Hoa Kim Ngan NHU-TARNAWSKA

Cracow Colloquium on f-electron systems (CCFES2021) April 18-21, 2021

Program and abstracts

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UNIWERSYTETU PEDAGOGICZNEGO KRAKÓW 2021

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Preface

Cracow Colloquium on f-electron systems (CCFES2021) is held as an online event on April 18-21, 2021. CCFES2021 is organized by Faculty of Exact and Natural Sciences, Pedagogical University of Cracow, in a cooperation with Faculty of Mathematics and Physics, Charles University in Prague. On-line CCFES2021 was originally planned as on-site CCFES2020 at the Pedagogical University of Cracow, Poland.

"Cracow Colloquium on f-electron systems" was held the first time in 2015 (CCFES2015), initiated by "Prague Colloquium on f-electron systems" (PCFES), organized every two years in Prague since 1992. After the success of CCFES2015, we decided to take a new format for the colloquium as "Prague/Cracow on f-electron systems" (P/CCFES), organized every two years with a change of its location, in Prague and in Cracow. PCFES2018 was then held in Prague in 2018. CCFES2020 was planned to be held in Cracow on June 28-July 1, 2020. CCFES2020 has been in the list of conferences which received the funding from Polish Academy of Arts and Sciences (PAU) in the scope of Krakow Scientific Conferences 2020 (KKN2020). Due to the pandemics, CCFES2020 was postponed to April 18-21, 2021 (CCFES2021). CCFES2021 is in the reserved list of conferences which received the funding from PAU in the scope of KKN2021.

CCFES2021 focuses on the topics such as electronic structure, magnetism and superconductivity of *f*-electron systems (both lanthanides and actinides). It covers both theoretical and experimental aspects. The colloquium is also devoted to the field of hydrides of *f*-metal based materials and their technical application. Relevant contributions from the related research topics in Condensed Matter, e.g. *d*-electron systems, nanomaterials, functional materials, are also included in the scientific program of CCFES2021.

CCFES2021 is an activity included to the Calendar of the Jubileefor celebration of 75 years of Pedagogical University in Cracow-the first Pedagogical University in postwar Poland founded on 11th May, 1946.

Hoa Kim Ngan Nhu-Tarnawska (N.-T.H. Kim-Ngan)
on behalf of the Organizing Committee of CCFES2021

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Wstęp

Cracow Colloquium on f-electron systems (CCFES2021) w dn. 18 - 21 kwietnia 2021r. odbywa się w trybie zdalnym. Konferencja CCFES2021 jest organizowana przez Wydział Nauk Ścisłych i Przyrodniczych Uniwersytetu Pedagogicznego w Krakowie, we współpracy z Wydziałem Matematyki i Fizyki Uniwersytetu Karola w Pradze. Wirtualna konferencja CCFES2021 była pierwotnie planowana jako CCFES2020 na Uniwersytecie Pedagogicznym w Krakowie.

Konferencja "Cracow Colloquium on f-electron systems" odbyła się po raz pierwszy w roku 2015 w Krakowie (CCFES2015) i jest cykliczną konferencją związaną z "Prague Colloquium on f-electron systems" (PCFES) organizowaną (w Pradze) co dwa lata od 1992. Po sukcesie konferencji CCFES2015, wspólnie zdecydowano o przekształceniu tej konferencji na "Prague/Cracow Colloquium on f-electron systems (P/CCFES), która obywa się co dwa lata na zmianę w Pradze i w Krakowie. PCFES2018 obyła się w Pradze w roku 2018. W roku 2020, CCFES2020 była zaplanowana w terminie 28 czerwca - 1 lipca, 2020 w Krakowie. CCFES2020 była na liście konferencji, które dostały dofinansowanie Polskiej Akademii Umiejętności (PAU) w ramach programu Krakowskie Konferencje Naukowe 2020 (KKN2020). Z powodu pandemii, CCFES2020 została przeniesiona na nowy termin 18-21 kwietnia, 2021 (CCFES2021). CCFES2021 znajduje się na liście rezerwowej konferencji, które dostały finansowanie programu Krakowskie Konferencje Naukowe 2021 (KKN2021).

Tematyka CCFES2021 obejmuje takie tematy jak struktura elektronowa, magnetyzm, nadprzewodnictwo i kwantowe zjawiska krytyczne układów *f*-elektronowych (zarówno lantanowców, jak i aktynowców). Konferencja ta poświęcona jest również tematyce wodorków materiałów opartych na *f*-metalach i ich zastosowaniu technicznym. Program naukowy CCFES2021 obejmuje także wybrane wykłady z powiązanych tematów badawczych w materii skondensowanej takich jak układy *d*-elektronowych, nanomateriały, materiały funkcjonalne.

CCFES2021 jest również aktywnością, która jest uwzględniona w „Kalendarium obchodów jubileuszowych" 75-lecia Uniwersytetu Pedagogicznego w Krakowie. Jest pierwszym Uniwersytetem Pedagogicznym w powojennej Polsce założonym 11 maja 1946.

Hoa Kim Ngan Nhu-Tarnawska (N.-T.H. Kim-Ngan)
w imieniu Komitetu Organizacyjnego CCFES2021

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Welcoming to CCFES2021!

Dear honored and invited guests, dear friends and colleagues,

We are glad to welcome you at Cracow Colloquium on f-electron systems held on April 18-21, 2021 (CCFES2021).

On-line CCFES2021 was originally planned as on-site CCFES2020 to be held on June 28-July 1, 2020, at the Pedagogical University of Cracow, Poland. CCFES2020 was already got the approval from Polish Academy of Science and Art for a financial support within the scope of Krakow Scientific Conferences 2020. All organizational issues have already been completed for welcoming all participants for the original dates. Due to the pandemics, we had to postpone CCFES2020 to 2021 (CCFES2021). We are well prepared for the case when the external conditions are available for an on-site conference, we will then organize CCFES2021 on-site or in the hybrid form. However, due to the actual situation, CFES2021 is held fully as an on-line event. We are aware, that on-line conference cannot replace face-to-face meetings. However, we think that it is necessary to have the forum for even if on-line informal discussions on current issues in rare earths and actinides science.

The scientific program of CCFES2021 consists of 11 sessions with 2 plenary lectures and 12 invited talks given by distinguished specialists, contributed talks and posters, as well as a special session for the PhD students in Physics at our University. There are contributions from participants from 12 countries in Europe, Asia and USA, with which we feel as a big success, especially in such a difficult time.

We thank all of you for your contributions.

We wish you a fruitful and enjoyable time at CCFES2021.

We wish you and your families always in a good health.

Best regards. Pozdrawiamy serdecznie.

Grzegorz Formicki
Dean of Faculty of Exact and Natural Sciences,
Pedagogical University of Cracow

Artur Błachowski
Chairman of Discipline Council
of Physics, Faculty of Exact and Natural
Sciences (WNŚiP), Pedagogical University
of Cracow (UP-Kraków)

Hoa Kim Ngan Nhu-Tarnawska
On behalf of the Organizing Committee
of CCFES2021,
Deputy Chairman of Discipline Council
of Physics, WNŚiP, UP-Kraków.

ORGANIZING COMMITTEE

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Ladislav Havela (CUNI)
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Hoa Kim Ngan Nhu-Tarnawska (PUC)
Ryszard Radwański (PUC)
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HONORED INVITED SPEAKER

Jaap Franse (The Netherlands)

INVITED SPEAKERS

Zbigniew Bukowski (Poland)
Jeroen Custers (Czech Republic)
Antonio António Pereira Gonçalves (Portugal)
Itzhak Halevy (Israel)
Dariusz Kaczorowski (Poland)
Tatsuya Kawae (Japan)
Claudine Lacroix (France)
Dominik Legut (Czech Republic)
Andrzej M. Oleś (Poland)
Peter Riseborough (USA)
Małgorzata Samsel-Czekała (Poland)
Jozef Spałek (Poland)
Eteri Svanidze (Germany)
Andrzej Ślebarski (Poland)
Gertrud Zwicknagl (Germany)

Program

Sunday, April 18, 2021			
SD	**Special Session for PhD students in Physics** ***(3 minutes – 3 slides presentation)*** **Chair persons: Dawid Nalęcz, Kamila Komędera**		
16:00-16:10	**Welcoming address**	Hoa Kim Ngan Nhu-Tarnawska	
16:10-16:15	*The fracture toughness of TiB_2 doped by tungsten measured by the nanoindentation method*	Sylwia Sowa	**SD-01**
16:15-16:20	*Is there a relationship between curvature and inductance in the Josephson junction ?*	Aleksander Jarmoliński	**SD-02**
16:20-16:25	*Electrical properties of sodium bismuth titanate $Na_{0.5}Bi_{0.5}TiO_3$ ceramics under various sintering conditions*	Kamila Kluczewska-Chmielarz	**SD-03**
16:25-16:30	*Effect of Fe doping electric properties of $Na_{0.5}B_{0.5}TiO_3$ ceramics in unpoled and poled state*	Marcin Wąs	**SD-04**
16:30-16:35	*Influence of E-poling on the structural, dielectric, vibrational and ferroelectric properties of $Na_{0.5}Bi_{0.5}TiO_3$ single crystals*	Michalina Nowakowska-Malczyk	**SD-05**
16:34-16:40	*The electrocaloric effect in $BaTiO_3$:Eu ceramics*	Przemysław Gwizd	**SD-06**
16:40-17:00	*Discussions*		

Monday, April 19, 2021			
SO	**Opening Session** **Chair persons: Hoa Kim Ngan Nhu-Tarnawska, Silvie Mašková-Černá**		
8:45-9:00	**Welcome address** Honorary guests of CCFES2021: Michał Rogoż, Vice-Rector of the Pedagogical University of Cracow. Grzegorz Formicki, Dean of Faculty of Exact and Natural Science, Pedagogical University of Cracow.		
S1	**Session 1: Plenary Lectures** **Chairperson: Ladislav Havela**		
9:00-9:45	*Quantum criticality driven by magnetic field*	Dariusz Kaczorowski	**PL-01**
9:45-10:30	*Superconductivity enhanced by atomic disorder*	Andrzej Ślebarski	**PL-02**
10:30-11:00	*Break*		
S2	**Session 2: Historical recall of f-electrons research** **Chairperson: Hoa Kim Ngan Nhu-Tarnawska**		
11:00-11:45	*Research on Magnetism and Superconductivity of f-metal intermetallic compounds starting in the seventies of the 20th century.*	Jaap Franse	**HI**
S3	**Session 3: Actinides I** **Chairperson: Silvie Mašková-Černá**		
11:45-12:15	*Effects of composition on the UFe_xSb_2 system*	Antonio Pereira Gonçalves	**I-01**
12:15-12:30	*Magnetic entropy analysis using a calculated phonon background – how does it work for UH_3 ?*	Ladislav Havela	**O-01**
12:30-14:00	*Lunch break*		

S4	**Session 4: Rare Earths** **Chairperson: Artur Błachowski**		
14:00-14:30	*High-spin Ni states in a model for doped NiO_2 planes in $NdNiO_2$*	Andrzej Michał Oleś	**I-02**
14:30-14:45	*Quest for new intermetallic f-electron compounds*	Tomasz Klimczuk	**O-02**
14:45-15:00	*Local origin of strong field-angular anisotropy in magnetic phase diagrams of $Ce_{1-x}La_xB_6$ measured in a rotating magnetic field*	Dmytro Inosov	**O-03**
15:00-15:15	*Investigating ground-states of 4f-based single-crystals by neutron diffraction*	Margarida S. Henriques	**O-04**
15:15-15:30	*The influence of annealing temperature on the magnetic properties of La-doped $BiFeO_3$ prepared by sol-gel method*	Karolina Siedliska	**O-05**
15:30-16:00	*Break*		
S5	**Session 5: Theory** **Chairperson: Ryszard Radwański**		
16:00-16:30	*Towards a better understanding of the RKKY interaction in heavy-fermion systems*	Gertrud Zwicknagl	**I-03**
16:30-17:00	*Enhanced Spin-Orbit Interaction in the Underscreened Anderson Lattice*	Peter Riseborough	**I-04**
17:00-17:15	*Electronic structure of the non-centrosymmetric heavy-fermion $CeRh_2As_2$*	Évrard-Ouicem Eljaouhari	**O-06**
17:15-17:30	*Non-s-wave superconductivity in noncentrosymmetric ThCoC-2 in view of ab initio calculations and Eliashberg formalism*	Gabriel Kuderowicz	**O-07**
Tuesday, April 20, 2021			
S6	**Session 6: Strongly correlated systems** **Chairperson: Andrzej Michał Oleś**		

