high pressure and strong magnetic field, together with the electronic properties of a divalent ytterbium compound $YbCu_2Ge_2$, will be reviewed. YbT_2Zn_{20}, which crystalizes in a cubic $CeCr_2Zn_{20}$-type structure, is a heavy fermion compound, indicating the huge electronic specific heat coefficient $\gamma = 8$ J/(K$^2\cdot$mol) in $YbCo_2Zn_{20}$, for example[1]. YbT_2Zn_{20} shows the typical heavy fermion metamagnetism at $H_m \cong 6$, 65, and 100 kOe below the temperature $T_{\chi max} = 0.32$, 5.8, and 7.4 K, where the magnetic susceptibility shows a broad maximum, for $YbCo_2Zn_{20}$, $YbRh_2Zn_{20}$, and $YbIr_2Zn_{20}$, respectively [2]. With increasing pressure, H_m decreases and the A-value of the Fermi liquid relation in the electrical resistivity, $\rho = \rho_0 + AT^2$, is enhanced. At the critical pressure P_c, the A-value becomes extremely large, reaching about 400 $\mu\Omega\cdot$cm/K^2, which corresponds to the huge γ value of about 15 J/(K$^2\cdot$mol) [3]. The significant change of the electronic states in $YbCu_2Ge_2$ is also realized under high pressures.

[1] M. S. Torikachvili et al., Proc. Natl. Acad. Sci. 104, 9960 (2007).
[2] Y. Hirose et al., J. Phys.: Conf. Ser. 273, 012013 (2011).
[3] F. Honda et al., J. Phys. Soc. Jpn. 79, 083709 (2010).

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Inhomogeneous magnetic ground state in CeAgGa and CeCoGa

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Many of cerium heavy fermion compounds order antiferromagnetically, nonetheless, there is known a groupof ferromagnetic heavy fermions or Ce-based Kondo lattices where atomic disorder leads to existence of aspin-glass-like state. Since the coupling constant J between the 4f spins and the conduction spins as well asthe hybridization energy V and the f-f correlations (Coulomb energy U) determine the ground state propertiesand simultaneously the exchange integrals are strongly dependent on the Ce-Ce distance and local symmetryof Ce ion, we have started to investigate the physical properties of the ternary CeTX compounds, where Tis the transition metal and X is Sb, Sn, Ga, or Al. In this presentation we study CeCoGa (symmetry C2/m)and CeAgGa (symmetry Imma). Our magnetic measurements (susceptibility, magnetization, specific heat, andresistivity) suggest that the both compounds are magnetically ordered Kondo lattices, and show evidence forthe formation of a spin-glass state above the temperature of magnetic ordering. The randomness in the Ce-Cemagnetic exchange interactions seem to arise from a statistical distribution of T and X elements. Complex magnetic behavior of the Kondo-lattice CeAgGa with ferromagnetic order below Tc = 3.6 K and antiferromagneticCeCoGa (TN=4.3 K) is discussed in terms of interplaying RKKY interactions, Kondo effect, and structuraldisorder, we also examine the contribution of the symmetry on the ground state properties. We present x-rayphotoemission valence band spectra as well as ab-initio band structure spin-polarized calculations.

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High pressure phase diagram of the heavy-fermion compound CeCoGe$_{2.2}$Si$_{0.8}$

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The pressure-tuned quantum critical point (QCP) of the antiferromagnetic heavy-fermion compound CeCoGe$_{2.1}$Si$_{0.9}$ was claimed to be dominated by different effects on both sides of the QCP: on the magnetic side spin fluctuations govern the criticality, while on the non-magnetic side the criticality is dominated by disorder that quenches the spin fluctuations [1].

Here we study high-quality CeCoGe$_{2.2}$Si$_{0.8}$ samples [2], with residual resistance ratios four times larger than those of the previously investigated CeCoGe$_{2.1}$Si$_{0.9}$ samples. Interestingly, while DC magnetic susceptibility measurements show that the Néel temperature of T_N = 4K at zero pressure is only slightly reduced by pressure up to 3.0 kbar, a much stronger decrease is observed for the specific heat anomaly. We will present electrical resistivity and specific heat measurements up to 15 kbar and down to 0.05 K, and establish the pressure – temperature phase diagram for CeCoGe$_{2.2}$Si$_{0.8}$. The critical behavior shall be compared to the one observed for both CeCoGe$_{2.1}$Si$_{0.9}$ and the pure reference compound CeCoGe$_3$ [3]. We hope that this investigation will elucidate the role of disorder.

[1] Alzamora M., Fontes M. B., Larrea J., Borges H. A., Baggio-Saitovitch E. M., Medeiros S. N. Phys. Rev. B **76** 125106 (2007).

[2] J. Larrea J, J. Teyssier, H. Ronnow, M. Müller, S. Paschen. Accepted for publication in J. Phys: Conf. Ser.

[3] G. Knebel, D. Aoki, G. Lapertot, B. Salce, J. Flouquet, T. Kawai, H. Murunaka, R. Settai, Y. Onuki . J. Phys. Soc. Jpn. **78**, 074714 (2009).

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Development of the specific heat in the Ce(Ni,Pd)In series

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A large group of the intermetallic ternary *RTX* compounds, where *R* is rare-earth element, *T* transition d-metal and *X* p-metal, crystallizes in hexagonal ZrNiAl-type of structure. Most of these compounds order magnetically at low temperatures, often with complex magnetic structures, but there are also some compounds without magnetic transition down to very low temperatures. The presented study of the development of magnetic behavior in Ce(Ni,Pd)In series is based mainly on the specific heat measurement.

Both parent compounds were previously studied by some experimental techniques as specific heat, magnetic susceptibility or electrical resistivity. CeNiIn is a valence fluctuator without magnetic order at least down to 50 mK and with Kondo like behavior. On the other end of the series, CePdIn orders as heavy-fermion antiferromagnet around 1.8 K. Moreover, there is the significant anisotropy along the crystallographic axes. Most of properties of these compounds are significantly influenced by external and chemical pressure.

The change of the magnetic properties and also the values of the specific heat in this series are caused by isoelectronic substitution of Ni by Pd. The Pd atoms have not only different character of the d-electrons but also larger radius. As a consequence, the lattice parameters change considerably in Ce(Ni,Pd)In series. Both these changes, character of the d-electrons and lattice parameters, are responsible for the dramatic development of the magnetic properties reflected in our study in the specific heat data.

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Investigation of the new heavy fermion compound Ce_2PtIn_8 : single crystal study

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The $Ce_nT_mIn_{3n+2m}$ (n=1, 2; m=1; T=transition metal) type compounds are subject of intense interest in the condensed-matter community. By adding an additional $CeIn_3$-stacking layer in the tetragonal crystal structure the dimensionality changes from 3D to more 2D. While selecting the proper transition metal, the compound might either order antiferromagnetically or becomes superconducting. It has been shown, that the superconducting state is closely linked to the presence of a quantum critical point. Thence, the group of $Ce_nT_mIn_{3n+2m}$ compounds is predestined to investigate the interplay between magnetism and superconductivity.

Recently, two new compounds from the $Ce_nT_mIn_{3n+2m}$ heavy fermion family have been found. Ce_2PdIn_8 is an ambient pressure superconductor while $CePt_2In_7$ orders antiferromagnetically.

Here, we report on the existence of a new heavy fermion (γ~370 mJ/molCe.K^2) compound Ce_2PtIn_8. Similar to Ce_2PdIn_8, the synthesis of Ce_2PtIn_8 is rather complicated. However, from our recent studies of solution growth of Ce_2PdIn_8 supported by differential thermal analysis optimal conditions for growing Ce_2PtIn_8, single crystals could be deduced. Single crystal X-ray diffraction confirmed that Ce_2PtIn_8 crystallizes in Ho_2CoGa_8-type structure with lattice parameters a=4.699 Å and c=12.185 Å.

We will present specific heat, resistivity (ambient and under hydrostatic pressure) and magnetization measurements. Ce_2PtIn_8 orders magnetically at 2.1 K. An order-to-order transition is observed just below at 2 K. Contrary to Ce_2RhIn_8, the two transitions merge at magnetic field around 4 T and split again in higher magnetic fields pointing on a different character of magnetic ordering. The magnetic field-temperature phase diagram will be discussed in the context of superconductivity and magnetism evolution in related compounds.

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Structure transitions in CeRuSn

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Recently reported CeRuSn is a very rare example of intermediate valent system undergoing both structure and magnetic transitions at ambient pressure. The former is manifested by significant anomalies in electrical resistivity, magnetic susceptibility, thermal expansion and specific heat, which were measured in a wide temperature and pressure range. The evolution of crystal structure was also studied as a function of temperature by X-ray single crystal diffraction. Our investigation has revealed that by passing the transitions, the structure mostly varies along the c-direction where changes in Ce-Ru distances give rise to a different number of crystallographically independent cerium sites, a part of them being in an intermediate valent state. External hydrostatic pressure strongly influences critical temperatures pushing them to higher temperatures, reminding the behavior of pure cerium metal.

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CePd₃: a strongly correlated system for low temperature thermoelectric applications

CePd$_3$: a strongly correlated system for low temperature thermoelectric applications

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The performance of a material for thermoelectric applications can be evaluated by the dimensionless figure of merit, zT,, which depends only on the material properties and is given by $zT = \alpha^2\sigma T/\lambda$ (where α is the Seebeck coefficient, σ is the electrical conductivity, λ is the thermal conductivity and T is the absolute temperature). Therefore a good thermoelectric material should simultaneously possess i) high electrical conductivity, characteristic of metals, and ii) high Seebeck coefficient and bad thermal conductivity, characteristic of insulators.

Kondo systems can have a narrow band with high density of states near the Fermi level, formed by the so-called Abrikosov-Suhl resonance that arises from the interaction between the localized f or d states and the conduction electron states. This can induce very large values of the Seebeck coefficient, which surpass those of normal metals by 10-100 times.

CePd$_3$ is a Kondo system that has been classified as a typical intermediate valence material. It crystallizes in the simple face-centered cubic AuCu$_3$ structure-type, which has a large void at the center of the unit cell, and presents a small homogeneity range. CePd$_3$ shows one of the highest Seebeck coefficients among rare earth intermetallic compounds ($\alpha > 100\mu$V/K) and, consequently, was considered as a potential material for thermoelectric cooling applications. However, pronounced sensitivity of the electrical transport properties to small stoichiometry deviations and high thermal conductivities have been reported. Substitutions on CePd$_3$ were also extensively studied with the objective of increase the figure of merit, but with a very limited success. Here we report the detailed study of arc-melted and splat-cooled CePd$_{3-x}$ ($0.1 \leq x \leq 0.1$) materials by X-ray diffraction, Scanning Electron Microscopy, electrical resistivity and Seebeck coefficient measurements, together with thermal conductivity measurements on selected samples. A peculiar microstructure and an increase of the thermoelectric properties were observed in the splat-cooled materials, when compared with the arc-melting ones, indicating this technique as a good method for preparing high performance CePd$_3$.

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Uranium-iron-germanium intermetallic compounds

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Uranium intermetallic compounds containing Ge and a transition element have shown a wide variety of properties. One of the most puzzling ground-states is the coexistence of superconductivity and ferromagnetism reported first for UGe$_2$ (under pressure) [1] and URhGe [2] and later for UCoGe [3].

The experimental investigation of the isothermal section U-Fe-Ge at 900ºC brought into light nine new intermetallic compounds. Here we present a short review on the structure and physical for three new compounds: U$_9$Fe$_7$Ge$_{24}$, U$_2$Fe$_3$Ge and U$_3$Fe$_4$Ge$_4$. U$_9$Fe$_7$Ge$_{24}$ crystallizes in an original tetragonal structure and the magnetic and specific heat measurements down to 2 K do not show any magnetic transition [4]. The Curie-Weiss behaviour with a negative paramagnetic Curie temperature and reduced effective magnetic moment of indicate that the compound is rather far from onset of magnetism, presumably due to a strong hybridisation of the 5f and ligand states.

The compound U$_2$Fe$_3$Ge crystallizes in the hexagonal Mg$_2$Cu$_3$Si structure, an ordered variant of the hexagonal MgZn$_2$ Laves structure (C14). U$_2$Fe$_3$Ge orders ferromagnetically at Curie temperature T_C=55K. Specific heat, however, does not display any anomaly in the vicinity of T_C. Magnetization isotherms along the principal axes indicate that magnetic moments lie in the basal plane of the hexagonal lattice and no anisotropy within the basal plane was detected. In contrast to typical U-based intermetallics, U$_2$Fe$_3$Ge exhibits surprisingly low magnetocrystalline anisotropy (10 T). The dominance of U in the magnetism of U$_2$Fe$_3$Ge follows from the Mössbauer spectroscopy study suggesting very low or even zero Fe moments [5].

U$_3$Fe$_4$Ge$_4$ crystallizes in the orthorhombic Gd$_3$Cu$_4$Ge$_4$ isotype and it orders ferromagnetically below T_C = 20 K [6]. The transition can be seen in the resistivity and in the specific heat experiments. The magnetic moment is reduced and, according to Mössbauer spectroscopy results, it is dominated by uranium.

UFeGe is a compound crystallizing in the orthorhombic TiNiSi-type structure, but it undergoes a monoclinic distortion below $\approx$500 K [7], being a weak paramagnet. The stabilization of the orthorhombic phase was attempted via substitution into the U sublattice. Specific heat studies revealed that the orthorhombic material UFeGe has the γ-coefficient $\approx$30 mJ/mol K^2, i.e. about 3 times higher than the monoclinic phase ($\gamma \approx$12 mJ/mol K^2). Based on these results and magnetization studies, we can speculate that the tendency to remove high density of states from the Fermi level is the reason for the structure distortion.

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The increase of the Curie temperature in UGa_2 under pressure

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UGa_2 is a uranium intermetallic with unusually high ferromagnetic ordering temperature T_C = 126 K. Despite that its $5f$ states cannot be treated as either fully localized or as fully itinerant [1]. This is corroborated by the finite $5f$ -density at ε_F detected by the photoelectron photoemission [2], low electronic contribution to the specific heat, and the easy-axis saturation magnetization short of the free-ion value for uranium. Our previous magnetization measurements at pressures up to 0.7 GPa have revealed the anomalous increase of the Curie temperature in UGa_2 at the rate of +4 K/GPa. The present work is aimed at further investigation of this phenomenon. For that purpose the resistivity measurements have been performed on a single crystalline needle of UGa_2 in the I // [001] geometry in an anvil cell with the solid transmitting medium. The monotonous increase (+4K/GPa) of the Curie temperature was observed in the whole experimentally available pressure range, $i.e.$ up to 7 GPa, reaching almost T_C = 155 K. No signs of saturation have been observed on the $T_C(P)$ dependence. Considering the crystallographic surrounding of the uranium atoms, with d_{U-Ga} being by more than 1 Å shorter compared to d_{U-U}, and d_{U-U} well exceeding the Hill limit, we have concluded that the observed behaviour of UGa_2 should be the consequence of the strengthened f-ligand hybridization.

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ORBITAL SPECIFICITY IN THE UNOCCUPIED STATES OF UO2 FROM RESONANT INVERSE PHOTELECTRON SPECTROSCOPY

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One of the crucial questions of all actinide electronic structure determinations is the issue of 5f versus 6d character and the distribution of these components across the density of states. Here, a break-though experimentis discussed, which has allowed the direct determination of the U5f and U6d contributions to the unoccupieddensity of states (UDOS) in Uranium Dioxide. A novel Resonant Inverse Photoelectron (RIPES) and X-rayEmission Spectroscopy (XES) investigation of UO2 is presented. It is shown that the U5f and U6d componentsare isolated and identified unambiguously.
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Hydrogen absorption in f-electron compounds of 221-type

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The family of 221 compounds with the tetragonal Mo_2FeB_2 structure comprises both rare earth and actinides representatives. Here we compare behavior upon H doping of several examples on the basis of U and RE (e.g. Nd). The U_2T_2In and U_2T_2Sn compounds absorb up to 2 H atoms/f.u. In the case of RE_2T_2X, the compounds can absorb much higher amounts of hydrogen. In Nd_2Ni_2In, the H doping produces a sequence of hydrides $Nd_2Ni_2InH_2$, $Nd_2Ni_2InH_4$ and $Nd_2Ni_2InH_7$.

The impact of hydrogenation on magnetic properties of U- and RE-compounds is different. In the case of U_2T_2X, the volume expansion leads to a band narrowing. As a consequence, it leads to the strengthening of magnetic interactions due to hydrogenation. For RE-compounds, the exchange coupling is reduced presumably by reducing the concentration of conduction electrons.

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NpPt$_2$In$_7$ and Np$_2$PdIn$_8$: new Np-based intermetallic compounds.

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The neptunium analogues of the CePt$_2$In$_7$ and Ce$_2$PdIn$_8$ layered intermetallic compounds have been synthesized and characterized by means of resistivity, magnetic susceptibility and heat capacity techniques. Rietveld analysis of the powder x-ray diffraction patterns of NpPt$_2$In$_7$ and Np$_2$PdIn$_8$ confirm tetragonal structure type for both compounds, with lattice parameters similar to those previously reported for CePt$_2$In$_7$ and Ce$_2$PdIn$_8$, respectively.

For NpPt$_2$In$_7$ an antiferromagnetic transition was observed with the Néel temperature T_N = 23 K. Rather complex magnetism is revealed for Np$_2$PdIn$_8$ with ferromagnetic and possibly antiferromagnetic transitions at T_C = 9.5 K and T_N = 8.5 K, respectively. For both NpPt$_2$In$_7$ and Np$_2$PdIn$_8$ a Curie-Weiss fit of the high-temperature magnetic susceptibility curve, $\chi(T)$, gives an effective magnetic moment as expected for trivalent Np.

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Evolution of ferromagnetism and quantum criticality in UCo$_{1-x}$(Fe,Ru)$_x$Ge compounds

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UCoGe is one of few examples of coexistence of weak ferromagnetism (T_C ~ 3 K) and ambient pressure superconductivity (T_{SC} ~ 0.6 K). We have prepared a series of polycrystalline samples of UCo$_{1-x}$Ru$_x$Ge compounds for x ≤ 0.35 and UCo$_{1-x}$Fe$_x$Ge compounds for x ≤ 0.24 in order to study development of magnetism and superconductivity of this compound with Fe and Ru doping. The both series adopts the orthorhombic TiNiSi-type structure of the parent UCoGe compound. Evolution of the lattice parameters follows well the Vegard's law. All samples have been subjected to magnetization, ac susceptibility, heat capacity and electrical resistivity measurements in wide temperature and magnetic field intervals. The Fe doping increases the Curie temperature and reaches its maximal value T_C ≈ 10 K for x ≈ 0.08. Then the Curie temperature goes down and ferromagnetic order vanishes for x ≈ 0.22. The Ru doping leads to the sharp increase of the Curie temperature up to the T_C = 8.5 K for x = 0.12. Further increase of Ru content destabilized ferromagnetic state through a ferromagnetic quantum critical point (FM QCP) for x ≈ 0.3. No sign of superconductivity has been detected in the Fe or Ru doped samples. We have succeeded in the growth of the single crystal of the UCo$_{0.88}$Ru$_{0.12}$Ge (maximum T_C) where we have studied strong magnetocrystalline anisotropy and change of the absolute value of spontaneous magnetization. The behavior of the UCo$_{1-x}$Ru$_x$Ge system is discussed on the basis of concept of magnetism influenced by quantum criticality.