9:00-9:30	*Coherence in Kondo alloys*	Claudine Lacroix	**I-05**
9:30-10:00	*Anisotropic Magnetic Field Dependence of Non-Fermi Liquid Behavior in Quadrupolar Kondo Compound* $Pr_{0.05}La_{0.95}Pb_3$	Tatsuya Kawae	**I-06**
10:00-10:15	*Spin-orbital entanglement in magnetic quantum materials*	Dorota Gotfryd	**O-08**
10:15-10:30	*Magnetism and crystal-field states in the Kondo-lattice antiferromagnet* $CeRh_2Si_2$	Ryszard Radwański	**O-09**
10:30-11:00	*Break*		
S7	**Session 7: Magnetism and superconductivity** **Chairperson: Zbigniew Tarnawski**		
11:00-11:30	*Magnetism, superconductivity and magneto-transport properties of Eu-based ternary pnictides*	Zbigniew Bukowski	**I-07**
11:30-12:00	*Probing the superconducting state of* Ce_3PtIn_{11}	Jeroen Custers	**I-08**
12:00-12:15	^{57}*Fe and* ^{151}*Eu Mössbauer studies of 3d-4f spin interplay in* $EuFe_{2-x}Ni_xAs_2$	Artur Błachowski	**O-10**
12:15-12:30	*Effect of Gd doping on the magnetic properties of* $CeNi_5$ *melt-spun ribbons*	Andrea Dzubinska	**O-11**
12:30-14:00	*Lunch break*		
S8	**Session 8: Actinides II** **Chairperson: Antonio Pereira Gonçalves**		
14:00-14:30	*Non-collinear magnetism in* β-UH_3	Dominik Legut	**I-09**
14:30-14:45	*Electrical Resistivity measured on FIB-structured microdevices*	Silvie Mašková-Černá	**O-12**
14:45-15:00	*Why the cubic phase of uranium ?*	Kim-Ngan N.-T.H.	**O-13**

15:00-15:15	*Photoelectron spectroscopy and magnetism of U hydrides*	Oleksandra Koloskova	**O-14**
15:15-15:30	*Magnetism and superconductivity in complex noncentrosymmetric $M_4Be_{33}Pt_{16}$ (M = Y, La-Nd, Sm-Lu, Th, and U) compounds*	Primož Koželj	**O-15**
15:30-16:00	*Break*		
S9	**Session 9: Novel materials and techniques Chairperson: Zbigniew Bukowski**		
16:00-16:30	*TOF-SIMS uranium isotopes spectrometry of small and around-natural enrichment in the nuclear forensic science*	Itzhak Halevy	**I-10**
16:30-17:00	*Revealing intrinsic properties of solid-state materials*	Eteri Svanidze	**I-11**
17:00-17:15	*^{57}Fe Mössbauer studies of 122-iron arsenides*	T.T.Ha Nguyen	**O-16**
17:15-17:30	*A typical heavy fermion system $CeRh_2As_2$*	Andrzej Ptok	**O-17**
Wednesday, April 21, 2021			
S10	**Session 10: Exotic f-electron systems Chairperson: Eteri Svanidze**		
9:00-9:30	*The dual U 5f electrons and phonon anomalies (rattling) in caged UTE_2Al_{10} systems (TE = Fe, Ru, and Os)*	Małgorzata Samsel-Czekała	**I-12**
9:30-9:45	*Origin of large low-temperature specific heat in topological Kondo insulator SmB_6*	Dawid Nałęcz	**O-18**
9:45-10:00	*Intermediate Valence Behavior of $Yb_2Cu_9Al_8$*	Martin Juckel	**O-19**
10:00-10:15	*The interplay of 4f states and superconductivity in $CeIr_3$: DMFT study*	Sylwia Gutowska	**O-20**
10:15-10:45	*Break*		

S11	**Poster *session (3 minutes – 3 slides presentation)* Chairperson: Hoa Kim Ngan Nhu-Tarnawska**		
10:45-11:15	*EXAFS as a Probe of Actinide Oxide Formation in the Tender X-Ray Regime*	James Tobin	**P1**
	Observation of c-f hybridization gap in heavy-fermion system $EuNi_2P_2$ by using Point-contact spectroscopy	Takuya Takahashi	**P2**
	Magnetism of $TmFe_4CoAl_7$ single crystal (authors: A.V. Andreev et al.)		**P3**
	Pseudogap state in untwinned $YBa_2Cu_3O_{7-\delta}$ single crystals (authors: Omelchenko L.V.)		**P4**
	Magnetization-Induced Band Shift in ferromagnetic Weyl Semimetal $Co_3Sn_2S_2$ (authors: Xianggang Qiu et al.)		**P5**
	Influence of strontium atoms substituting on the electronic properties of the $K_{0.5}Bi_{0.5}TiO_3$ studied by ab initio methods	Grzegorz Jagło	**P6**
	Summary and Closing		
11:15-11:30	*Summary*	Silvie Mašková-Černá	
	Closing	Hoa Kim Ngan Nhu-Tarnawska	
11:30:12:30	***On-line round-table discussion***		

PL - Plenary lecture
HI - Honored invited talk
I - Invited talk
O - Oral talk
P - Poster
SD - Studia doktoranckie

Plenary lectures
and
invited talks

Research on Magnetism and Superconductivity of *f*-metal intermetallic compounds starting in the seventies of the 20th century

Jaap J.M. Franse
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An overview is presented of the evaluation of research on d-metals, Rare Earths and Actinides in the past fifty years at the University of Amsterdam. Special attention is given to the intense cooperation with research groups in Poland and the Czech Republic.

After finishing my own PhD program in the year 1969 on the magneto-crystalline anisotropy energy of Nickel and its interpretation in terms of energy bands shifting through the Fermi level upon rotation of the magnetisation vector, I was invited to join the Academic Staff of the Physics Laboratory at the University of Amsterdam. My first task was to start a research program on magneto-volume phenomena in weakly ferromagnetic alloys and intermetallic compounds. I developed equipment for magnetisation measurements under high hydrostatic pressures, a capacitance cell for thermal expansion measurements at low temperatures and techniques for measuring volume magnetostriction, susceptibility, specific heat, resistivity, Hall effect, etc. It was a period in which experimental equipment was designed by physicists themselves and constructed in the instrumental workshop of the institute. The results of the experiments on magneto-volume phenomena could successfully be combined in an analysis within the Stoner-Edwards-Wohlfarth theory. In my role as researcher, I was involved in the start of fruitful cooperation with many researchers from Eastern European countries as Poland, Czechoslovakia, Romania, Ukraine and Russia apart from the regular contacts with colleagues from West-European countries, the United States and Japan.

During the seventies of the 20th century large progress was made in the field of hard magnetic materials. Intermetallic compounds like $SmCo_5$ and Sm_2Co_{17} opened a new frontier in the search for better permanent magnets. In Amsterdam, it did realise us that there was reason to include the Rare-Earth (RE) metals in our research program as well. Our institute disposed of an unique semi continuous high magnetic field installation with magnetic fields up to 40 tesla and a pulse duration up to one second [1] that made the installation suited for RE metals research. I mention two examples of high-field experiments by Roeland and co-workers: (a) the high field magnetic susceptibility of Gd metal was measured in order to check the results from energy band calculations by Freeman and (b) an energy level crossing of the two lowest energy levels of Praseodymium metal was observed around 20 tesla. Parallel to these investigations research was carried out by Schinkel, De Boer and co-workers on, what were called, valence fluctuation or intermediate valence compounds like YbCuAl and $CeSn_3$. Those years, we had regular visitors from the Institute of Low Temperature and Structure Research in Wroclaw, contacts that started at the ICM'76 in Amsterdam.

Together with Peter de Châtel, I was responsible for the Proceedings of that conference and in that position I met many physicists from East and West, among them Henryk Szymczak from Warsaw and Jozef Spałek from Krakow with whom fruitful interactions developed in the following years.

My first attempts in the study of RE metals was a series of experiments on the magnetocrystalline anisotropy energy of a Gd metal single crystalline sample in order to trace the effects of temperature and pressure on the 5d electron states that contribute appreciably to the magnetic moment of Gd (7.63 μ_B per Gd atom, 7 μ_B from the 4f electron spins in the half-filled 4f shell and 0.63 μ_B from polarisation of conduction, mainly 5d, electrons). In high-pressure magnetic anisotropy measurements at low temperature we could show that 5d electron states near the Fermi level are in an appreciable way responsible for the magnetic anisotropy, in line with the De Haas–Van Alphen studies on Gd under high pressure. These results were reported in 1980 at the Crystalline Electric Field Conference in Wrocław [2]. My visit to Wrocław in 1980 was the start of my collaborations with this institute on uranium-antimony or arsenic compounds [3,4]. The emphasis at the Wrocław conference was directed to the energy-level schemes in pure RE metals and in their (inter)metallic compounds and followed the research lines of preceding conferences. At that time a lively discussion emerged on the valence state of several of the RE metals like Ytterbium and Cerium and their intermetallic compounds. The term 'valence fluctuations' expressed the unstable valence state in which some of these metals and (inter)metallic compounds behaved as function of temperature, composition, pressure etc. Subsequent Rare Earth conferences were devoted to these phenomena and step by step the Actinides were included as can be seen from the name of the Grenoble Conference in July 4-7, 1986: International Conference on the Anomalous Rare Earths and Actinides (ICAREA). Within these anomalous metals and intermetallic compounds, a new class already emerged in the early eighties which became known as the 'heavy fermion' compounds. Characteristic for these compounds are the large values for the effective electron mass that is developed at low temperatures. Values for the electron mass enhancement of 100 to 1000 were reported. As a big surprise superconductivity was found in several heavy-fermion compounds like $CeCu_2Si_2$, UBe_{13} and UPt_3. It gave rise to a new series of conferences under the name that was fixed in 1991 'Strongly Correlated Electron Systems' (SCES), a series of conferences that still exists. Professor Kasuya, one of the founders of the RKKY interaction, played a major role in these discussions. In order to describe these materials, the Kondo effect was mentioned and the term Kondo Lattice was introduced. The systems, however, turned out to be too complex to define them with a single expression.

Prior to my stay in Wrocław in 1980, I visited the Physics Department of the Charles University in Prague where I met the research group of Vladimir Sechovsky and co-workers. In 1985 Sechovsky paid a visit to our institute in Amsterdam which was the start of a longstanding cooperation with our institute, a cooperation that still holds on and was focused on ternary uranium intermetallics [5]. During many years, Vladimir Sechovsky and Ladislav Havela brought their research programme on UTX (U is Uranium, T is Transition Metal, X = Al, Ga, Sn) and other U-based compounds to Amsterdam for performing high-field magnetisation measurements and stimulated young scientists to join this programme in Amsterdam. Alexander Andreev became member of this research team and was a regular visitor to Amsterdam as well.

The entrance into the Rare Earth and Actinide systems forced us to upgrade our sample preparation facilities. It happened that I received in 1978 a letter by Alois Menosky from Prague, in which he proposed to arrange a visit for him in The Netherlands. That suggestion fitted well with my growing interest in the actinide intermetallics. Our institute was a relatively 'open' institute. Visitors from abroad were always welcome to carry out part of their research programme in our institute, especially in the unique 40 tesla high-magnetic-field installation. It brought us in contact with scientists from all over the world and with regular visitors from Poland, Czechslovakia, Austria, Romania, in particular. And later on, from Vietnam, Japan, China and Russia. The world of magnetism research in actinide compounds was rather small in the seventies. A leading position was taken by the Institute for Low Temperatures and structure Research in Wrocław and its director W. Trzebiatowsky. By the intensive international contacts physicists at other places were stimulated to enter into the magnetic research on these actinide compounds. And Menovsky, before he started to work on uranium compounds at the Charles University in Prague, worked for some time in Wrocław and took advantage of the sample preparation knowledge that was developed in the institute. At arriving in Amsterdam in 1979, it took Menovsky one to two year to finish a three-arc Czochralski crystal-growth equipment for highly reactive materials as all of the rare-earth metals and uranium are [6]. intermetallic compounds of the 4f and 5f series were no longer out of our view and could be produced as single-crystalline samples of high purity. And, being in the position to prepare the uranium intermetallics, we had to make choices where to concentrate our research efforts. We started with the Laves-phase compounds and performed high-pressure and high-magnetic-field studies on the Laves-phase compounds UFe_2, UCo_2, UNi_2 and UAl_2. We extended these experiments to other UX_2 compounds (X = Pt, Ge, Ga) with different crystallographic structures and studied the neighbouring compounds as well (UX, U_4X_3, UX_3 etc.) by preference on single-crystalline samples. Most fascinating we found the U:Pt series to be with complex magnetic behaviour of UPt and strong indications for heavy-fermion behaviour in UPt_3. This latter compound turned out to be one of our most intriguing intermetallic compounds and I shall return to it later.

But not only the uranium compounds like UBe_{13} and UPt_3 were at the centre of solid-state research. The discovery of $Nd_2Fe_{14}B$ opened new routes for application of RE compounds in magnetic devices and renewed the interest in the magnetic properties of the RE intermetallics worldwide. The European Commission started in 1984 a Concerted European Action on Magnets (CEAM) with Michael Coey and Dominique Givord as driving forces in which research groups all over the European Union participated, including associate countries in Eastern Europe. High-magnetic field experiments on single-crystalline samples brought better understandings of the crystal-field and exchange interactions in these materials with the immediate consequence that financial support was more easily available for rare-earth compared to uranium research. The group of Karol Krop at the Solid State Physics Department of the University of Mining and Metallurgy in Krakow (at present the AGH University of Science and Technology) worked as well on the RE intermetallic compounds and a very fruitful cooperation was established [7]. Two of his co-workers spent several years in Amsterdam, working on crystal-field calculations for RE intermetallic compounds (Ryszard Radwański) and on the Amsterdam programme for UPt_3, high T_c

superconductors and specific-heat measurements down to 100 mK (Zbigniew Tarnawski).