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The cubic γ-phase in U-Mo alloys synthesized by splat-cooling

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U-Mo alloys (with Mo concentration of 1–17 at.%) were prepared by splat cooling technique and characterized by X-ray diffraction (XRD) method for phase determination. The double-phase (α+γ) structure was obtained in the alloys with 0 – 10 at.% Mo, while those with minimum 11-12 at.% molybdenum show a stable γo-phase and those with ≥ 13 at.% molybdenum revealed 100% pure γ-phase at room temperature. The XRD analysis and EBSD mapping revealed that a small amount of the high-temperature γ phase was retained at room temperature in the splat-cooled pure uranium specimens, something which was hitherto considered impossible. The results obtained on U-Mo alloy with 15at.% Mo clearly indicated the presence of a γ-U phase structure with no evidence for α or α-related phases.

The superconducting transition was investigated for the as-formed samples by low-temperature resistivity and specific heat measurements down to 0.3 K in magnetic fields up to 5 T. All the splats become superconducting with Tc in the range from 1.24 K (pure U splat) to 2.11 K (U-15 at.% Mo) [1,2].

The phase transformation and/or stabilization of γ-uranium phase in U–Mo alloys upon aging, annealing at 500∘C and 800∘C for different time (1 h-144 h) and hydrogenation were described. For a comparison the phase characterization of pure U specimen with different annealing history were also presented. All phases formed in the splats are very stable in exposing to ambient conditions (no ageing). The γ-phase in U-Mo alloys undergoes eutectoid decomposition to form equilibrium phases of orthorhombic α-uranium and body centered tetragonal U$_2$Mo intermetallic compound (tetragonal γ'-phase) upon annealing at 500ºC, while annealing at 800ºC has stabilized the initial γ phase. Hydrogen absorption at room temperature was tested for pure-U splat and γ-phase U-15at.% Mo alloy. Unlike α-U which easily absorbs a large amount of hydrogen, the cubic *bcc* phase does not absorb any detectable amount of hydrogen at pressures below 1 bar and at room temperature. At high pressure, the U-15at.% Mo splat become powder consisted of elongated particles of 2-4 mm which revealed an amorphous state.

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Superconductivity in the cubic γ-phase uranium molybdenum alloys synthesized by ultrafast cooling

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Uranium can exist in three allotropic phases, namely α - (orthorhombic), β - (tetragonal) and γ - (body-centered cubic). The γ-uranium phase is thermodynamically stable in the temperature range 1048-1408 K. But we retain γ-phase to room temperature by doping 0-15 at.% of Mo and consequently fast cooling from the high-temperature solid solution using splat cooling technique with cooling rate of 10^6 K/sec. In this work we present the electrical resistivity, magnetic susceptibility and specific-heat data of the γ-phase U-Mo alloys. Special attention was given to low temperature properties where γ-phase exhibits transition to a superconducting state. Electrical resistivity in the normal state increases with increasing of Mo concentration, which can be attributed to an atomic disorder and/or disorder imposed by ultrafast cooling. The disorder also leads to progressive flattening of $\rho(T)$, resulting even into a negative slope (dρ/dT < 0) for alloys with $x \geq 11$ at.% Mo. Such behavior observed earlier in alloys with very strong scattering. Low-T resistivity exhibits superconductivity at all samples, from T_c=1.24 K (pure U splat) to 2.11 K (x = 0.15) with a quite sharp transition. We also observed the shift of T_c to lower temperatures in applied magnetic fields. The H_c dependence for the U-Mo alloys revealed neither a quadratic dependence as the temperature approaches 0 K expected for type-I superconductors, nor a linear dependence typically exhibited by strongly interacting Fermi liquid superconductors e.g. U_6Fe. We can conclude that we observe two different types of superconductivity, one type in α -U, not necessarily intrinsic, which has lower T_c and critical field. The other type, belonging to the *bcc* phase, has a higher T_c and much higher critical field. Specific heat measurements at low temperatures revealed for all samples discontinuites related to superconductivity transitions. With increase of applied magnetic field the height of peaks decreased and they shift to low temperatures. The most pronounced anomaly appears for 15% Mo. Its temperature coincides with T_c from electrical resistivity. The size of the step ΔC even exceeds the BCS prediction 1.43*$\gamma_e T_c$. 11% Mo exhibits clearly two broad anomalies, at 1.7 K and 1.0 K attributed to γ° and γ-phase. Only a weak and broad peak was observed for pure U splat sample around 0.7 K, indicates that here the superconductivity is inhomogeneous and probably not intrinsic. Magnetic susceptibility was measured in temperatures from 4 K to 300 K. It does not reveal any anomalies. A weak paramagnetic behavior was observed for all splat samples with values of magnetic susceptibility approximately 5*10^{-9} m^3/mol.

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Structure and magnetic properties of UO_2/Fe_3O_4 thin films

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Uranium compounds, where the magnetism is determined by the state of 5*f* electrons, are rather exotic and interesting research objects [1]. Uranium dioxide UO_2 is an antiferromagnet with Néel temperature T_N = 30.8 K [2]. It plays an important role in science and technology, and investigation of its magnetic properties in a low-dimensional state is an attractive task. The present work is conducted on antiferromagnetic/ferromagnetic UO_2/Fe_3O_4 heterostructures separated by Au spacer with various thicknesses of the layers. The samples are grown by reactive sputter deposition and characterized by X-Ray Photoelectron spectroscopy, HRXRD (High-Resolution X-ray Diffraction) and magnetic methods using a vibrating sample magnetometer and a SQUID magnetometer (Quantum Design). The exchange coupling mechanism is studied by measuring the temperature evolution of the hysteresis loops (crossing T_N of UO_2) under various cooling conditions. The magnetic properties of UO_2/Au/Fe_3O_4 are compared to those of the UO_2/Fe_3O_4 bilayers in order to clear up the effects of a non-magnetic spacer layer on the exchange coupling mechanism.

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Thermodynamic constraints for magnetic systems approaching Quantum Criticality

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Based on specific heat (C_m) and entropy results, three distinct types of phase diagrams are recognized [1]:
i) with the entropy of the ordered phase (S_{MO}) decreasing with the order temperature (T_{MO}), ii) those showing a transference of degrees of freedom from the ordered phase to a non-magnetic component, with their $C_m(T_{MO})$ jumps (ΔC_m) vanishing at finite temperature and iii) those ending at a Critical Point at T > 0 because their ΔC_m do not decrease sufficiently with T_{MO} producing a $S_{MO}(T)$ bottleneck at low temperature.

Only the systems belonging to i) ($S_{MO} \rightarrow 0$ as $T_{MO} \rightarrow 0$) can be regarded as candidates for QC behavior. In these systems their 2nd. order magnetic phase boundaries (MPB) deviate from the classical negative curvature below T ≈ 2:5 K, denouncing usual monotonous misleading extrapolations of $T \rightarrow 0$. A pre-critical region is identified where the characteristics of the MPB undergoes significant modifications like to become of 3rd order, in coincidence with the presence of a 1st order MPB centered a that critical region. The mentioned 3rd order transition is suppressed by magnetic field whereas the 1st order one is even weakly enhanced. An increasing remnant entropy up to 0.4 RLn2 is observed at $T \rightarrow 0$. The ii) group includes well known pressure induced superconductors (sc), showing that the MPB does not reach the sc dome, whereas the iii) group compares with the well known phase diagram of URu_2Si_2 under magnetic field.

Also related to the $T \rightarrow 0$ phenomenology is the upper limit of $\partial S_m / \partial T = \gamma$ in systems not showing magnetic order. In this case, the physical constraints arising from the third law can be recognized and discussed for Ce based compounds.

[1] J.G. Sereni; arXiv: cond-mat.1108.0197 and Phil. Mag. B (2012) accepted.

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Synthesis of uranium sesquicarbide and rediscovery of its physical properties

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Among the uranium carbides, three intermediate phases are reported and correspond to UC, UC_2 and U_2C_3. Relatively to the two formers compounds, U_2C_3 has been less studied and still many questions relative to its physical properties are pending[1,2]. Indeed while it is reported as an antiferromagnet below 60 K, neutron diffraction measurement failed to observe a magnetic moment in this phase [3,4]. Because of its presence in nuclear reactors, an investigation of the chemical bonding and physical properties is indispensable. U_2C_3 crystallizes in the cubic Pu_2C_3-prototype, space group I-43d (n°220) with lattice parameter a = 8.0901(2) Å. In this study we report the synthesis of U_2C_3, obtained as major phase with either UC or UC_2, following an adequate heat treatment of arc melted UC_x (1.5 < x < 1.9) ingots. Also we report the complete measurement of the U_2C_3 specific heat down to 2K, while previous data were reported only above 10K. The estimated Sommerfeld coefficient and Debye-Temperature are $\gamma(U_2C_3)$ = 40.7 mJ/mol (U)K^2 and $\Theta_\Delta(U_2C_3)$=256K, respectively. A possible anomaly mentioned 50 years ago [4] for U_2C_3 could be observed in this study at 3.3K.

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THE DISORDERED-LOCAL-MOMENT STATE IN D-AND F-ELECTRON ITINERANT MAGNETS

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The contribution is devoted to applicability of the so-called disordered-local-moment (DLM) state in an abinitio theory of metallic magnetic systems. Particular attention will be paid to magneto-volume phenomena(spontaneous volume magnetostriction) and to transport properties (spin-disorder resistivity). Existing resultsfor systems containing transition-metal and rare-earth elements will be reviewed and analyzed. First resultsobtained for actinide systems (UC, UN) within a fully relativistic treatment of the DLM state will also be presented and discussed.

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Antiferromagnetic ordering on frustated fcc lattice in the intermetallic compound GdPtBi

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The type of antiferromagnetic magnetic order in the half-Heusler intermetallic compound GdPtBi, where the Gd atoms form a magnetically frustrated fcc lattice, has been investigated using exchange constants calculated from first principles within the framework of the Green's function based magnetic force theorem. It is found that the degeneracy of the magnetic states on the fcc lattice with antiferromagnetic nearest neighbor interaction is removed by strong fourth-nearest neighbor interaction along the cube diagonal. We show that an antiferromagnetic ordering of so-called "third kind" occurs at low temperatures. The Monte Carlo simulations using our derived exchange constants predict an experimental Neel temperature (TN) with good accuracy. The estimated temperature dependence of the correlation functions in the paramagnetic region exhibit a typical behavior for frustrated system – a massive short range order is retained for temperatures which are one order of magnitude higher than TN. Thus it is appears that GdPtBi is a perfect material to study effects of magnetic frustrations in metallic systems.

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Electronic structure of compressed americium metal

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We report a theoretical investigation of changes of the electronic structure of americium metal due to lattice compression. We employ a variant of the LDA+DMFT method that incorporates strong correlations among the 5f electrons as well as a feedback of these correlations on the rest of the electrons by means of an appropriate adjustment of the electronic charge density [1]. We observe only relatively minor modifications of the electronic structure under pressure that appear to be in accord with the recently measured RXES spectra [2].

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Electronic structure theory of PuCoGa$_5$ and PuCoIn$_5$ unconventional superconductors

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PuCoGa$_5$, discovered in 2002, has the highest critical temperature of 18.5 K among heavy-fermion superconductors [1]. Spin and charge valence fluctuations may have an important role in mediation of the superconducting phase in PuCoGa$_5$, but the specific character of the coupling mechanism remains uncovered. Very recent point-contact spectroscopy experiments [2] unambiguously prove that the paired superconducting electrons have wavefunction with the *d*-wave symmetry. Moreover, the gap value and its temperature dependence can be well reproduced making use of the Eliashberg equations with the spin-fluctuations-like spectral function.

The electronic structure and the magnetic character of PuCoGa$_5$ are investigated making use of a combination the local density approximation (LDA) with an exact diagonalization (ED) of the Anderson impurity model. The band structure obtained by the relativistic version of the full-potential linearized augmented plane wave method (FP-LAPW) is consistently extended to account for the *f*-orbital atomic multiplets and their hybridization with the conduction bands. The results show an intermediate valence nature of the Pu *f*-shell that consists of a mixture of a magnetic f^5 sextet and a non-magnetic f^6 singlet, which is similar to the case of δ-Pu [3]. The Pu *f*-shell carries a non-vanishing average moment as it fluctuates between the singlet and the sextet. In the same time, the ground state of the entire impurity model is a singlet that corresponds to all angular momenta being equal to zero. Thus, the magnetic fluctuations in the *f*-shell are accompanied by canceling antiferromagnetic fluctuations in the conduction bands, resulting in temperature-independent magnetic susceptibility at low temperatures. The role of hybridization strength is investigated, and comparison between PuCoGa$_5$ and PuCoIn$_5$ is given. Our findings can be important for understanding the superconductivity in these materials.

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Strongly correlated 5f-electrons in actinides: Unusual ground states and electron spectroscopies

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Intermetallic compounds containing actinide ions exhibit a broad spectrum of different physical phenomena at low temperatures. The latter include heavy quasiparticles, unconventional superconductivity and various forms of magnetic ordering. We present results for calculated ground state properties of the tetragonal compound UPt$_2$Si$_2$. We compare the predicted variation with magnetic field of the Fermi surface derived from two different models for the 5f-electrons. Assuming a 5f^2 ground state seems inconsistent with the observed anomalies. The Dual Nature ansatz, on the other hand, predicts field-induced instabilities and points to the possible existence of a Lifshitz transition.The complex and sometimes enigmatic properties of these compounds derive from the strong correlations among the 5f electrons. Previous model calculations suggested that the intra-atomic Hund's rule-type correlations may lead to partial localization which is reflected e. g. in the co-existence of itinerant 5f-derived heavy quasiparticles and local magnetic excitations. The conjectured Dual Nature of 5f electrons which is closely related to the question of the 5f valence of the actinide ions affects the ground state and the low-energy excitations but it cannot be directly probed by them. Here we present microscopic calculations for core level spectroscopy in actinides emphasizing the consequences of strong intra-atomic correlations of the 5f shell.

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Multipole state in 5d transition metal oxides

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To clarify a crucial role of a spin-orbit coupling in the emergence of novel spin-orbital states in 5d-electron compounds such as Sr_2IrO_4, we investigate ground-state properties of a t_{2g}-orbital Hubbard model including the spin-orbit coupling by numerical techniques [1]. Note that due to the spin-orbit coupling, the t_{2g} level is split into a j_{eff}=1/2 doublet and a j_{eff}=3/2 quartet, where $j_{eff}=-l+s$ is an effective total angular momentum. Since the effective total angular momentum gives a good representation of the electron state, we envisage that the complicated spin-orbital state can be described from the viewpoint of multipole, in the same way as the multipole physics of f-electron systems.

Considering the low-spin state of Ir^{4+} ions, the number of electrons per site is set to be five, in which the lower j_{eff}=3/2 quartet is fully occupied, while the upper j_{eff}=1/2 doublet is half-filled. In the absence of the spin-orbit coupling, the ground state is a spin singlet. With increasing the strength of the spin-orbit coupling, the ground state turns into a singlet state in terms of the effective total angular momentum. We find the so-called complex orbital state, in which real *xy*, *yz*, and *zx* orbital states are mixed with complex number coefficients. Regarding the multipole state, we observe that the Γ_{4u} dipole and octupole correlations are enhanced in the spin-orbit-induced phase. We will also discuss the spin, orbital, and multipole states for other electron numbers.

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From magnetism to superconductivity: a unified approach to high Tc and heavy fermion systems

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We have recently developed the statistically-consistent approach to both t-J model and periodic Anderson-Kondo model. This approach was used to analyze the properties of high-temperature superconductors [1] in a quantitative manner, as well as the hybrid pairing induced by the Kondo interaction. We see that the overall doping dependence in the superconducting phase (SC) is properly reproduced for the first time. In the case of heavy fermions, the pairing evolves from the Kondo insulating [2]. The universal aspects pf real space pairing are raised [3].

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Unconventional superconductivity at the border with magnetic and Kondo insulating states

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We discuss a detailed phase diagram and other microscopic characteristics on the number of electrons - hybridization strength plane for a heavy-fermion almost localized Fermi liquid with strongly renormalized characteristics. Our approach includes effects of large (but finite) f −f intraatomic interaction U for the Anderson-lattice model, with both the hybridization and the Kondo interaction incorporated in a systematic manner. In effect, we analyse the effective Hamiltonian which can be termed the Anderson-Kondo lattice model. We discuss normal, magnetic, and superconducting phases as well as their interplay. In analogy to high-Tc, we observe that the superconducting state evolves from the (Kondo) insulating phase. Also, in the Kondo insulating state we observe total compensation of magnetic moments. The superconducting pairs can form a singlet state and have the mixed heavy f-electron - conduction c-electron nature.

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Magnetic field effect on the heavy-fermion state

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In heavy-fermion systems, a magnetic field can change the electronic state drastically, such as a metamagnetic transition. To investigate magnetic field effects on the heavy-fermion state, we study the periodic Anderson model. We set the Coulomb interaction between f electrons infinity, and consider a variational wavefunction, in which the double occupancy of the f electrons at the same site is removed. Then, by using the Gutzwiller approximation [1,2], we evaluate the energy and find the variational parameters that minimize energy. The magnetization and the effect of a magnetic field on the effective mass will be discussed.

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Aspects of the hidden order phase in URu_2Si_2: Remarkable nesting and spin-orbital hybridization

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The intermetallic uranium compound URu_2Si_2 undergoes a mysterious phase transition to an unknown phase below 17.5 K. Here we analyze the Fermi surface (FS) nesting properties of URu_2Si_2 with particular focus on their implication for the "hidden order" phase.

We show that there exist two Fermi surfaces that exhibit unusually strong nesting at the antiferromagnetic wavevector, Q_0=(0, 0, 1). The corresponding energy dispersions fulfill specific relations at eight FS hotspot lines: $e_1(k) = -e_2(k \pm Q_0)$. Notably, the spin-orbital characters of the involved 5f states of the two Fermi surfaces are *different:* $j_z=\pm5/2$ versus $\pm3/2$. As an implication electrons on one FS sheet cannot `jump´ to the other FS, rendering the occurring degenerate Dirac crossings symmetry protected in the nonmagnetic normal state. Pairing of the electrons in these two FSs can however commence through interaction with a quasiparticle with wavector Q_0 and it requires additionally a transfer of spin-angular momentum Δj_z between the Fermi surface states. We point out that dynamical symmetry breaking through an Ising-like spin-orbital excitation mode at Q_0 with $\Delta j_z=\pm1$ fulfills these criteria and can thus induce a hybridization of the two states, causing substantial Fermi surface gapping. Concomitant spin and orbital currents in the uranium planes give rise to a rotational symmetry breaking in the hidden order state.

Recent neutron and ARPES experiments have shown the pronounced appearance of the unusual Ising-like spin-orbital excitation mode at Q_0 upon entering the hidden order state, in good agreement with the microscopic model.

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A NOVEL PHASE TRANSITION IN THE UNDERSCREENED ANDERSON LATTICE MODEL: A CANDIDATE CONCEPT FOR THE UNDERSTANDING OF HIDDEN ORDER IN URu_2Si_2

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We analyze a novel type of phase transition that appears in the spin-rotationally invariant form of the underscreened Anderson Lattice Model and we obtain, with decreasing temperature, a continuous transition withopening of a gap. We suggest that this model might describe the "Hidden Order" transition in URu_2Si_2, We also examine the gaps that appear in the electronic dispersion relations of the bands of different orbital characterand compare our results with those found through photo-electron spectroscopy.

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^{119}Sn Mössbauer spectroscopy of 3d-, 4f-, and U-intermetallic compounds

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The results of Mössbauer spectroscopy (MS) investigation of the magnetic hyperfine fields (HFs) on ^{119}Sn probe nuclei for the intermetallic compounds based on the 3d-, 4f-elements, and uranium are presented in this work. It has been shown that the mechanisms of electron polarization on ^{119}Sn nuclei are different for the following groups of the compounds.