These circumstances prevented, in fact, a full devotion of our research programme towards the actinide compounds. When I now observe the more recent publications on materials like UGe_2 or UGa_3, I get the feeling that we missed some important findings. On the other hand, the work on the RE intermetallics and on the compound UPt_3, in particular, was fascinating and I am satisfied with the choices we made at that time. I have to add to this point that, from the year 1979 on, I became involved in a scientific collaboration with Vietnamese physicists from the University of Hanoi, a collaboration that was based on the study of magnetism in the RE intermetallics with an open eye for possible applications. Within this cooperation programme, Hoa Kim Ngan Nhu-Tarnawska performed her research on spin-fluctuation phenomena in $REMn_2$ compounds and received the doctors title at the University of Amsterdam [8]. During her stay in Amsterdam she was involved in the research programme on RE- and U-based compounds in general. Karol Krop took part in this cooperation on several occasions. This cooperation with Vietnam was certainly another argument to continue magnetism research on the rare-earth intermetallics in Amsterdam for which we had, as mentioned before, fruitful cooperation with Polish and Czech research groups as well [9-11]. In that same period Frank de Boer extended his cooperation with scientists from the Academica Sinica in China on the RE intermetallics.

Before the discovery of the heavy-fermion superconductors and (a few years later) the high-temperature superconductors, there were some simple rules that governed superconductivity: the mechanism behind superconductivity is the electron-phonon interaction; the maximum value for the superconducting transition is around 25 K, magnetism is in competition with s-wave superconductivity and a coexistence of magnetic order and superconductivity is not expected, especially not for itinerant-electron systems. p-wave and d-wave superconductivity was hardly mentioned, just like other interaction mechanism between electrons in the superconducting state. That picture has been changed by the observation of superconductivity in strongly correlated electron systems and in high-temperature superconductors. Work on the high-T_c superconductors was carried out in cooperation with co-workers from the Institute of Physics of the Polish Academy of Science in Warsaw and from the Solid State Department of the University of Mining and Metallurgy in Krakow [12,13].

I mentioned the compound UPt_3 for which three different superconducting phases in the B-T plane have been observed below 500 mK, besides spurious short-range antiferromagnetic fluctuations below 6 K. The present report is too short to mention all the peculiarities of this system. Apart from the antiferromagnetic fluctuations that further have been studied in alloying experiments for the series $U(Pt,Pd)_3$ with Pd concentrations up to 10 at% Pd, long-range antiferromagnetism has been observed for Pd concentration above 2 at% with a maximum value of T_N of 6 K for 5 at% Pd and with uranium moments up to 0.5 μ_B per uranium atom. Lowering the Pd concentration makes the antiferromagnetic order weaker. In detailed experiments (μSR and neuron scattering) the critical composition has been established as 0.6 at % Pd. On the occasion of the hundredth issue of the Journal Acta Physica Polonica A, I reviewed the anomalous superconductivity and antiferromagnetism in the $U(Pt,Pd)_3$ system [14]. At the SCES Conference of 2002 in Krakow, I was approached by Josef Spałek to present

the summary of that conference, an honour that I shared with Jacques Flouquet and Gerry Lander. And since in later years new experimental and theoretical findings failed to appear for this class of materials, the interests of the scientists moved to new directions like topological semiconductors/superconductors and other phenomena that trigger the imagination but fall outside the experience of the author.

The long-term fruitful cooperation with the Amsterdam research groups and the possibility of working with all the facilities of the research laboratory in Amsterdam became a firm background for further developments of many Eastern European scientists. And not only in the development and achievement of their own research topics, the experience for years with the scientific life in Amsterdam has motivated them to build up research facilities in their own institutions. From my side, I had the privilege to attend several conferences on magnetism and magnetic materials in Poland in the eighties and nineties of last century and I could profit from inspiring contacts with many Polish scientists.

In this report for CCFES2020/2021, a conference that is jointly organised by scientists from Prague and Krakow, I would like to thank the Czech and Polish people, with whom I had long-term contacts that continued for years after their visits and stays in Amsterdam. I am grateful for having received an Honorary Professorship at the Institute for Low Temperatures and Structure Research of the Polish Academy of Sciences in Wroclaw in 1998 and for being elected as Foreign Member of the Polish Academy of Sciences in 2001.

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Notes from the Organizing Committee of CCFES2021:
This historical recall from Prof. Jaap Franse has been prepared for CCFES2020. A special celebration gathering has been then scheduled (on-site) to highlight the significant personal and professional contribution of Prof. Jaap Franse to the fruitful cooperation in the f-electron research.

Quantum criticality driven by magnetic field

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For the past few decades, the unsettling thrust to understand the enigmatic physics near a quantum phase transition (QPT) has motivated condensed-matter research community to explore more about this precarious point of instability. In contrast to a conventional classical phase transition that is driven by temperature, QPT can be tuned by nonthermal parameters such as external pressure, chemical pressure (doping), or magnetic field. However, there are some difficulties while employing pressure and chemical doping as tuning parameters. Namely, it can be fairly challenging to carry out thermodynamic measurements at ultra-low temperatures and under high pressure, whereas alloying tends to introduce disorder-driven effects, which cannot be separated from the quantum criticality of the translationally invariant parent phase. In this regard, magnetic field appears to be of particular usefulness as it can reversibly and continuously tune the system towards QPT, without encountering the aforementioned complexities.

In our lecture, we will first recall a few examples from the literature of successful research into quantum critical phenomena driven by an external magnetic field. We will then present our own results of our recent studies on the metamagnetic behavior in the novel cerium compound $CePtIn_4$ [1-3]. By analyzing the magnetic field dependencies of its magnetic susceptibility, magnetoresistance and specific heat at very low temperatures, we constructed a fascinating magnetic phase diagram, where continuous suppression of the Néel temperature in a mean field-like manner is terminated at a tricritical point, which is likely also a triple point in the system, separating antiferromagnetic, paramagnetic, and intermediate metamagnetic states. Beyond this point, the transition splits into two first-order metamagnetic-like boundaries, which approach two separate quantum critical end points as $T \rightarrow 0$. Our findings significantly expand the frontier of QPTs controlled by the magnetic field, thus generating an opportunity to further exploit experimental and theoretical understanding of the associated perplexing physics.

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Superconductivity enhanced by atomic disorder

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We investigated the effect of enhancement of superconducting transition temperature T_c by nonmagnetic atom disorder in the series of filled skutterudite-related compounds ($La_3M_4Sn_{13}$, $Ca_3Rh_4Sn_{13}$, $Y_5Rh_6Sn_{18}$, $Lu_5Rh_6Sn_{18}$; M= Co, Ru, Rh), where the atomic disorder is generated by various defects or doping. We have shown that the disorder on the coherence length scale ξ in these nonmagnetic quasiskutterudite superconductors additionally generates a non-homogeneous, "*high-temperature*" superconducting phase with $T_c^* > T_c$ (dilute disorder scenario), while the strong fluctuations of stoichiometry due to increasing doping can rapidly increase the superconducting transition temperature of the sample even to the value of $T_c^* \sim T_c$ (dense disorder leading to strong inhomogeneity).

This phenomenon seems to be characteristic of high-temperature superconductors and superconducting heavy fermions, and recently have received renewed attention.

We documented experimentally the stronger lattice stiffening of the inhomogeneous superconducting phase T_c^* in respect to the bulk T_c one and propose a model that explains the $T_c^* > T_c$ behavior in the series of nonmagnetic skutterudite-related compounds.

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Effects of composition on the UFe_xSb_2 system

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Uranium-based materials show a vast and rich diversity of physical properties and electronic ground states, some of them unique. Their fascinating behavior is driven by factors like the large 5*f* spin-orbit coupling, which can control properties as the magnetic anisotropy, or the degree of delocalization of the 5*f* states, that can induce a large renormalization of the electric and magnetic polarizabilities.

Renormalization effects have been observed in the binary antimonide USb_2 that crystallizes in the anti-Cu_2Sb tetragonal structure. This compound orders antiferromagnetically below T_N = 203 K, with the magnetic structure formed by uranium moments aligned parallel to the *c*-axis, forming a sequence of + + - - + + - - ferromagnetic sheets along the *c*-axis. USb_2 has anisotropic electronic properties and a Sommerfeld coefficient of γ = 25 mJ/mol.K^2, typical for correlated uranium compounds. Recently, the uniqueness of USb_2 was highlighted by the discovery of non-trivial phase transitions induced by pressure and magnetic field, indicating a remarkably rich phase diagram.

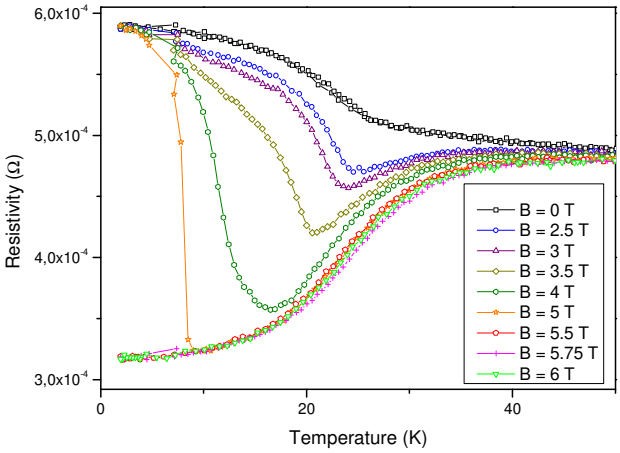
Interestingly, it is possible to intercalate layers of transition elements into the USb_2 tetragonal structure, forming stable ternary intermetallic alloys, UT_xSb_2 (T = Fe, Co, Ni, Cu, Ru, Pd, Ag, Au; $0 \leq x \leq 1$), that also crystallize in the *P*4/*nmm* space group but with the isotype $HfCuSi_2$ structure. Large stoichiometric variations are observed, changing the U-(nearest neighbors) distances and, consequently, the ligand-driven hybridization. Therefore, the study of UT_xSb_2 compounds can give important information that complements the USb_2 investigations.

The first systematic studies made on UT_xSb_2 alloys indicated a magnetic ground-state, except in the case of Fe and Co, where its existence was not possible to determine due to the presence of magnetic impurities [1]. The mechanism for the magnetism was first pointed out to be the interplay between superexchange via the metalloid ions and Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction via the conduction electrons. However, the variety of magnetic ground-states displayed by UT_xSb_2 lead to the evidence that *f-p*, *d* hybridization is a key factor determining their magnetic behavior. Among them, $UCuSb_2$ and $UAuSb_2$ were reported to be ferromagnets, while $UNiSb_2$, $UPdSb_2$ and $URuSb_2$ are antiferromagnets. The electronic states of these compounds are most likely quasi-two-dimensional, as in USb_2, which was confirmed for $UCo_{0.5}Sb_2$ that shows a strong ferromagnetic Kondo behavior with two-dimensional weak localization.

Recently, the physical properties of a $UFeSb_2$ polycrystalline sample and $UFe_{0.6}Sb_2$ single crystals were investigated [2,3]. In those studies it was evidenced a ferromagnetically ordered state below T_C = 31 K for both compositions. ^{56}Fe

Mössbauer spectroscopy measurements clearly indicated that the main contribution to the magnetic ordered state comes from the uranium sublattice, pointing to a non-negligible hybridization of uranium and to magnetism of itinerant character. $UFe_{0.6}Sb_2$ was found to be anisotropic, with the easy-magnetization direction being [001]. However, the adjustment of the high temperature magnetic susceptibility data of $UFe_{0.6}Sb_2$ to a modified Curie-Weiss law yielded an effective moment of μ_{eff} ~ 3.61 μ_B/U, which strongly contrasts with the value obtained for $UFeSb_2$ polycrystalline samples (1.2 μ_B/U).

In order to contribute to a better understanding of this large family of compounds we decided to prepare and characterize other compositions from this system, UFe_xSb_2 (x = 0.5, 0.7). *Ab* initio calculations of UFe_xSb_2 (x = 0.5, 1) electronic structures, which would allow a better understanding on the origin of the unusual physical properties observed, were also performed. In this talk, we will present the results obtained for both samples, $UFe_{0.5}Sb_2$ polycrystalline materials and $UFe_{0.7}Sb_2$ single crystals, which evidence a complex magnetic behavior that can be explained by an unusually steep local minimum in the density of states close to the Fermi level.



Electrical resistivity $UFe_{0.7}Sb_2$ as a function of temperature for different applied magnetic fields (B // [001] and I // [010]).

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High-spin Ni states in a model for doped NiO_2 planes in $NdNiO_2$

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Superconductivity found in doped $NdNiO_2$ is puzzling as two local symmetries of doped NiO_2 layers compete, with presumably far-reaching implications for the involved superconductivity mechanism. In spite of great similarity between CuO_2 and NiO_2 planes, there are substantial differences in the electronic structure. While La_2CuO_4 is a charge-transfer system, the NiO_2 planes in $NdNiO_2$ have large charge-transfer energy $\Delta \sim 7$ eV which indicates more a Mott-Hubbard system [1]. Perhaps the most important difference between the above two classes of materials is that only one band crosses the Fermi level in cuprates, while two bands cross the Fermi level in nickelates [2].