1. The compounds TFe_2 (T=Sc, Ti, Y, Zr, Lu, Hf, U) with Laves structures are ferromagnets (FM) except $TiFe_2$ that is an antiferromagnetic (AFM). In the FM compounds TFe_2, the HFs for ^{119}Sn atoms localized on T-sites (HF = B_1) are positive and proportional to the Fe magnetic moments: $B_1=A_1 \times \mu_{Fe}$, where A_1=28 T/μ_B is the hyperfine coupling constant. The HF B_1 reaches the value of about 50 T for ^{119}Sn in $ZrFe_2$. The HFs for ^{119}Sn atoms localized on Fe-sites (HF = B_2) are negative: $B_2=A_2 \times \mu_{Fe}$, where A_2=−3.8 T/μ_B.

2. In the ordered alloys of rare earth metals (RE) with p-metals, the HFs for ^{119}Sn atoms reach the values of 40 T. Systematics of the HFs for ^{119}Sn in the FM and AFM binary Gd - X compounds (X is a p-metal) is presented in work. The HF values on ^{119}Sn nuclei in $REAl_2$ и $REGa$ compounds are proportional to the spin magnetic moment of RE ions.

3. Huge HFs reaching 56 T have been found for ^{119}Sn atoms localized on RE-sites of RE-3d compounds. This value is the maximum of the known HF values on ^{119}Sn nuclei in the metallic magnets. It has been shown that the HFs are created due to two additive contributions of RE- and 3d-magnetic sublattices. The temperature dependencies of the HFs for ^{119}Sn atoms in $REFe_2$, $RECo_2$, $RECo_5$ compounds are related to the temperature changes of 3d-4f and 3d-3d interactions.

4. The selectivity of the magnetic hyperfine interaction for ^{119}Sn atoms to the certain 3d-3d or 4f-4f magnetic exchange interactions of the ternary RE-based intermetallic compounds has been observed. The HFs on ^{119}Sn nuclei localized at Si sites of GdMnSi and GdCoSi ferrimagnetic compounds are induced only by Gd magnetic moments. On the contrary, the HFs for ^{119}Sn atoms located at Ge-positions of $REMn_2Ge_2$ compounds are formed only by the Mn-magnetic moments.

5. The HFs on ^{119}Sn nuclei in UTM (T is a d-metal, M is a p-metal) compounds with ZrNiAl-type crystal structure are proportional to the full magnetic moment of U-ions: $B = A \times \mu_U$, where A= 6.5(4) T/μ_B. The results of ^{119}Sn MS study on UNiSn, UGa_3, UIn_3, UPb_3, UGa_2, UGe_2, USn_2 compounds indicate a strong anisotropy of the magnetic hyperfine interaction caused by the significant nonsphericity of 5f-electron shell of uranium ion.

Among the 3d-, 4f-, and U-magnetic moments, the ability to create a spin polarization on the ^{119}Sn nuclei is the largest for 3d-moments (in equivalent of the unit moment) and this one is the smallest for the unit magnetic moment of RE-ions.

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Magnetic states of $UCuGe_{1-x}Sn_x$ compounds studied by ^{119}Sn Mössbauer spectroscopy

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The non-collinear antiferromagnetic (AFM) compounds UCuGe and UCuSn with competing exchange interactions crystallize in the ordered derivatives of hexagonal CaIn2 structure: hexagonal SrPtSb type and orthorhombic P21cn structure, respectively. In these compounds, uranium magnetic moments are equal to about 2.0 µB and are ordered below TN =62(2) K [1, 2].

The hyperfine interactions on 119Sn nuclei of UCuGe1-xSnx compounds (x=0.0 – 1.0) have been studied at this work. It was found that substitution of Ge atoms by Sn atoms leads to the appearance and coexistence of two local ordered magnetic states of these compounds. For the whole region of x, the Mössbauer spectra represent a superposition of two magnetic sextets with two sets of hyperfine parameters. Two subspectra with significantly different values of magnetic hyperfine fields, B1 and B2, correspond to two magnetic states: low-field (LF) and high-field (HF). LF-component corresponds to AFM ordering of U magnetic moments in the neighborhood of some part of 119Sn atoms. HF-component indicates a ferromagnetic (FM) nearest environment of other 119Sn group of atoms. With the increase of x, B1 decreases smoothly from 6.3 T to 5.4 T, and B2 increases from 9.8 T to 11.7 T.

Temperature dependences of magnetic hyperfine fields B1 and B2, corresponding to AFM and FM local magnetic states, are very different. B1 (T) tends to zero at the magnetic ordering temperatures of parent compounds, T 1=60–62 K. The hyperfine field B2 vanishes at higher temperature T2 which increases from 70 K to 83 K with the increase of x.

The ratio of intensities of the LF and HF components of spectra varies in a regular manner with the increase of x, symmetrically with respect to x = 0.5. The HF-component reaches 80% of the total spectrum for x = 0.2 and x = 0.8.

The intensity of the HF-component correlates with the probability of occurrence of single Sn atom in the nearest neighborhood (NN) of the uranium ion at Ge-rich region (x <0.5), and with one of single Ge atom in the NN of uranium ion at Sn-rich region (x> 0.5).

The results are discussed together with 119Sn MS data for GdCuSn, GdAgSn and GdCuGe compounds.

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An investigation concerning the corrosion and recrystallization characteristics of laser beam welded gadolinium

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The safe long term containment of radioactive waste is an essential goal for the UK nuclear community. Within the UK radioactive waste inventory, metallic uranium fuel is a key 'reactive' material requiring long term containment. To better understand the long-term behavior of uranium in both storage and disposal environments, we have been studying gadolinium, an f block element, but a close chemical surrogate to uranium.

The corrosion of gadolinium is a relatively undeveloped area of research, but one that is becoming increasingly important as its availability and applications prosper; particularly in the nuclear industry. Gadolinium has the highest thermal neutron capture cross section that is known (49 000 barns), therefore making it a suitable candidate for neutron shielding material in nuclear power stations, nuclear waste storage, transportation vessels and even protective clothing [1] [2]. For example copper and aluminum gadolinium alloys have been proven to have a high neutron capture cross section, whilst also being stable at high temperatures, resistant to low temperature embrittlement and possessing good working and mechanical properties at a moderately low cost [3]. Many of these processes require the welding of gadolinium as a pure metal or alloy, but the corrosion behavior is not well understood.

We have developed the first quantitative microstructure study of gadolinium, using electron back scatter diffraction (EBSD), on a series of laser beam welds. The aim of the laser beam welding was to apply a localized stress on the metal, to show that areas of high stress encourage preferential corrosion. In a repository environment, this is important because 'stressed' uranium and gadolinium may be a significant source of corrosion and therefore hydrogen production, leading to hydriding of these metals in the repository environment. Differentiating corrosion characteristics allows us to contribute towards the comprehension of the mechanisms involved in these processes.

The current experiments so far have shown that as a result of laser beam welding under inert conditions the microstructure of the weld metal is significantly finer grained ≤ 50 μm, and the surface over-layer exhibits substantial Ca and F concentrations towards the margins of the weld, indicating diffusional expulsion from the parent metal on heating. This initial study has demonstrated that gadolinium exhibits similar recrystallization characteristics to uranium after 'flash' melting.

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Effect of hydrogenation on structural properties of multilayered Ti-TiO$_2$ thin films

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Thin film multilayers of Ti–TiO$_2$ system have been prepared by the reactive sputtering with the ultimate aim to study the interlayer properties and the influence of annealing, ion mixing and hydrogen intake on the microstructure and electronic structure.

Single-, bi- and trilayer thin films have been deposited on Si(111) substrates, i.e. Ti/Si(111), Ti/TiO$_2$/Si(111) and Ti/TiO$_2$/Ti/Si(111), respectively, by d.c. pulsed magnetron sputtering from metallic Ti target in an inert Ar or reactive Ar + O$_2$ atmosphere with nominal layer-thickness over the range of 50 – 500 nm. The film chemical composition, depth profile, layer thickness and structure were determined by combined analysis of RBS, XRD, XRR and optical reflectivity spectra. The results showed that the as-sputtered Ti film, crystallizing in the hexagonal structure, exhibit a strong preferred orientation with (00.1) plane parallel to the substrate, i.e. the *c*-axis of the hexagonal cell of Ti crystallites is perpendicular to the substrate. There is a strong influence of single layer thickness on the crystal growth as evidenced by XRD, XRR and optical measurements. Hydrogen charging at 1 bar at 300ºC revealed that in the case of the three-layered structure of Ti/TiO$_2$/Ti/Si(111) hydrogen diffused through TiO$_2$ without any accumulation in it. For structures covered with palladium, up to 40-50% of hydrogen is built (is stored) in the topmost and the bottom Ti layers. Palladium is known to act as a catalyst and facilitates dissociation of H$_2$ into atomic hydrogen. The XRD pattern of single and three layered films upon hydrogenation at 10 bar and 100 bar at RT consisted of more Ti reflections. Kiessing fringes in XRR of the film disappeared upon hydrogenation at 100 bar. The results indicated that the preferential orientation in the Ti films is destroyed in this case.

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Effect of La doping on the thermoelectric properties of Kondo lattice compound $CeFe_2Al_{10}$

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The effect of La substitution on the Ce site of $CeFe_2Al_{10}$ has been also studied on a series of $Ce_{1-x}La_xFe_2Al_{10}$ alloys by means of electrical resistivity (ρ), Seebeck coefficient (S), and thermal conductivity (κ) measurements. It is found that the substitution of La on the Ce sites in $CeFe_2Al_{10}$ initially causes a substantial increase in ρ, attributed to the increase of disorder. For all the presently investigated $Ce_{1-x}La_xFe_2Al_{10}$ alloys, the sign of S is positive, suggesting that the majority carriers for the thermoelectric transport are holes. As the Ce sites are completely substituted by La ($LaFe_2Al_{10}$), the majority carriers become electrons. We further attempt to analyze the ρ and S data by using two band model where the dominant contribution to the electrical transport arises from the scattering between electrons from broad $5d$-$6s$ conduction band and the narrow Lorentzian-shaped $4f$ band. An estimation from the Wiedemann-Franz law the total thermal conductivity of these Kondo lattice compounds is mainly due to lattice phonons rather than the charge carriers. A clear trend found in the lattice thermal conductivity (κ_L) for the $Ce_{1-x}La_xFe_2Al_{10}$ series is that the height of the low-temperature peak gradually decreases while the peak position shifts to higher temperatures with increasing substitution level. A theoretical analysis of thermal conductivity indicates that the point defect scattering mechanisms provide a reasonable explanation for the observed low-T behavior in $\kappa_L(T)$.