A cuprate-like regime with Zhang-Rice (ZR) singlets is then replaced by the regime of local triplet states for increasing values of charge-transfer energy, which would suggest a rather different scenario of high-T_c superconductivity [3]. The latter transition occurs in an abrupt way in the impurity model [1], while here we find a gradual change. We address this competition by exact diagonalization of Ni_4O_8 clusters with periodic boundary conditions [4]. The model contains Ni—O hopping t_{pd}, interoxygen hopping t_{pp}, and the Kanamori parameters at Ni $\{U_d,J_d\}$ and O $\{U_p,J_p\}$ ions. With increasing value of charge-transfer energy we observe the expected crossover from the cuprate regime dominated by ZR singlets (S=0) to local triplet (S=1) states upon hole doping. We find that a smaller charge-transfer energy Δ is able to drive this change of the ground state character when realistic values for nickel-oxygen repulsion U_{dp} are taken into account. For large values of the charge-transfer energy, oxygen orbitals are less important than in superconducting cuprates as their finite spectral weight is found only at rather high excitation energies. Orbital-resolved hole densities are shown in Fig. 1(a)—they change from an almost equal density distribution between x^2-y^2 and $2p$ orbitals in ZR singlets at small Δ to nearly complete hole localization in x^2-y^2 (b_1) orbitals at large $\Delta \sim 7$ eV. While the parameter U_{dp} (intersite Ni—O Coulomb repulsion) has almost no influence here, it changes radically the hole distribution in doped systems and reduces (extends) there the region of ZR $|b_1 L_{b1}\rangle$ singlets ($|a_1 b_1\rangle$ triplet states) [4], see Fig. 1(b). The Hubbard subbands survive the doping and change from the hybridized d—p states known from cuprates to triplet $|a_1 b_1\rangle$ states for nickelates with increasing charge-transfer energy Δ.

To illustrate the nature of the electronic states, we studied the occupied/empty hole states in the thermodynamic limit by variational cluster approximation (VCA) [5]. As the $(NiO_2)^{3-}$ plane is negatively charged, we use the hole notation. In the undoped systems this means the filling of one hole per each NiO_2 unit. We consider such a system and show that the undoped NiO_2 plane is insulating. Whether or not this

corresponds to the real situation in $NdNiO_2$ is an open question—we suggest that this system is in a poor metallic state with considerable self-doping when electrons are transferred from Nd ions to NiO_2 planes. It increases the hole concentration beyond one hole per NiO_2 unit.

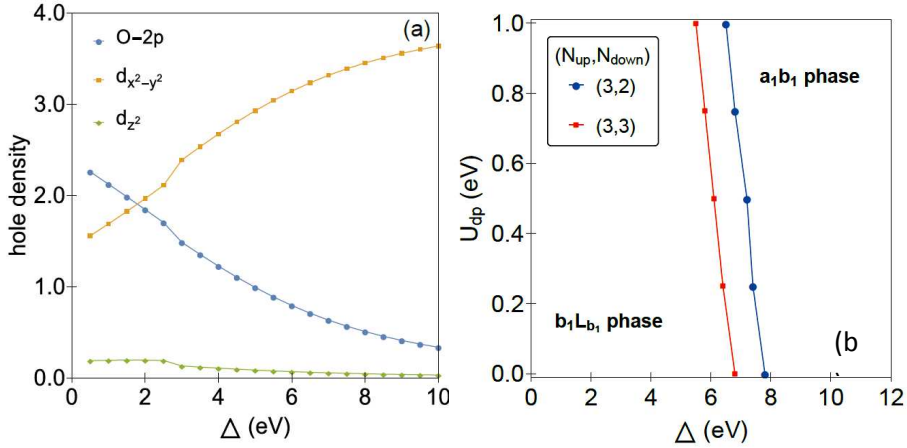

Fig. 1. For increasing Δ in the periodic Ni_4O_8 cluster: (a) hole densities as obtained for the undoped cluster with N(up)=N(down)=2 holes, and (b) phase diagram for doped cluster with (3,2) or (3,3) holes in the {Δ,U_{dp}} plane. Lines in (a) show the hole number in Ni(x^2-y^2) orbitals (orange), in O(2p) orbitals (blue), and in Ni(z^2) orbitals (green). Other parameters (all in eV): t_{pd}=1.3, t_{pp}=0.55, U_d=8.34, J_d=1.18, U_p=4.4, J_p=0.8.

Next to x^2-y^2, a second Ni(3*d*) a_1 orbital, either *xy* or z^2, becomes relevant in doped materials [6] and provides another possibility of triplet $|a_1b_1>$ states formation, with x^2-y^2 holes. Both the above orbitals may be occupied by holes following quantum chemical calculations [7]. While it is natural to consider two e_g orbitals, in nickelate films *xy* orbitals are preferentially occupied which we simulate by large crystal-field splitting of z^2. Using VCA we have verified that the results are qualitatively the same and a triplet arises at Ni ions, independently of the symmetry of the occupied orbitals. Our result that U_{dp} favors local triplets implies that correlation effects beyond purely on-site interactions should be taken into account when obtaining effective two-band models.

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Towards a better understanding of the RKKY interaction in heavy-fermion systems

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The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between 4f-magnetic moments plays an important role in intermetallic rare-earth compounds. At low temperatures, these materials exhibit very rich phase diagrams with a plethora of co-existing or competing quantum phases including heavy fermions, unconventional superconductivity and unusual magnetism.

The central focus of the present paper is a comprehensive computational scheme which allows for a more quantitative understanding of the RKKY interaction in Ce- and Yb-based heavy-fermion compounds. The scheme fully accounts for the anisotropies in the 4f-states resulting from the Crystalline Electric Field (CEF). In addition, realistic conduction band dispersions with several bands intersecting the Fermi energy are used in the derivation. Starting from a periodic Anderson model, we show that the anisotropy of the CEF ground state manifests itself in the anisotropy of the effective exchange coupling constant J(**R**, **R**') between two moments at sites **R** and **R**' while the interaction between two Kramers doublets is isotropic in pseudo-spin space.

We evaluate the exchange constant for various models of the conduction states in tetragonal Ce- and Yb-122 compounds.

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Enhanced Spin-Orbit Interaction in the Underscreened Anderson Lattice

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We investigate the effect of many-body interactions on the spin-orbit coupling of anisotropic metals. We use the Underscreened Anderson Lattice Model that was proposed to describe uranium and plutonium compounds [1]. By using a rotationally invariant approximation [2], we show that Coulomb interactions induce off-diagonal correlations that enhance the components of the spin-orbit coupling [3]. Even modest values of the Coulomb interaction U can enhance the spin-orbit coupling by factors of about 4 and have significant effects on the occupied and unoccupied portions of the electronic spectrum, but the enhancements are most pronounced for systems that are on the verge of magnetic instabilities. The enhancement is anisotropic in crystals with non-cubic symmetries and can lead to giant magnetic anisotropies in paramagnetic states.

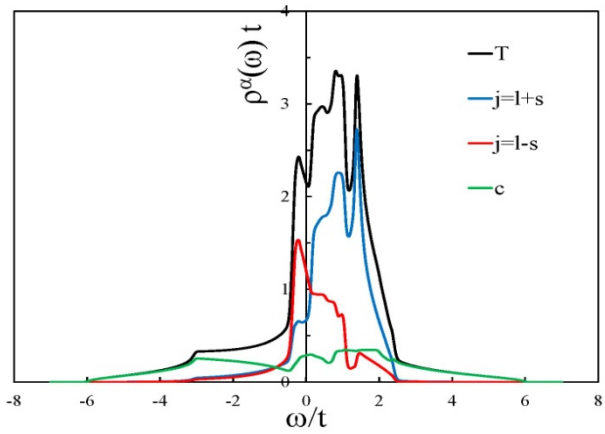

Fig. 1. Total density of states and its decomposition into (j, j_z) eigenstates and conduction states.

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Coherence in Kondo alloys

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Kondo alloys are realized in many different families of strongly correlated systems where magnetic impurities are distributed randomly in a metallic crystal and interact with conductions electrons. For small concentration, x, of Kondo impurities, Kondo effect leads to the formation of local singlets, while in the case of Kondo lattice (x=1), a coherent Fermi liquid state can be stabilized. While these 2 limits are well understood, the nature of the ground state for intermediate values of x was not so well understood.

We have studied the influence of different parameters within a Kondo alloy model: in particular we point out the importance of the number of conduction electrons per site, n_c, besides the relative values of Kondo interaction, J_K, and the bandwidth W.

Several new results will be presented, concerning both magnetic and non-magnetic phase-diagrams of a Kondo alloy. In the non-magnetic phase we show that photoemission experiments may reflect the breakdown of coherence when concentration decreases.

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Anisotropic Magnetic Field Dependence of Non-Fermi Liquid Behavior in Quadrupolar Kondo Compound $Pr_{0.05}La_{0.95}Pb_3$

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New phenomena associated with quadrupolar or higher order multipolar moments in *f*-electron compounds have been attracting much attention in the past few decades. Among these compounds, Pr-based compounds with a Γ_3 doublet ground state in the cubic crystal-electric-field have been studied extensively in connection with the quadrupolar Kondo effect (QKE) [1,2]. Because of *c*–*f* hybridization, the QKE is characterized by two electron channels owing to the correlation between the Γ_3 doublet and the charge of conduction electrons, leading to non-Fermi liquid (NFL) behavior characterized by a divergent logarithmic temperature dependence of the electronic specific heat coefficient (C_{el}/T) and the quadrupolar susceptibility at sufficiently low temperatures. In $Pr_xLa_{1-x}Pb_3$ for $x \leq 0.05$, NFL behavior with $-\ln T$ dependence is observed in the electronic specific heat C_{el}/T below $T \sim 2$ K, where C_{el}/T at each concentration can be scaled by a characteristic temperature [3].

To examine the realization of QKE as the origin of NFL behavior in $Pr_xLa_{1-x}Pb_3$ for $x \leq 0.05$, we focus on the dependence of the NFL behavior on the magnetic field along the three principal axes. The field dependence of the antiferro-quadrupolar ordering temperature is well known to be strongly anisotropic owing to the mixing of the higher order multipolar moments induced by the magnetic field. Similarly, in the QKE, the anisotropic dependence of NFL behavior on the field direction should be observed owing to the splitting of the Γ_3 doublet caused by the magnetically coupled Van Vleck process with the triplet excited states.

The magnetic field dependence of C_{el}/T with $-\ln T$-divergent NFL behavior in $Pr_{0.05}La_{0.95}Pb_3$ is strongly anisotropic in all three directions. In H//[100] and [111], the suppression of $-\ln T$ dependence appears at $T \sim 0.65$ K in $H = 4$ T and ~ 0.48 K in $H = 6$ T, respectively, whereas in H//[110], it survives at temperatures as low as the lowest temperature, $T = 0.2$ K. The observed features can be understood by considering the characteristics of the cubic symmetric QKE [4]. Additionally, the field dependence of the quadrupolar susceptibility measured from the nonlinear susceptibility Γ_3 in $Pr_{0.05}La_{0.95}Pb_3$ is consistent with that expected from QKE. Γ_3 shows $-\ln T$ dependence in the [100] and [110] directions below $T \sim 2.5$ K, whereas in the [111] direction, Γ_3 stabilizes to a constant value below $T \sim 2.5$ K [5]. These results indicate that the anisotropic field dependence of NFL behavior is a key feature for manifesting QKE as the origin of the observed NFL behavior.

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Magnetism, superconductivity and magnetotransport properties of Eu-based ternary pnictides

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Europium in intermetallic compounds most often occurs as Eu^{2+}. In this state, it has a large pure spin magnetic moment, which orders ferro- or antiferromagnetically at low temperatures. In most cases, the localized 4f electron system has little effect on the conduction band electrons. Although superconductivity originating from the *3d* Fe electrons and the magnetism of localized 5*f* Eu electrons are electronically separated, a clear interaction of both systems is observed in all compounds investigated. In this presentation, I will overview a few selected groups of Eu-based ternary pnictides, in which the interaction of a magnetically ordered system of localized Eu^{2+} moments with conduction electrons leads to many interesting phenomena.

In $EuFe_2As_2$, a parent compound of iron-based superconductors, the magnetic moments of Eu^{2+} are ordered in an A type antiferromagnetic structure. When $EuFe_2As_2$ is substituted in order to obtain superconductivity, the magnetic structure evolves through the canted antiferromagnetic to ferromagnetic with Eu spins aligned along c axis. As a consequence, Eu ferromagnetism coexists with superconductivity. One of the most interesting phenomena is the occurrence of spontaneous vortices generated by an internal field in a ferromagnetic superconductor. At lower temperatures, coexistence of ferromagnetism with superconductivity leads to the formation of the composite domain and vortex-antivortex structure [1,2].

Another member of the family of Eu-based iron-pnictides is the stoichiometric $AEuFe_4As_4$ with A=Rb [3,4] and Cs [5] in which every second layer of Eu in the parent material is replaced with the layer of nonmagnetic Rb or Cs. These materials have the superconducting transition temperature of T_{sc} = 36.5 K. The resonant X-ray scattering and neutron diffraction measurements demonstrated that the magnetic structure is helical ie. the Eu moments align ferromagnetically inside the layers and rotate 90° from layer to layer [6].

Recently, a new parent compound $EuFeAs_2$ has been synthesized which upon La-doping exhibits superconductivity with the T_{sc} up to 11 K [7]. Further study of $EuFeAs_2$ revealed that the magnetic transition around 100 K is associated with the SDW ordering in the Fe sublattice while the low temperature anomaly at 46 K is attributed to the antiferromagnetic transition of Eu^{2+} sublattice [8]. It is reported that Ni substitution of $EuFeAs_2$ suppresses the SDW transition and superconductivity emerges at T_{sc} = 17.5 K [9]. We have found that Co doping also leads to disappearance of the SDW transition and induces superconductivity with the transition temperature up to 27 K.

Eu-based ternary arsenides of the $CaAl_2Si_2$-type structure attracted great attention of solid state physicists due to the discovery of interesting topological properties in these compounds e.g. $EuCd_2As_2$ is a candidate for an antiferromagnetic Dirac

semimetal [10.11]. Colossal magnetoresistance was recently reported in $EuCd_2P_2$ [12]. Here, we present magnetic and magnetotransport properties of $EuZn_2As_2$ and $EuZn_2P_2$ single crystals.

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Probing the superconducting state of Ce_3PtIn_{11}

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Recently, Ce_3PtIn_{11} a new member of the $Ce_nT_mIn_{3n+2m}$ series has been synthesized [1]. At ambient pressure the compound displays two consecutive magnetic transitions at T_{N1} = 2.2 K and T_N = 2.0 K. Below T_c = 0.34 K the compound becomes superconducting (SC) with an estimated penetration depth λ = 229 nm utilizing BCS theory. Ce_3PtIn_{11} takes an exceptional position in this series of compounds being the only compound exhibiting magnetic and SC ordering at ambient pressure. More intriguing, the compound possesses two inequivalent crystallographic Ce-sites. An analysis of the entropy suggested that the Ce2-sublattice is responsible for the magnetic ordering while the Ce1 is largely Kondo screened, so to say being quantum critical, like the Ce-ion in $CeCoIn_5$ and hence is associated with SC [1]. Very recent ^{115}In NQR experiments corroborate this viewpoint [3,4]. These experiments show, that the critical spin fluctuations are aliated only with the Ce1-site, and the magnetic moment of Ce2 appears to be 20 times larger than the moment of Ce1. A scenario of microscopic coexistence of magnetism and SC as a result of two distinct but likely interacting Kondo lattices is unprecedented in HF physics and opens a whole new realm of states of matter.

Yet, little is known about the SC state in Ce_3PtIn_{11}. In this presentation we will try to shed some light on the SC properties. A pressing question is what is at the origin of the Cooper-pairing as the critical point where the AFM state goes to zero is still far away (the critical pressure needed equals $p_c \approx 1.5$ GPa). Moreover, as shown ^{115}In NQR a sudden drop of spin-relaxation rate $1/T_1$ emerges upon entering the superconducting state suggesting a first order type of transition from the AFM state into the SC one [3]. Such would indicate a breaking of symmetry and implies that magnetic order and superconductivity compete [5]. Interestingly, far below T_c a Korringa-type of evolution of $1/T_1$ at the In-sites is observed. Such behavior can be explained by the existence of a finite density of states (DOS) deep inside the superconducting phase. Low temperature specific heat measurements confirm the presence of uncondenstated heavy quasi-particles in down to lowest temperatures (Fig.

1b) but also reveal a logarithmic temperature dependence of the normal state indicative of the existence quantum critical fluctuations. Likely, Ce_3PtIn_{11} exhibits a second QCP which already affects the physical properties of this compound at ambient pressure.

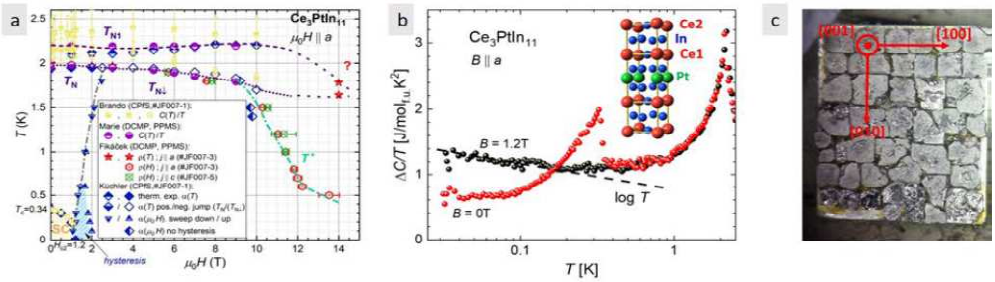

Figure 1: The H - T phase diagram of Ce_3PtIn_{11} for μ_0H // a. Data were collected from specific heat, thermal expansion, magnetostriction, resistivity, and magnetoresistance experiments. Lines are a guide to the eyes. (b) The zero field specific heat and in an applied field of $\mu_0H = 1.2\ T \geq \mu_0H_{c2}$ after subtracting the nuclear contribution arising from In. The log T-dependence points to the presence of quantum critical fluctuations of a nearby QCP. The inset shows the Ce_3PtIn_{11} unit cell. (c) Sample mosaic used for μSR experiment. It consists of 36 co-aligned single crystals ($m_{total} \approx 150$ mg) and covers an area of 4.5 × 5 mm^2.

We conducted zero-field (ZF) and longitudinal field (LF) μSR experiments at temperatures above the magnetic transitions, at temperatures inside the magnetically ordered state and at temperatures below *T*c to solve other important question, which is if SC and magnetism coexist or compete. Despite the small sample size we observed a subtle oscillatory component in the spectra for $T < T_N$ on top of the exponential relaxation decay indicating the presence of an ordered magnetic structure. A weak magnetic field in of only 1 kG was enough to fully decouple the muon and resulting in a time dependence of the spectra which can be described by an exponential. This, combined with the ZF observation of an oscillatory component indicates the presence of a static or quasi-static internal field. For $T < T_c$, the static field increases upon lowering the temperature suggesting that we are tracking an order parameter in the form of a static internal field. Our analysis also implies a microscopic coexistence of AFM and SC in Ce_3PtIn_{11}. Intriguing, at lowest temperatures < 0.2 K this internal field seems to collapse for yet unknown reasons. This deserves more attention in the future.

To conclude, The SC state of Ce_3PtIn_{11} hides even more secrets possibly related to the presence of two distinct Ce-sites.

Acknowledgments

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Non-collinear magnetism in β-UH_3

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Uranium with hydrogen forms 3 different cubic compounds, α-UH_3, β-UH_3 and UH_2, all undergoing ferromagnetic ordering. Our first-principles calculations revealed a complex (non-collinear) magnetic order in β-UH_3. Unlike the other uranium hydrides, α-UH_3 and UH_2, β-UH_3 with two different U sites exhibits a site dependent size and direction of U magnetic moments. While the U moments at the 2*a* sites are locked in the body diagonal direction, the moments at the 6*c* sites are inclined by approx. 15 degrees. The difference stems from 5*f* orbital moments. Comparison of results for all 3 species reveals that the U-U spacing is not the primary parameter to control the magnetism in uranium hydrides. Further insight is provided by evaluating individual exchange interactions between different neighbours, yielding the transition temperatures in a reasonable agreement with experiment.

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TOF-SIMS uranium isotopes spectrometry of small and around-natural enrichment in the nuclear forensic science

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The aim of this research is to explore the methodology for uranium-enrichment identification using TOF-SIMS, establish the reliability of the enrichment detection as compared to traditional ICP-MS isotope detection and develop the technique to apply as part of the evidence chain in the field of nuclear forensics. The need for -improving the forensic techniques for uranium enrichment levels for faster, more reliable tests is ever-growing and might improve the control of nuclear materials. A special emphasis is put on the very small range of sizes, 0.1-20 µm. Measuring bigger samples is much easier but it is averaging and sometimes even causing loss of data. It is averaging between different particles or different inhomogeneous parts of the samples.

The enrichment is defined as $E = {}^{235}U/\sum U$, it is trivial that in the range of enrichment around the natural U, more sensitive parameter will be ${}^{235}U/{}^{238}U$. We mark this ratio to be Θ. In Figure 1, which shows ratio of ${}^{235}U/{}^{238}U$, the difference in slopes is very clear due the different enrichments.

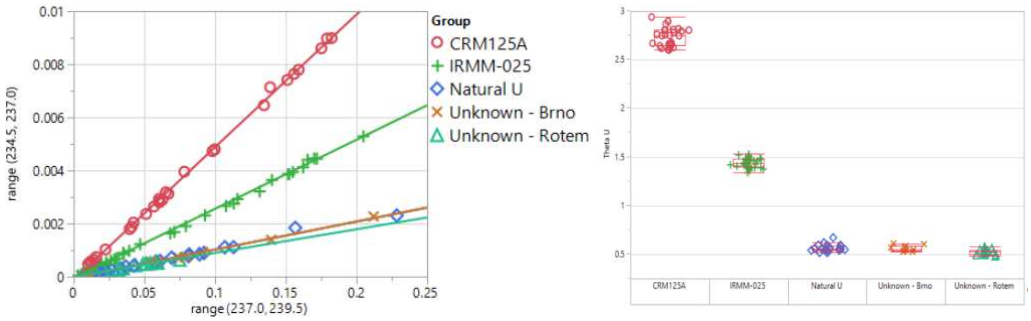

*Figure 1: U^{235}/U^{238} correlation and Θ by **reference** material (CRM125A, IRMM-025 and IAEA-314)*

Using the TOF-SIMS technique, we measure the U, UO and UO_2 intensity of emitted ions simultaneously.

Combining that data from each small sample in increase the sensitivity and reduce the measurements error. Example is given in figure 2.

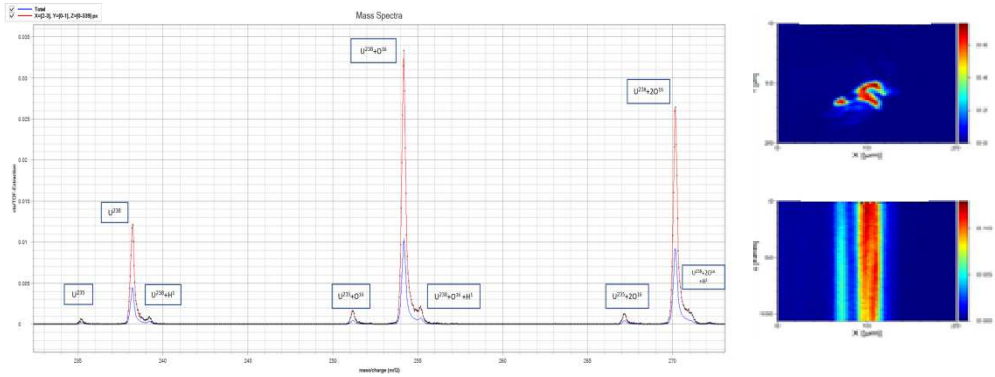

Figure 2: title missing. The entire sample U, UO, UO_2 peaks are marked blue and the zoomed-in peaks are marked red, x,y and z map is given in the right.

The technique used allows to measure the depth profiles of the sample. It means obtaining the TOF-SIMS data as a function of depth.

Since usually the samples in nuclear forensics are very small (picogram range), we have decided to measure several small samples and add the data to get better sensitivity and reduce the measurement error. We measured five different particles and compared the result with one particle with the same number of layers (from the depth profile). SEM photographs and results are given in figure 3 and table 1.

P10	P11	P20	P31	P32

Figure 3: Microscope images of different studied samples chosen by their morphology.

Table 1: enrichment of the different particles or different layers in the depth profile.

Different Particles	P10	P11	P20	P31	P32	Average
Enrichment	0.006503	0.006476	0.008344	0.007397	0.007188	**0.007190**
Recombined	Slice 1	Slice 2	Slice 3	Slice 4	Slice 5	Average
Enrichment	0.007405	0.007151	0.007292	0.007232	0.007121	**0.007249**

Data from all samples measured and their sum are given in figure 4. It is clearly seen that the sensitivity is not good enough for each sample by itself. From the other hand, the sum of those results can give a measurable data.

We proved that choosing samples with the same morphology by SEM gives us more accurate result.

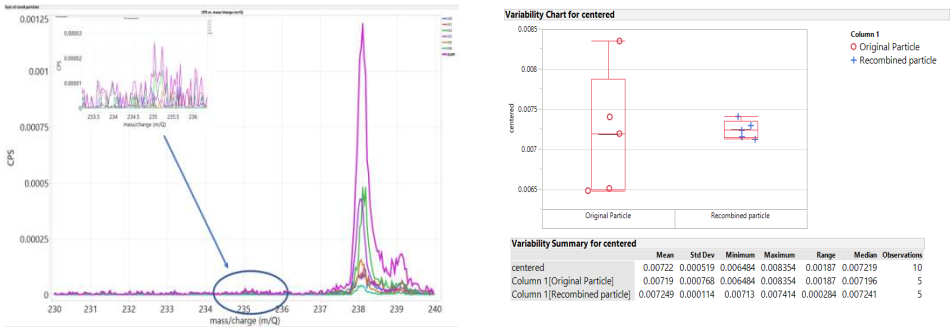

Figure 4: TOF-SIMS analysis of cumulative uranium particles, the isotopes ^{235}U and ^{238}U can be seen and the enrichment is calculated.