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Experimental study of alloys close to $Co_{11}Zr_2$ stoichiometry and modeling of electronic and crystal structure

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Comparing to other Co-rich stable magnetic materials of Co-Zr system with well defined crystal structure, $Co_{11}Zr_2$ intermetallic crystal structure is still unknown despite significant transmission electron microscopy and x-ray diffraction efforts. According to suggestions proposed in previous studies, the crystal structure of high temperature phase belongs to the rhombohedral crystal system and transforms on cooling into orthorhombic one. As there is no information about the correct space group with proper atomic coordinates for any suggested structure of $Co_{11}Zr_2$ compound, Ohodnicki et al. (2008), while studying in detail the binary Co-Zr system with the help of *ab-initio* approach, were forced to exclude $Co_{11}Zr_2$ compound from their calculations. It can be seen that the crystal and electronic structure of this compound still remains a mystery. So, the aim of the present study was to clarify the structure of the $Co_{11}Zr_2$ compound using experimental structural and thermal methods in combination with *ab-initio* modeling.

Co-rich alloys of the Co-Zr system in the concentration range up to 30 at.% of Zr subjected to different heat treatment conditions were experimentally investigated by means of differential thermal, electron microprobe, X-Ray diffraction and metallographic analyses.

The high precision *ab-initio* FLAPW method, implemented in WIEN2k software, was used for the electronic structure and total energy calculation of the ordered Co-Zr structures. Application of this method for band structure calculations allowed extracting quite precise information concerning atomic and electronic crystal structure.

Structures modeling Co_5Zr and $Co_{11}Zr_2$ intermetallic compounds were calculated with different atomic distribution in respective unit cells. The comparison of the modeled crystal and electronic structure with experimental data will be discussed.

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Fermi surface and magnetic order in UPt_2Si_2

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U intermetallic compounds exhibit highly complex phase diagrams at low temperatures with unusual and often enigmatic orders. The high sensitivity with respect to variations in external parameters like pressure or magnetic field reflect the strong correlations within the U 5f shell.

The present contribution focusses on the tetragonal compound UPt_2Si_2. We calculate the magneticfield dependence of the Fermi surface for itinerant and partially localized U 5f electrons and discuss consequences for field-induced instabilities.

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Heat capacity and electrical resistivity of hexagonal Ce-Ni-Ge system

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Metallic Ce compounds are of great interest for the intriguing physical properties associated with the 4f electrons. One notable example of compound intensively studied for many years is $CeNi_5$ crystallizing in the hexagonal $CaCu_5$ type, which results to be a Stoner enhanced paramagnet characterized by a spin fluctuation contribution on its transport properties.

Here the effect of the Ni/Ge substitution on the ground state of $CeNi_5$ is presented. Several ternary germanides $CeNi_{5-x}Ge_x$ (x=0, 0.1, 0.2, 0.5, 0.8) were prepared by argon arc-melting the elements on a water cooled copper hearth with a tungsten electrode starting from the nominal compositions. All the alloys crystallize in the $CaCu_5$ structure. Single phase of the polycrystalline samples was confirmed by X-ray diffraction and by electron microscope analysis. The measurements of heat capacity between 0.4 and 300 K, resistivity between 2 and 300 K and magnetic susceptibility up to 800 K are provided and the results are presented. No phase transition was observed in heat capacity and resistivity measurements. Small anomaly at about 6 K on heat capacity is attributed to Ce oxide. The resistivity measurements show a typical metallic behavior. Sommerfeld electronic coefficient γ from $C(T)/T^2$ vs T^2 and coefficient A in AT^2 term of electrical resistivity have been determined. The results are compared to the isostructural $CeNi_5$.

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High field Hall measurements on UPt₂Si₂ at very low temperatures

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Tetragonal UPt_2Si_2 has recently been characterized as a moderately mass enhanced antiferromagnet with a transition temperature T_N = 32 K in zero magnetic field [1-4].

In magnetic fields the antiferromagnetic phase transition was found to shift down to lower temperatures with increasing fields for both crystallographic axes as it is typical for antiferromagnets. However, below ~15 K and for magnetic fields *B* applied parallel to the *a* axis the transition splits up and becomes hysteretic, forming a new and distinct region between ~ 34 T and ~ 48 T in the magnetic phase diagram. Similarly, with the magnetic field applied parallel to the *c* axis a hysteretic magnetization and qualitative changes of the resistive signature of the phase transition are found. These features indicate the presence of multiple high field phases. Such phases, together with signs of Fermi surface effects in the data, point to a significant role of the Fermi surface in UPt_2Si_2 [5].

Here, we present new magnetoresistivity and Hall effect data on UPt_2Si_2 at temperatures 50 mK to 2K in high magnetic fields up to 34 T. For the *a* axis this field range only covers the antiferromagnetic phase. Instead, for the *c* axis, we observe hysteretic behavior of the magnetoresistivity at all temperatures, with multiple steps appearing upon decreasing magnetic field at temperatures below ~ 350 mK. Additionally, in the Hall signal we observe a significant change in the field region 22 – 27 T, independent of temperature. These findings are discussed in the context of the magnetic phase diagrams proposed in Ref. 5, in particular with respect to the possibility of a Lifshitz transition.

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Hydrogenation-mediated structure transformations in UPtSn

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UPtSn intermetallic compound exists in two structure modifications: hexagonal low temperature modification (ZrNiAl structure type) which is formed after annealing below $T = 300°C$ or in as-cast alloys and cubic high-temperature modification (MgAgAs structure type) which is formed after annealing above $T = 600°C$.

An as-cast sample of the nominal composition UPtSn, containing hexagonal UPtSn as the majority phase (70 wt.%) and U_2Pt_2Sn and $U_3Pt_3Sn_4$ as spurious phases, has been hydrogenated under hydrogen pressure of 140 bar and applying thermal cycling up to 500°C. It resulted in the formation of hydride $UPtSnH_x$ with isotropic lattice expansion ($\Delta a/a = 0.33\%$, $\Delta c/c = 0,32$), whereas the additional phases remained intact. It allowed to estimate the hydrogen content as $x \approx 0.3$ H/f.u. Hydrogenation weakens the ferromagnetic interactions in the parent intermetallic, resulting in the decrease of T_C from 25 K for UPtSn to 19 K and the reduction of magnetic moment of uranium at $T = 2$ K from 0.8 μ_B to 0.6 μ_B (on randomly oriented fixed powder). Similar performance has been already observed for other uranium stannides with heavy d-metals (e.g. URuSn [2]) upon hydrogenation, leading to the assumption that the reduction of the density of states at Fermi level may serve as a possible mechanism for the suppression of magnetism in such compounds.

The thermal decomposition of hydrogenated sample by heating in vacuum up to $T = 750°C$ resulted in the transformation of most of UPtSn compound into high-temperature cubic modification, while after heating up to $T = 700°C$ only ≈30% of UPtSn adopts MgAgAs structure type. Hence, hydrogenation can be regarded as an alternative less time-consuming method for the synthesis of cubic UPtSn. Taking into account the paramagnetic nature of cubic UPtSn phase, the total magnetic moment reduced substantially compared to the initial and hydrogenated compounds. Further attempts to hydrogenate cubic UPtSn phase ($p(H_2) = 140$ bar, $T = 500°C$) have been unsuccessful what makes the hydrogenation-desorption process irreversible in this particular case.

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Magnetic, magnetocaloric and magnetoacoustic properties of $Er_2Fe_{14}B$

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The aim of the present work is the combined study of magnetic, magnetocaloric and magnetoacoustic properties of the $Er_2Fe_{14}B$ compound at temperatures corresponding to spin-reorientation transition (SRT) range. The $Er_2Fe_{14}B$ compound exhibits the first-order SRT at 325 K; at this temperature, the abrupt reorientation of the magnetic moment from the basal plane to the c-axis direction takes place. This fact is confirmed by measurements of field and temperature dependences of magnetization for single-crystal $Er_2Fe_{14}B$ samples. Effect of hydrogen on the magnetic properties of $Er_2Fe_{14}B$ also was investigated. Magnetocaloric effect (MCE) characterized by ΔT_{ad} was studied by a direct method at a field change of to $\Delta H = 18$ kOe; $|\Delta T_{ad}|$ is not high and equals 0.2-0.4 K for $Er_2Fe_{14}B$. However, the following fact is of most importance. The ΔT_{ad} value plotted vs temperature clearly demonstrates the sign alternation of MCE at T = 325 K, i.e., in applying magnetic field, below T_{SR}, the heat absorption takes place (negative MCE), whereas above T_{SR}, the heat evolution (positive MCE) is realized. The SRT is accompanied by an anomaly of ultrasound velocity variations. Since T_{SR} is close to room temperature, the material shows promise as working medium in heat sensors for various applications. The work is supported by RFBR, pr. no. 10-03-00848.

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Magnetism study in $NdMn_{1-x}Fe_xO_3$ doped system.