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Revealing intrinsic properties of solid-state materials

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Synthesis optimization is a rather lengthy and costly process, during which many obstacles are encountered and, rather frequently, cannot be overcome. This is particularly true when it comes to the *f*-electron materials which have fragile ground states, that are easily affected by crystallographic imperfections. We have previously shown that the physical properties of the heavy-fermion superconductor UBe_{13} are strongly affected by its synthesis conditions [1]. In order to solve this experimental challenge, we have implemented a new approach to study solid-state materials on the micro-scale. In particular, this method allows to examine the intrinsic electrical resistivity of UBe_{13} material by extracting micro- sized domains from a polycrystalline specimen by menas of focused-ion-beam structuring [2]. In order to showcase the proof of principle, we have also applied this technique to Be_5Pt [3] and TaIrGe [4] – materials for which ground state properties can be predicted by theoretical means.

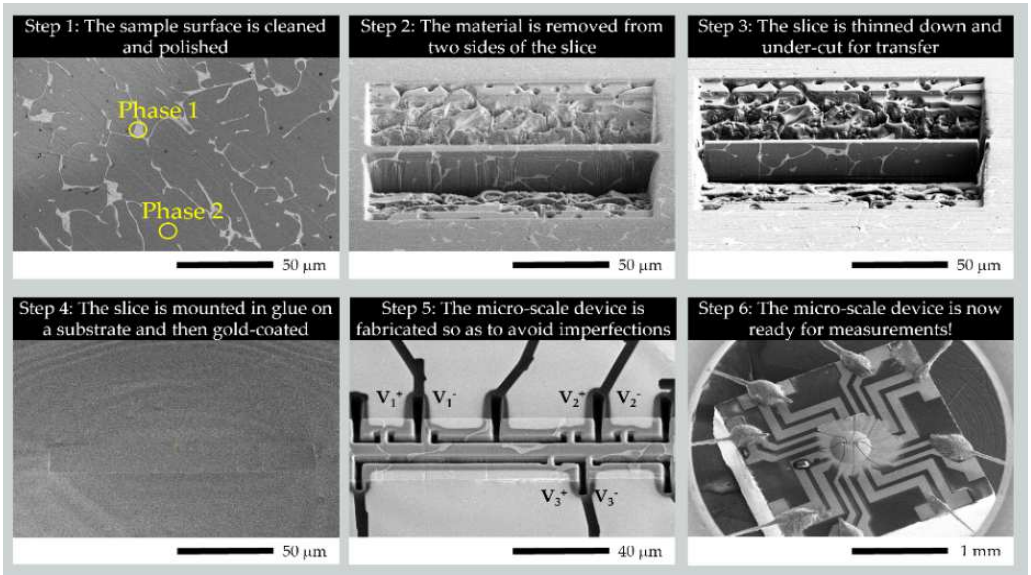

Fig. 1: A polycrystalline material in which Phase 1 is an impurity phase and Phase 2 is the main phase. A micro-scale piece of this material is first isolated using focused-ion-beam structuring. Voltage contacts are then placed so as to avoid Phase 1, which allows to study intrinsic electric resistivity of Phase 2.

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The dual U 5*f* electrons and phonon anomalies (rattling) in caged UTE_2Al_{10} systems (*TE* = Fe, Ru, and Os)

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In memoriam Prof. Dr. Robert Troć (1935-2019)

The orthorhombic (U/Th)TE_2Al_{10} systems exhibit rattling vibrations of the central U/Th atom of the oversized cage formed by the surrounding *TE*-Al atoms [1-5]. Thus anharmonic low-energy Einstein vibrations and their coupling with the conduction electrons lead to a variety of fascinating properties of such materials.

In this review [1-5], electronic structures of these caged compounds, calculated by DFT methods and measured by X-ray photoemission spectroscopy are discussed in the context of a dual nature of the U 5*f* electrons. Their dual character, unveiled also in other experimental data, supported by effective crystal-field calculations, and its influence on the rattling effect, reflected in the transport properties, is considered as well.

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Oral talks

Magnetic entropy analysis using a calculated phonon background – how does it work for UH_3 ?

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Magnetic entropy belongs to key indicators of the character on magnetic moments. In the extreme case of weak itinerant ferromagnets, where magnetic moments collapse right at T_C, the total entropy change ΔS between the 0 K limit (fully ordered moments) and paramagnetic state (no moments) has to be zero. In an opposite case of stable magnetic moments, ΔS should be Rln2 or higher, depending on the multiplicity of the magnetic state just above T_C.

Magnetic entropy contributes to heat capacity $C(T)$, and in practical life one can subtract other contributions due to the lattice C_{latt} and electronic C_e terms so as to asses the magnetic entropy $\Delta S_m(T) = \int_0^T \left(\frac{C_m}{T_1}\right) dT_1$, where C_m the magnetic part of the heat capacity. This can be very well done if T_C is located at low temperatures, where C/T (T^2) is usually a linear function, as $C(T) = C_e + C_{latt}$ can be approximated as $\gamma T + \beta T^3$. As a bonus one obtains the density of electronic states at the Fermi level (from γ) and Debye temperature Θ_D (from β).

However, the linearity does not extend higher than $\approx\Theta_D/10$. Non-Debye character of crystal lattice makes the situation even worse and the ultimate trick to use non-magnetic surrogate data to subtract C_{latt} can be used with some confidence in selected cases only.

This is exactly the case of UH_3, ferromagnet with $T_C \approx 170$ K, which has no non-magnetic analogue and H-related high energy optical modes make the lattice strongly non-Debye like. In this situation we attempted to use advanced ab-initio calculations of lattice vibrations to calculate the phonon spectra. From the density of phonon states $g(E)$ one can obtain $C_{latt}(T) = \frac{\partial}{\partial T}[\int_0^\infty E\, g(E) f(E,T) dE$, where $f(E,T)$ is the Bose-Einstein distribution function.

The results in Fig. 1 shows that C_{latt} really well reproduces even the upturn of $C(T)$ in the paramagnetic state, if we use γ= 60 mJ/mol K^2, which is double comparing with the experimental low-temperature value γ= 28 mJ/mol K^2, obtained for a sample with 11% U substituted by Zr so as to maintain the α-UH_3 structure [1]. This gives γ= 31.4 mJ/mol K^2 if normalized per mole U. The γreduction in the ferromagnetic state reveals that the spin splitting of the 5*f* states, which gives already an effective moment in the paramagnetic state, proceeds in the ferromagnetic state. This fact is corroborated by magnetostriction effects as well as by DLM calculations [1]. Hence the calculations of crystal lattice dynamics (here using the GGA+*U* method within the VASP package, 2x2x2 supercell of 64 atoms) provide a realistic lattice specific heat, fully suitable for a quantitaive analysis of specific heat.

And what is the entropy? Using the background of C_{latt} + γT from high temperatures, the entropy is not close to 0 as in weak itinetant systems, but 0.63*Rln(2) if normalized per mole of U, i.e. still considerably below Rln2 (the green line in Fig. 2). We can also try to get the real C_m and ΔS_m if we assume the change of γ from 60 to 30 mJ/mol K^2 in the ferromagnetic state. In Fig. 2 we rather arbitrarily changed γ in one step at 80 K, where the volume magnetostriction effect starts to saturate, giving the black line. In this case ΔS_m comes close to Rln2. If we considered the low temperature $\gamma \approx$ 30 mJ/mol K^2 all the way up, the entropy becomes too high and unplysically increasing in the high-T range.

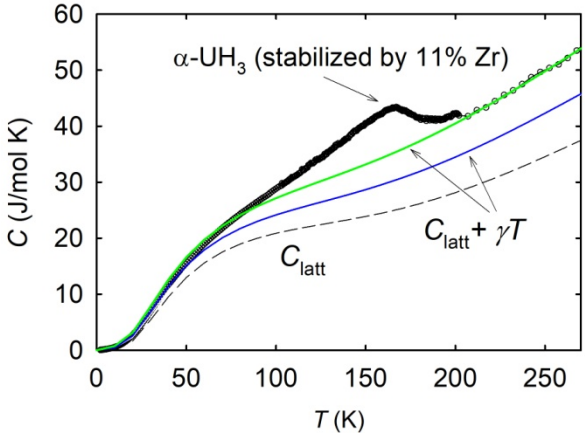

Fig. 1. Temperature dependence of specific heat of α-UH$_3$, the calculated bare lattice part and lattice and electronic part for different γ. The maximum at T = 170 K is the magnetic phase transition.

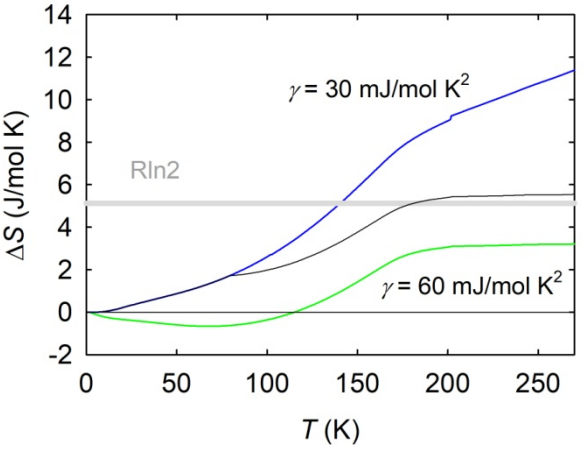

Fig. 2. Related changes of entropy ΔS(T) counted from T = 0. It compares the entropy including the change of electronic part at T = 80 K (green) with purely magnetic one (black).

As a conclusion, we achieved a consistent description of electronic and magnetic heat capacity using the calculated lattice part. It demonstrates that α-UH$_3$ is definitely not a purely band ferromagnet, which could be expected from U-U in the vicinity of the Hill limit, although the magnitude of magnetic moments is sensitive to magnetic order.

Acknowledgments

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Quest for new intermetallic f-electron compounds

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In the quest for new intermetallic compounds we aim to synthesize chemical compounds that reveal interesting physical properties, i.e. superconductivity, long range magnetic ordering, etc. In this lecture we will present recently reported ferromagnetism in $NdIr_3$ [1] and superconductivity in $CeIr_3$ [2]. Both compounds form in a complex rhombohedral structure in centrosymmetric space group R-3m (No. 166).

We will also discuss crystal structure and magnetism of the Yb-based 2-dimensional triangular lattice $Rb_3Yb(PO_4)_2$ compound [3].

Acknowledgment

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Local origin of strong field-angular anisotropy in magnetic phase diagrams of $Ce_{1-x}La_xB_6$ measured in a rotating magnetic field

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Cubic *f*-electron compounds commonly exhibit highly anisotropic magnetic phase diagrams consisting of multiple long-range ordered phases. Field-driven metamagnetic transitions between them may depend not only on the magnitude, but also on the direction of the applied magnetic field. Examples of such behavior are plentiful among rare-earth borides, such as RB_6 or RB_{12} (R = rare earth). For example, in this work we used torque magnetometry to measure anisotropic field-angular phase diagrams of La-doped cerium hexaborides, $Ce_{1-x}La_xB_6$ (x = 0, 0.18, 0.28, 0.5).

One expects that field-directional anisotropy of phase transitions must be impossible to understand without knowing the magnetic structures of the corresponding competing phases and being able to evaluate their precise thermodynamic energy balance. However, this task is usually beyond the reach of available theoretical approaches, because the ordered phases can be noncollinear, possess large magnetic unit cells, involve higher-order multipoles of 4*f* ions rather than simple dipoles, or just lack sufficient microscopic characterization.

Here we demonstrate that the anisotropy under field rotation can be qualitatively understood on a much more basic level of theory, just by considering the crystal-electric-field scheme of a pair of rare-earth ions in the lattice, coupled by a single nearest-neighbor exchange interaction. Transitions between different crystal-field ground states, calculated using this minimal model for the two well studied compounds CeB_6 and HoB_{12}, possess field-directional anisotropy that strikingly resembles the experimental phase diagrams. This implies that the anisotropy of phase transitions is of local origin and must be easier to describe than the ordered phases themselves.

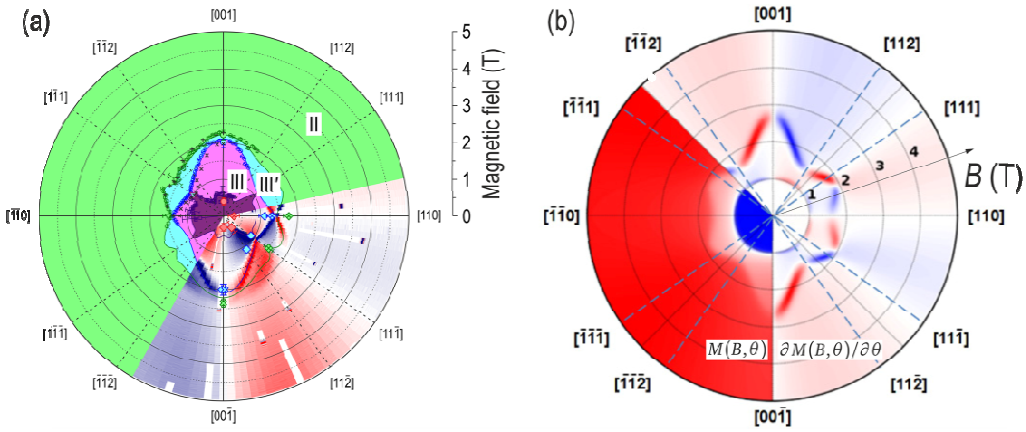

Fig. 1. (a) Field-angular magnetic phase diagram of CeB_6 measured using torque magnetometry. (b) Angle derivative of the magnetization, calculated ab initio for a two-site model.