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We will present effect of iron substitution for manganese on magnetic properties and heat capacity in the $NdMn_{1-x}Fe_xO_3$ family of compounds. Both boundary compounds ($NdMnO_3$ and $NdFeO_3$) exhibit interesting magnetic properties due to two different magnetic sublattices (Nd sublattice and Mn sublattice) and the fact that manganese atoms in these compounds are in ionic state Mn^{3+} and Mn^{4+}. Thence the compounds comprise properties of canted antiferromagnets and ferrimagnets. In case of $NdMnO_3$, the Mn sublattice orders at T_N = 82 K with magnetic moments parallel to *b*-axis and Nd sublattice orders feromagnetically (moments parallel to *c*-axis) at $T_1 \approx$ 20 K [1]. In $NdFeO_3$, Fe sublattice orders above room temperature and undergoes spin reorientation in temperature range 70 – 160 K [2], but Nd sublattice orders only at very low temperatures ($T \approx$ 1.5 K). Up to now, the only referred substitutional compound is $NdMn_{0.9}Fe_{0.1}O_3$ [3].

We prepared polycrystalline samples of $NdMn_{1-x}Fe_xO_3$ ($0 \leq x \leq 1$) compounds and attempted to prepare single crystals by melting the stoichiometric amount of starting oxides in the vertical floating zone mirror furnace. We have measured magnetization, susceptibility and specific heat properties and studied their evolution with doping. We found that for small iron doping T_N decreases, but hysteresis loop broadens and changes from simple, ferromagnetic-like, to more complicated multistep "butterfly type" hysteresis loop. Measurements of temperature dependence of magnetization revealed compensation temperature and magnetization reversal effect on sample with x = 0.2. In the heat capacity data of un-doped sample we observed another small anomaly at about 0.5 K which can be signature of another magnetic phase transition. The studies of higher iron concentrations (x > 0.2) are still in progress. We believe that we will be able to present the complete set of experimental data and interpretation for the full concentration range.

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Metamagnetic behavior in cubic heavy fermion compounds YbT_2Zn_{20} and UT_2Zn_{20} (T : transition metal)

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Yb and U-based ternary compounds YbT_2Zn_{20} (T = Co, Rh, Ir) and UT_2Zn_{20} (T = Co, Ir) crystallize in the cubic $CeCr_2Al_{20}$-type structure with a large lattice constant $a \simeq 6$ Å and show heavy fermion features at low temperatures[1-3]. Among YbT_2Zn_{20}, an exceptionally large electronic specific heat coefficient γ = 8 $J/K^2 \cdot$mol was observed in $YbCo_2Zn_{20}$. UCo_2Zn_{20} and UIr_2Zn_{20} also possess large γ = 350 and 400 $mJ/K^2 \cdot$mol, respectively, and are reported to be non-magnetic heavy fermion compounds[3]. Recently, we succeeded in growing high-quality single crystals of YbT_2Zn_{20} (T = Co, Rh, Ir) and UT_2Zn_{20} (T = Co, Ir), and studied a metamagnetic like behavior, which appears in the heavy fermion state below the characteristic temperature $T\chi_{max}$ at which the magnetic susceptibility takes a broad maximum.

For $YbCo_2Zn_{20}$, $YbRh_2Zn_{20}$, and $YbIr_2Zn_{20}$, the metamagnetic anomaly was observed at H_m = 6, 63, and 97 kOe below $T\chi_{max}$ = 0.32, 5.8, and 7.4 K, respectively. These values approximately satisfy a relation of $15T\chi_{max}(K) = H_m(kOe)$, which is applied for metamagnetic behaviors of several Ce-, U-, and Yb-based heavy fermion compounds[4]. On the other hand, metamagnetic behavior was observed at H_m = 80 kOe below $T\chi_{max}$ = 8.5 K in UCo_2Zn_{20} and at H_m = 20 kOe below $T\chi_{max}$ = 5.2 K in UIr_2Zn_{20}. The metamagnetic field H_m = 20 kOe in UIr_2Zn_{20} is substantially smaller than the expected value from the above relation $H_m(kOe) = 15T\chi_{max}(K) \simeq 80$ kOe, showing a clear contrast to YbT_2Zn_{20}.

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Metamagnetic behavior of YbT$_2$Zn$_{20}$ (T : Co, Rh, Ir) and UT$_2$Zn$_{20}$ (T : Co, Ir)

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YbT$_2$Zn$_{20}$ (T : Co, Rh, Ir) and UT$_2$Zn$_{20}$ (T : Co, Ir) crystallize in the CeCr$_2$Al$_{20}$ type cubic structure with the large Yb-Yb and U-U distances ($d \sim 6$ Å). These compounds do not ordermagnetically and indicate a large electronic specific heat coefficient γ, in particular $\gamma = 8000$ mJ/K^{2}mol for YbCo$_2$Zn$_{20}$, without a magnetic ordering at low temperatures[1,2]. The magnetic susceptibility follows the Curies-Wiess law down to a characteristic temperature $T_{\chi max}$, indicates a maximum at $T_{\chi max}$ and decrease slightly below $T_{\chi max}$, meaning that an f electron nature is changed from localized into itinerant, forming heavy quasiparticles. One of characteristic features in heavy fermion compounds is the metamagnetic behavior at the magnetic field H_m at temperatures lower than $T_{\chi max}$. We found the metamagnetic transition in heavy fermion compounds YbT$_2$Zn$_{20}$ (T : Co, Rh, Ir) and UT$_2$Zn$_{20}$ (T : Co, Ir)[3,4]. In addition to this metamagnetism, YbCo$_2$Zn$_{20}$ shows an another metamagnetic behavior at 6 T derived from the field-induced quadrupolar ordering. In order to investigate the ordering phase, we measured the magnetoresistance under high fields and at low temperatures.

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NMR STUDY OF THE POSSIBLE CHARGE-DENSITY-WAVE TRANSITION IN Ce$_3$Co$_4$Sn$_{13}$

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We present a study of the phase transition behavior in Ce$_3$Co$_4$Sn$_{13}$ using 59Co nuclear magnetic resonance (NMR) spectroscopy. The quadrupole splitting, Knight shift, and spin-lattice relaxation rate (1/T1) below and above the phase transition temperature T0 have been identified. All measured NMR quantities exhibit pronounced features at around T0=155 K except for the Knight shift. It thus excludes the magnetic origin for the observed transition. Since the x-ray diffraction results below and above T0 show the absence of a crystal structural change, we speculate that the peculiar phase transition is possibly related to an electronic origin and/or electron-lattice coupling such as the formation of a charge-density-wave (CDW). As a matter of fact, the disappearance of the double-peak feature of 59Co NMR central line below T0 can be realized as the spatial modulation of the electric field gradient due to incommensurate CDW superlattices. Also, a distinct peak found in the spin-lattice relaxation rate near T0 manifests a phase transition and its feature can be accounted for by the thermally-driven normal modes of the CDW. From the NMR analyses, we obtained a consistent picture that the change of electronic structures below T0 is mainly due to the weakening of the p-d hybridization. Such an effect could result in possible electron-lattice instability and thus the formation of a CDW state in Ce$_3$Co$_4$Sn$_{13}$.

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Properties of the two novel polar intermetallics $Yb_3Pd_2Sn_2$ and $Eu_3Pd_2Sn_2$

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Ytterbium and europium compounds show a great variety of anomalous physical properties due to the fact that these lanthanides can exist in the trivalent or in the divalent state. The divalent and trivalent oxidation states may coexist in some compounds called heterogeneous mixed valence systems, with inequivalent crystallographic R-sites (R = rare-earth). A different situation is that of an intermediate valence system, where each lanthanide has the same, non-integer valence due to hybridization between f- and conduction electrons. Here we present a comparison between the structure and the physical properties of two novel compounds with inequivalent crystallographic R-sites, namely $Yb_3Pd_2Sn_2$ and $Eu_3Pd_2Sn_2$. In fact, during our investigation on the Yb-Pd-Sn system, a compound with the formula $Yb_3Pd_2Sn_2$ and an orthorhombic cell was found. The crystal structure of this compound has been determined *ab initio* from powder X-ray diffraction data and it is representative of a new structure type with Yb-atoms occupying four inequivalent crystallographic positions. Searching for other $R_3Pd_2Sn_2$ compounds, the existence of $Eu_3Pd_2Sn_2$ crystallizing in the $La_3Ni_2Ga_2$ structure-type (with Eu-atoms occupying two inequivalent sites) has been found. The structure of $Yb_3Pd_2Sn_2$ is closely related to the $La_3Ni_2Ga_2$ structure-type, and therefore to the structure of $Eu_3Pd_2Sn_2$. In both cases, polyanionic networks $[Pd_2Sn_2]_\infty$ have pronounced 2D characters and, making an analogy with structural organic chemistry, could be defined as *cis*-$[Pd_2Sn_2]_\infty$ and *trans*-$[Pd_2Sn_2]_\infty$ conformations for $Eu_3Pd_2Sn_2$ and $Yb_3Pd_2Sn_2$, respectively.

$Yb_3Pd_2Sn_2$ shows no phase transition down to 0.3 K and it behaves as an ordinary metal. The magnetic susceptibility shows a very weak temperature dependence in the whole temperature range with a small upturn at low temperatures likely due to paramagnetic impurities. The nearly constant susceptibility indicates a close to divalent Yb-behaviour, although a tiny broad bump above 200 K may indicate some degree of hybridization between 4f and conduction electrons. Also the Sommerfeld coefficient determined from heat capacity, showing a slightly enhanced value of 67 mJ mol^{-1} K^{-2}, suggests a certain degree of c-f hybridization. Nevertheless, a possible scenario where $Yb_3Pd_2Sn_2$ is a heterogeneous mixed valent compound is ruled out by the results of ^{170}Yb-Mössbauer spectroscopy.

For $Eu_3Pd_2Sn_2$ the susceptibility in the paramagnetic regime follows the Curie-Weiss law, with an effective moment of 7.94 μ_B, in agreement with the value for the free ion Eu^{2+}. The paramagnetic Curie temperature θ_p = -5 K is negative indicating the presence of antiferromagnetic exchange. In fact, magnetic susceptibility at lower temperatures shows a main magnetic transition at 22 K with two other effects likely due to spurious phases. Eu-Mössbauer measurements confirm the existence of an intrinsic magnetic transition at 22 K.

Neutron powder diffraction patterns recorded at 40 K and 3.6 K using a large-area flat-plate geometry sample holder confirm the $La_3Ni_2Ge_2$ type-structure and the divalent state of the Eu atoms in $Eu_3Pd_2Sn_2$. The appearance of additional magnetic peaks at low temperature indicates antiferromagnetic order of the Eu sublattice.

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Role of structural state of Gd in the formation of its magnetocaloric effect value

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The magnetocaloric effect (MCE) was measured by direct method (ΔT_{ad}) using samples which differ in both purity and structural state, namely, polycrystalline (commercial purity), distilled, and single-crystal. Distilled Gd is characterized by low contents of gas-forming elements (10^{-2}-10^{-3} wt %); the content of basic metal is 99.96 wt%. Distilled Gd was found to have a complex structure, whose elements are present as micron-sized elongated "fibers" from 0. to 2.5 µm in lateral section (directed along the growth axis of distillate) and nano-sized crystallites 30-50 nm in size. The MCE of Gd samples subjected to hydrogenation and severe plastic deformation (SPD) was also studied. It was found that depending on the structural state of sample the difference in MCE value can reach more than 1 K, which is ~20-25% of the maximum MCE value for Gd. The possibility of the increase in MCE value to 4.5-5.0 K is shown can be obtained at the expense of hydrogen-induced structure ordering of sample; the decrease in MCE value takes place after SPD, which is related to the structure disturbance. The work was supported by the RFBR (project no. 10-03-00848) and Russian Academy of Sciences (program no. 5).

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Specific heat of the $CeCu_4Mn_yAl_{1-y}$ compounds

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Specific heat of the $CeCu_4Mn_yAl_{1-y}$ compounds has been studied. The samples are prepared by induction melting and it is found, based on the X-ray diffraction, that all the compounds keep the $CaCu_5$-type structure. This series exhibits a transition from the heavy fermion (HF) state for $CeCu_4Al$ to the spin-glass (SG) behavior for $CeCu_4Mn$. The magnetic measurements indicate a spin-glass-like order for all Mn containing compounds. However, the increased values of the electronic specific heat coefficient γ suggest a possible coexistence of the heavy fermion and SG states, especially in the case of the Al-rich compounds ($y<0.3$). In the present research we explore the behavior of the specific heat for various y. Heat capacity measurements were performed using the PPMS device in the temperature range 1.9–300 K. The relaxation method based on the 2 model has been employed. The specific heat has been analyzed considering the electronic, phonon, Schottky (Crystal Electric Field - CEF), Kondo and SG contributions. The assumption that the CEF splitting of the energy levels is similar for all the compositions allows us to estimate the spin glass and Kondo contribution to the heat capacity

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Structure transformation of $EuNi_5In$ under hydrogenation.

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RT_5X compounds (R= rare earths, T= transition metals, X= p-elements) have been found to be very attractive in terms of crystal chemistry and physical properties. A good example is UCu_5In, which crystallizes in three polymorphic modifications. $CePt_5Sb$ exhibits first order phase transition with low-temperature modification showing Kondo behaviour. A series of hexagonal $CeNi_5Sn$-type indium and tin based compounds were shown to absorb hydrogen up to 2.5H/f.u. The common feature of the RT_5X structures are very simple highly symmetrical structural motifs: $CaCu_5$, $MgCu_2$ and NiAs types. It can be postulated that structure of RT_5X is tuned by some external conditions. Here we present the result of hydrogenation of rhombohedral $EuNi_5In$ compound.

The $EuNi_5In$ intermetallic sample was prepared by arc melting of pure components under argon atmosphere. The sample inside of evacuated quartz tube was heated up to 1170K and subsequently cooled down to 870 K and annealed at this temperature for 3 weeks. The XRPD confirmed purity of the sample and rhombohedral structure of the compound (space group R-3m) with cell parameters a=4.8924(9)Å, c=29.754(8)Å.

$EuNi_5InH_{1.5}$ hydride was synthesised by the reaction of gaseous hydrogen with $EuNi_5In$ compound at room temperature and hydrogen pressure 700 mbar. The pressure increasing to 100 bar does not cause additional hydrogen absorption; however, experimental conditions of hydrogen insertion with slow cooling of the system lead to the formation of single crystalline hydride with size of about 0.2 mm. XRPD pattern showed the structural change of formed hydride, which was proven by X-ray single crystal investigation. $EuNi_5InH_{1.5}$ crystallizes in the hexagonal symmetry with P-6m2 space group and cell parameters a=4.9400(7)Å, c=10.640(2)Å, exhibiting a new structural arrangement. Therefore the unit cell of the new hydride is ~1/3 of the initial intermetallic compound along the c direction. Hydrogen absorption causes a strongly anisotropic expansion of the unit cell ($\Delta a = 1.0\%$, $\Delta c = 7.3\%$) and results in a volume increase of 9.4 %. The temperature-induced H desorption, which starts at about 330 and completes below 870 K, recovers the original crystal structure.

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Uranium magnetic materials - is it possible?

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Uranium intermetallics where the 5f electrons play the dominant role in the formation of magnetic properties are a subject of intensive studies. U atoms can carry a large magnetic moment and produce a huge magnetic anisotropy, the anisotropy field of many U compounds is estimated to be hundreds of Tesla. However, most of the interesting properties of the majority of the U intermetallics are manifest at low or very low temperatures. A "pulling out" the f-electron magnetism to elevated temperatures by employing the f-3d intersublattice exchange interactions, which was very successful in the 4f-electron R compounds and led to discovery of perfect magnetic materials, seems to fail in the case of 5f electrons of uranium. In metallic systems containing both uranium and the 3d metals (T), strong 5f-3d hybridization tends to delocalize the 5f electrons thus reducing strongly (down to zero) the U magnetic moment. At the same time the 5f-3d hybridization reduces (down to zero) the magnetic moment of T atoms. As an extreme example, one can consider UFeAl with two of three atoms with potentially large magnetic moments (3 $_B$ and 2 $_B$ per U and Fe). In reality, UFeAl is a paramagnet down to the lowest temperatures. Nevertheless, in contradiction with this general trend, several U-T-containing intermetallics are known, in which both U and T are magnetic and can be considered as potential magnetic materials. This is shown on the examples of $U_2(T,Si)_{17}$ and $UT_{12-x}M_x$ (M = Al, Si) compounds studied systematically in the framework of collaboration between Prague and Sendai groups.

The following conclusions are made:

1. Magnetic ordering of the U and 3d-metal sublattices can coexist in the same intermetallic compound.

2. Inter-sublattice exchange interaction between U and 3d metal can pull the U magnetism to rather high (room and higher) temperatures.

3. Nevertheless, perspectives of real magnetic materials with uranium currently look rather pessimistic from several viewpoints.

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Epitaxial growth and exchange bias in Th-diluted $U_{1-x}Th_xO_2$/Fe_3O_4 thin film bilayers

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The exchange bias (EB) effect, i.e. shifted hysteresis loop [1] of coupled bilayers of ferromagnetic (F) and antiferromagnetic (AF) thin film systems, has initiated large scientific and industrial interest. It is generally believed that EB is an effect resulting from the exchange interaction of interfacial F and AF spins. The strength of EB is related to the density of the interfacial uncompensated AF spins [2]. Therefore, an increase of uncompensated interfacial AF spin density, e.g. by dilution of the U-sublattice, may result in an enhancement of EB.

Here we present the study of thorium (Th) diluted $U_{1-x}Th_xO_2$ ($0.02 \leq x \leq 0.19$) thin films grown by DC-sputter deposition, representing the AF component and the magnetite as the F component of the bilayer. X-ray diffraction and X-ray photoelectron spectroscopy studies indicate the stoichiometric and epitaxial nature of the films. The magnetic study performed using VSM (PPMS9) indicates an enhancement of exchange bias in $U_{1-x}Th_xO_2$ with x > 15%.

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Optical spectroscopy on Heusler compounds

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Heusler compounds are versatile material class allowing to design desired properties through various constituent atoms, i.e. properties intrinsically related to the modification of the atomic electronic structure. Among the studied classes are half-metallic and thermoelectric materials. Although Heusler compounds are throughly studied by number of techniques, optical spectroscopies are often omitted. However, they can provide information of phonon energies, gap size and its purity, shape of critical points, presence of quasi-particles such as exciton, conductivity estimation from IR absorption, etc. Knowledge of complex refraction index is important for mass production control check of thin films, to check e.g. their thickness and roughness. Also, half-metallic Heusler compounds are promising materials for magneto-optical applications, due to low photon absorption for energies below half-metalic gap.

Within this contribution we present complex refractivity index, determined in wide spectral range from far-infrared to near-ultraviolet, of half-metallic Heusler compounds Co_2FeSi, $Co_2FeAl_{0.4}Si_{0.6}$ and $Co_2FeGa_{0.5}Ge_{0.5}$, on thermoelectric CoTiSb and on topological insulator PtYSb. The features of optical spectra are related with details of the electronic structure. The experimental optical properties are compared with ab-initio calculations and phonon spectra calculations.

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Phonon spectrum, thermal expansion and heat capacity of UO_2 from first-principles

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We report first-principles calculations of the phonon dispersion spectrum, thermal expansion, and heat capacity of uranium dioxide. The so-called direct method, based on the quasiharmonic approximation, is used to calculate the phonon frequencies within a density functional framework for the electronic structure. The phonon dispersions calculated at the theoretical equilibrium volume agree well with experimental dispersions. The computed phonon density of states (DOSs) compare reasonably well with measured data, as do also the calculated frequencies of the Raman and infrared active modes including the LO/TO splitting. To study the pressure dependence of the phonon frequencies we calculate phonon dispersions for several lattice constants. Our computed phonon spectra demonstrate the opening of a gap between the optical and acoustic modes induced by pressure. Taking into account the phonon contribution to the total free energy of UO_2 its thermal expansion coefficient and heat capacity have been computed from first-principles. Both quantities are in good agreement with available experimental data for temperatures up to about 500 K.

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