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Investigating ground-states of 4f-based single-crystals by neutron diffraction

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New materials exhibiting complex physical behaviors related to magnetism may play a paramount role in future technologies. Such systems often require detailed analysis of their crystalline and magnetic structures in the ground states and/or when submitted to multi-extreme conditions.

Laue diffraction can probe large reciprocal space areas, imaging the rich physics frequently found in these systems, manifested as incommensurability, diffuse scattering and magnetoelastic effects. The characterization of the magnetic phases can be completed with higher resolution data from monochromatic diffraction.

In rare-earth-based intermetallic compounds, the oscillatory character of the RKKY (Ruderman-Kittel-Kasuya-Yosida) exchange causes competing interactions which often frustrate magnetic moments. It is the case of the compounds belonging to the families $R_3Ru_4Al_{12}$ (R is a rare-earth element), $R_2Co_3Al_9$ and RFe_5Al_7 [1,2]. They display multiple spontaneous and induced phase transitions and complex magnetic structures that provide an opportunity to study the interplay among magnetic frustration, exchange interactions, and magnetic anisotropy. Here, we will present studies of the magnetic ground states using the neutron Laue diffraction combined with monochromatic neutron diffraction.

The Ho atoms in $Ho_3Ru_4Al_{12}$ form a kagome lattice and their magnetic ordering below the Néel temperature is not complete. Furthermore, Laue diffraction images taken in the antiferromagnetic state indicate that the magnetic structure needs to be described by two independent propagation vectors. Similarly, the $TmFe_5Al_7$ compound exhibits an incommensurate magnetic ground state and the propagation vector is determined from the Laue data despite the very weak magnetic scattering and the presence of a large twin crystal on the sample.

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The influence of annealing temperature on the magnetic properties of La-doped $BiFeO_3$ prepared by sol-gel method

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Perovskite bismuth ($BiFeO_3$) ferrite has attracted significant attention over the past few decades due to its outstanding physical properties. $BiFeO_3$ is a room temperature multiferroic material with T_C=1043 K and T_N=647 K. It has a magnetic incommensurate cycloid spin structure with a periodicity of about 64 nm [1]. This structure cancels the macroscopic magnetization and inhibits the observation of the linear magnetoelectric effect. The decrease in particle size has been proven to be effective in suppressing the cycloid structure and enhancing the magnetic moment of $BiFeO_3$. Ion substitution is an alternative efficient method to increase the magnetization in the $BiFeO_3$ system, e.g., rare-earth ions were used to partial replacement of Bi which led to the boost in the room temperature ferromagnetism [2].

We report the effect of La^{3+} cation substitution on structural and magnetic properties in $Bi_{0.9}La_{0.1}FeO_3$ prepared by sol-gel method and subjected to subsequent annealing at various temperatures in the range 723-1073 K. X-ray diffraction studies proved the formation of the rhombohedral $BiFeO_3$ phase. However, specimens annealed at 873 and 1073 K contained $BiFeO_3$ and some amount of parasite phases. Mössbauer spectroscopy investigations revealed the partial suppression of cycloidal spin order by La doping. Moreover, it enabled the observation of further cycloid destruction with the decrease of mean grain size. Measurements of magnetization showed a gradual appearance of hysteresis loop with the decrease of annealing temperature revealing weak ferromagnetic behavior of fine-grained La-doped $BiFeO_3$.

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Electronic structure of the non-centrosymmetric heavy-fermion $CeRh_2As_2$

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Non-centrosymmetric heavy-fermion materials have gained much interest in the past decade. In these materials, the lack of inversion symmetry in combination with strong spin-orbit interaction and magnetic interactions can lead to novel phenomena.

In this talk we present electronic structure calculations of the non-centrosymmetric heavy-fermion $CeRh_2As_2$ which shows a strong Kondo interaction (T_K ~ 20 - 30 K), a potential quasi-quartet crystal electric field (CEF) ground state and unconventional superconductivity [1].

The calculations have been performed by means of the Renormalised Band method which proceeds from a Dirac relativistic description of the electronic structure and accounts for CEF effects and the mass renormalisation.

We also present results obtained for its non-magnetic counterpart $LaRh_2As_2$

Reference

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Non-s-wave superconductivity in noncentrosymmetric $ThCoC_2$ in view of *ab initio* calculations and Eliashberg formalism

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The lack of inversion symmetry lifts the parity constraint on Cooper pairs and thus a mixture of spin-singlet and spin-triplet states can be formed in noncentrosymmetric superconductors. Recently characterized $ThCoC_2$, a nonmagnetic type-II superconductor with $T_c \approx 2.5$ K, shows several non-BCS features [1]. The upper critial field $H_{c2}(T)$ exhibits positive curvature. The electronic specific heat at low temperatures deviates from the exponential temperature dependence and the normalized specific heat jump $\Delta C_e/\gamma T_c = 0.86$ is much smaller than the BCS prediction. Normalized Sommerfeld coefficient exhibits a square root magnetic field dependence $\gamma_0 \sim \sqrt{H}$ [2], which suggest existence of nodes in the superconducting order parameter. Based on the magnetic field penetration depth measurement, superconductivity was proposed to be nodal d-wave and mediated by the spin fluctuations [3].

In this work we study electronic structure, phonons and electron-phonon coupling in $ThCoC_2$ with density functional theory implemented in Quantum Espresso [4]. Thermodynamic properties of the superconducting state were determined by solving Eliashberg equations [5]. Calculated electron-phonon coupling constant $\lambda \approx 0.59$ is in a decent agreement with the experiment and is strong enough to mediate superconductivity in $ThCoC_2$. Electronic specific heat and magnetic penetration depth calculated from Eliashberg equations strongly differ from the BCS model. However, neither of them can explain the experimental results, therefore, the non-s-wave superconductivity hypothesis is supported.

Acknowledgment

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Spin-orbital entanglement in magnetic quantum materials

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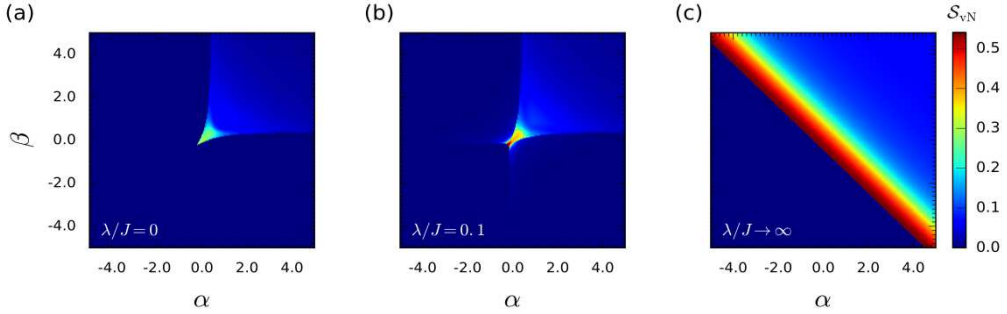
Strong relativistic spin–orbit coupling (SOC) in 4d and 5d materials leads to novel phenomena such as the complex phase behaviour observed in the extended Kitaev-Heisenberg model [1]. In this context we investigate spin–orbital entanglement (SOE) which plays a crucial role in the understanding of strongly correlated electrons in transition metal oxides. We study a transparent example of the intimate relation between quantum entanglement and SOC. To this end we numerically diagonalize one-dimensional spin–orbital model with the SU(2)⊗SU(2) 'Kugel – Khomskii' exchange supplemented by SOC of the Ising type for chains up to L = 20 sites [2,3]. We observe a substantial difference in the entanglement for small versus large SOC. While most of the features of the ground state with small SOC resemble the vanishing SOC limit, the phase diagram for large SOC regime is divided between the classical fluctuation—free region and surprisingly vast region where quantum fluctuations persist, including highly quantum 'stripe'—like area with maximal SOE. From a broader perspective, these results provide a basis to infer the generic properties of entanglement in transition metal oxides with finite SOC at higher dimension.



Evolution of the spin-orbital entanglement entropy SvN in the on-site spin-orbit coupling parameter λ . Figure has been published in [2].

***Acknowledgment**: We kindly thank National Science Centre (NCN) Projects No. 2016/23/B/ST3/00839 and 2016/22/E/ST3/00560*

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Magnetism and crystal-field states in the Kondo-lattice antiferromagnet $CeRh_2Si_2$*

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$CeRh_2Si_2$ is considered as a Kondo-lattice antiferromagnet due to large specific heat with λ-type peak at the magnetic-ordering temperature T_N of 36.5 K [1]. We have theoretically analyzed, within developed by us the Quantum Atomistic Solid-State Theory (QUASST), temperature dependence of the specific heat at temperatures both in the paramagnetic and the magnetic region. Our description of $C(T)$ reproduces very well $C(T)$ in the wide temperature range including the λ-type peak. Our description substantially improves a description in Ref. [1] based on two theories used for Kondo-lattice antiferromagnets [2,3]. In our description the large specific heat at low temperatures originates from splitting of the Kramers-doublet ground state of the Ce^{3+} ions realized during the formation of the magnetically-ordered state.

We have derived a set of crystal-field parameters, which, apart of the reproduction of crystal-field excitations of 30 and 52 meV, of the temperature dependence of the specific heat and of the paramagnetic susceptibility, reproduces a value of the magnetic moment, of 1.60 μ_B. Our results for the temperature dependence of the specific heat and of the entropy are physically adequate and substantially improved compared to other recent theoretical descriptions reported in a recent publication in Nature Comm. [4].

Good quantitative description proves that all Ce ions in $CeRh_2Si_2$ are in trivalent state Ce^{3+} ($4f^1$ configuration). A large value of the entropy removed in the magnetic transition, very close to Rln2, indicates that the hybridization effects and a broadening of crystal-field states in $CeRh_2Si_2$ are very small.

The QUASST approach can be used for the theoretical description of magnetic and electronic properties of other Ce, rare-earth and actinides compounds, let mention $ErNi_5$ [5], UPd_2Al_3 [6] and UGa_2 [7]. Owing to the integer *f*-shell occupation the QUASST approach has the start like the Kondo limit of the single-ion Anderson model and in the LDA+U, with infinite value of U, first-principles calculations.

** dedicated to Prof. Jaap Franse from University of Amsterdam and Prof. Karol Krop from AGH in Krakow for their anniversaries 80+. Good health and prosperity for further days.*

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^{57}Fe and ^{151}Eu Mössbauer studies of 3*d*-4*f* spin interplay in $EuFe_{2-x}Ni_xAs_2$

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The $EuFe_2As_2$-based compounds are unique laboratory for investigations of interplay between magnetism and superconductivity, as well as they are a playground for peculiar competition between itinerant 3*d* magnetic order of the spin-density-wave (SDW) type and the localized 4*f* magnetic moments. On the other hand, the Mössbauer spectroscopy is a useful local probe for investigation of the iron-based superconductors [1]. ^{57}Fe and ^{151}Eu Mössbauer spectra were obtained versus temperature for $EuFe_{2-x}Ni_xAs_2$ compounds with 3*d* and/or 4*f* magnetic order. Special attention was paid to the Ni-substitution level x corresponding to the spin reorientation, hence the compounds with x = 0.04, 0.07, 0.10, 0.12, and 0.40 were studied. Additionally, results for the end members of this system, i.e. $EuFe_2As_2$ and $EuNi_2As_2$, are reported for comparison.

It was found that spin-density-wave (SDW) order of the Fe itinerant moments is monotonically suppressed by Ni-substitution. However, the 3*d* magnetic order survives at the lowest temperature up to at least x = 0.12. The Eu localized moments order regardless of the Ni concentration with the spin reorientation (canting) from the *a*-axis in the parent compound toward *c*-axis with the increasing replacement of the Fe atoms above x = 0.07.

The change of the 4*f* spins order from antiferromagnetic to ferromagnetic is due to the disappearance of the 3*d* spins order and it is evidence of a strong coupling between the magnetism of Eu^{2+} ions and the conduction electrons of $[Fe_{2-x}Ni_xAs_2]^{2-}$ layers. The Fe experiences the transferred hyperfine magnetic field due to the Eu^{2+} ordering for Ni-substituted samples with x > 0.04, while the transferred field is undetectable in $EuFe_2As_2$ and for compound with a low Ni-substitution level. It seems that the 4*f* ferromagnetic component arising from a tilt of the Eu^{2+} moments to the *c*-axis of the unit cell leads to the transferred magnetic field at the Fe atoms.

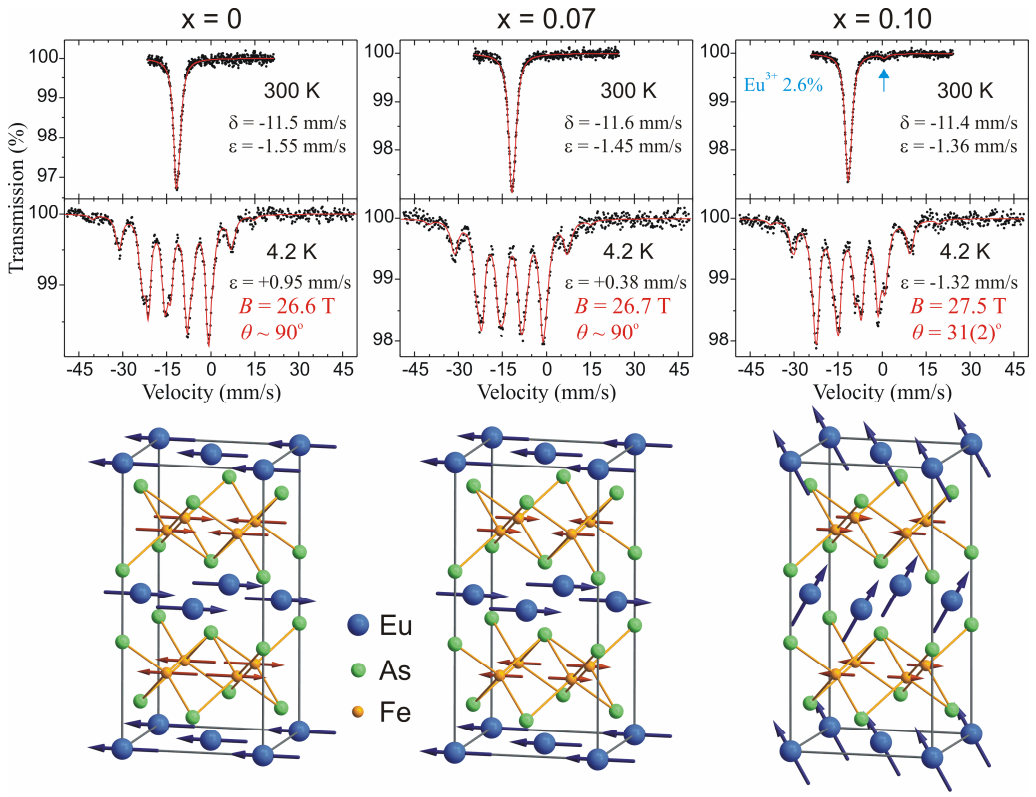

Figure 1: ^{151}Eu Mössbauer spectra of $EuFe_{2-x}Ni_xAs_2$ with x = 0, 0.07, 0.10. The hyperfine magnetic field for Eu^{2+} is denoted by B, while the symbol θ stands for the angle between the c-axis of the unit cell and the Eu magnetic moment. Sketches of the corresponding magnetic structures of $EuFe_{2-x}Ni_xAs_2$ system at the ground state emerging from the ^{57}Fe and ^{151}Eu Mössbauer results at 4.2 K.

Acknowledgment

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Effect of Gd doping on the magnetic properties of $CeNi_5$ melt-spun ribbons

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When the temperature approaches zero Kelvin, the highly correlated state of the electron system arises. It is usually caused by the enhanced electronic density of electron states close to the Fermi energy in metals, especially in sharp 4*f* electron states in rare earth elements. The emerging field of study is arising due to the undergoing quantum phase transitions. A fascinating variety of values of the temperature and magnetic field properties can be observed in the vicinity of quantum phase transition. The mentioned phenomena, which can arise at the quantum mechanics effects level, lead our group to study the selected intermetallic systems connected with these effects. These materials belong to a group of advanced materials and potential magnetic actuators. Because of the interesting properties, the effect of Gd doping on the magnetic properties of $CeNi_5$ melt-spun ribbons was investigated.

$CeNi_5$ is well known as a Stoner enhanced paramagnet, e.g. [1], and $GdNi_5$ is a ferromagnetic compound, e.g. [2]. The X-ray diffraction at room temperature shows the hexagonal $CaCu_5$ crystal structure with P6/mmm space group as it is typical for those class of compounds. The obtained results display that with the increase of the Ce content, the unit cell is expanding. It is consistent with the larger Ce volume concerning Gd.

To see the effect of spin fluctuations, observed and published in several publications, e.g. [1, 3], the $CeNi_5$ compound in a ribbon form was prepared. It was observed between T = 100 K and T = 150 K a shoulder, which corresponds with the maximum observed in polycrystalline $CeNi_5$ compound [4]. It can be explained in several ways. The first one is based on [5, 6], where the authors suppose that it is an intrinsic feature of the material. It is well-known that only a small percentage of magnetic impurities can change the characteristic behaviour of M(T) [4].

Moreover, the previous study did not show a low-temperature change [7, 8]. This maximum is therefore created due to the spin fluctuation effect, where magnetic moments are pressed to be ordered, and no magnetic field can diminish it. An effective paramagnetic moment for this sample is 3.52 μ_B/f.u., which is a little higher than for free Ce^{3+} ion. It can be due to the fact of CEF splitting of Ce^{3+} ion.

The magnetic properties studies have shown that only a small percentage of Gd creates the existence of transition temperature in dosed material as it will be presented for studied ribbons. The temperature dependencies of magnetic properties have a character typical for antiferromagnetic materials. This conclusion is partially supported by a negative value of paramagnetic Curie temperature. The question of

antiferromagnetic interaction was introduced in [9]. During the systematic investigations performed in the last decades, temperature dependencies of magnetization were done only at higher applied magnetic fields ($B \geq 1$ T). However, the antiferromagnetic character is manifested at lower magnetic fields. However, the study of other physical properties does not confirm antiferromagnetic ordering. In the paramagnetic region, a Curie-Weiss fit was provided. The obtained effective paramagnetic moment is 7.52 μ_B/f.u., which is lower than the bulk sample value. This deviation can be explained so that the piece of the sample was not homogenous and, on its surface, there could be more Ce than Gd, which yields from the microstructural analysis.

Two-τ techniques heat capacity measurements performed by the DynaCool (Quantum Device) equipment, and its analyses support observations collected from magnetic measurements. More details will be shown during the conference.

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Electrical resistivity measured on FIB-structured microdevices

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One of the most striking features of the light-actinide compounds is a giant magnetic anisotropy, originating from sizeable orbital magnetic moments induced in the system of bonding itinerant electrons by a strong spin–orbit interaction. The strong coupling of the magnetic anisotropy and anisotropy of underlying electronic structure makes absolutely essential studies of physical properties along different crystallographic directions. Any standard measurement of electrical resistivity requires macroscopic samples accommodating all the electrical contacts needed. In many cases such big single crystals are not available. This difficulty can be overcome by using FIB (Focused Ion Beam)-structured microdevices [1]. Aligned crystalline samples can be cut from polycrystals, microcrystallites, or even powders.

After choosing the proper area of the sample using SEM (scanning electron microscopy), thin lamellas having the desired orientation (fig. 1) are cut using FIB. The lamella (100x30x2 μm^3) is then transferred onto a substrate where suitable electric contact pads have been prefabricated by conventional lithography (fig. 2). Gold is sputtered over the whole surface of the lamella. Finally, the proper shape of the device is cut using FIB (fig. 3). The contact 1 and 2 are used for current and the sets of contacts 3-4, 5-6 and 7-8 are used to measure voltage for different directions of the material.

As an example, we will present results obtained using such device fabricated from U_2Ni_2Sn [2], (uniaxial antiferromagnet (T_N = 25 K) with pronounced anisotropy), for which conventional resistivity data are available for comparison.

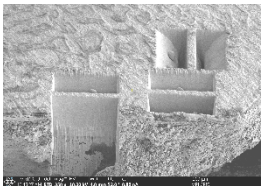

Fig. 1. SEM image showing cutting the lamellas.

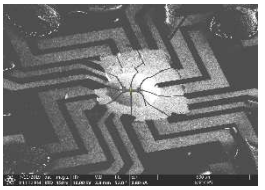

Fig. 2. Lamella placed on prefabricated substrate.

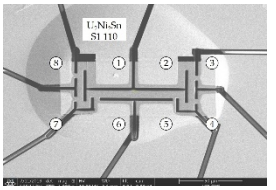

Fig. 3. SEM image of a microdevice of U_2Ni_2Sn

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Why the cubic phase of uranium?

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Physical properties of metallic uranium crystallised in the orthohombic structure (α-U) were well-known, since this phase exists at room temperature, e.g. the superconductivity in the natural uranium was first discovered in 1942 (T_c = 1.3 K). The body-centered cubic phase of Uranium (bcc; γ-U) is stable only at high temperatures (1045 - 1405 K). The large interest in the U-based systems with the γ-U phase was started from the search of materials fulfilling the requirements of using the low enriched uranium (LEU, <20% U) fuel for research nuclear reactors, since they have a higher thermal conductivity and higher resistance to irradiation. From a fundamental standpoint, it is of interest to determine the basic thermodynamic properties of these systems, since they exhibit a superconducting ground state around 2 K.

We have stabilized the γ-U phase in U-T systems (T = Mo, Nb, Zr, Ru, Pt, Ti) at room temperature by a combination of using (minimal possible) T concentration and splat cooling technique with a cooling rate of about 10^6 K/s [1, 2], so-called U-T splats. We summarize hereby our investigations of the low-temperature properties of U-T splats. All investigated samples exhibit the superconducting phase transition (Fig. 1) below 2.1 K [3,4]. The upper critical magnetic field ($\mu_0 H_{c2}(0)$) is in the range of 2 - 7 T, and the slope at T_c ($-\mu_0(dH_{c2}/dT)_{Tc}$) is about 2 - 5 T/K. A good agreement between the experimental specific-heat jump and that expected from BCS theory was obtained in U-15 at.% Mo splat ($U_{0.85}Mo_{0.15}$) crystallizing in the ideal cubic A2 structure and exhibiting the highest critical temperature (T_c = 2.1 K).

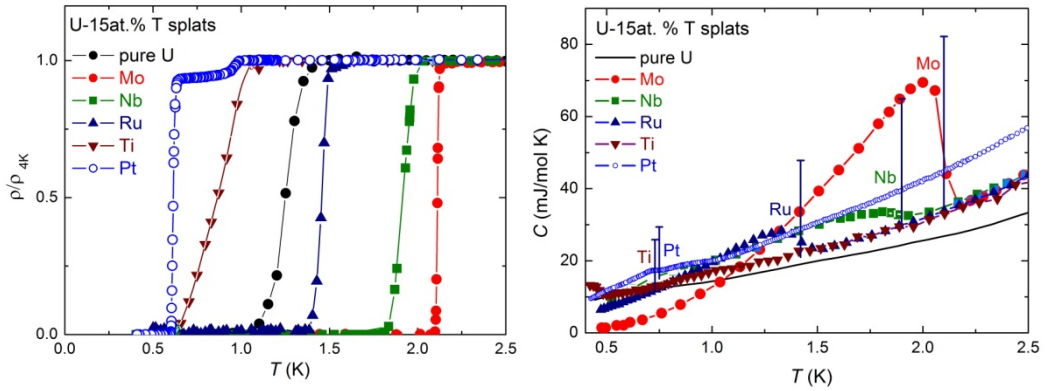

Fig. 1. Superconducting phase transition in U-15 at.% T splats revealed by drops of the electrical resistivity and anomalies in the specific heat (in zero magnetic field). The lines are for guiding the eyes.

The U-T splats absorb a large amount of hydrogen, but only at high hydrogen pressures (> 5 bar), forming hydrides of the $(UH_3)_xT_{1-x}$ type. $(UH_3)_{0.85}Mo_{0.15}$ is analogous to β-UH_3, but it is almost amorphous (the grain size smaller than 2 nm) [5]. The pure hydride of the α-UH_3 type (without admixture of β-UH_3) was found in $(UH_3)_{0.70}Zr_{0.30}$ (the grain size is in the range of 10-20 nm) [6]. Other hydrides consist of α-UH_3 and β-UH_3 mixture [7]. These hydrides are ferromagnetic with enhanced Curie temperature, T_C, reaching 200 K (in a comparison with β-UH_3 (T_C ~173 K) [8]). The T-concentration dependence of the Curie temperature for the $(UH_3)_{1-x}T_x$ hydrides (Fig. 2) revealed a maximum for T concentrations in the range x = 0.12-0.15. The magnetic moment of uranium is about 1μ_B/U, much smaller than the expect value ~ 3.2μ_B/U for f^{2+} and/or f^{3+} ground state.

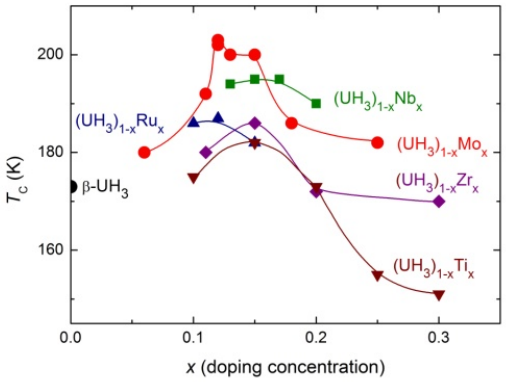

Fig. 2. T-concentration dependence of the Curie temperature of the $(UH_3)_{1-x}T_x$ hydrides. The lines are for guiding the eyes.

One important finding is that these hydrides (hydrides of γ-U based splat cooled alloys) are not pyrophoric and it is safe to handle them. (Fine powders β-UH_3 show spontaneous ignition at room temperature in air.) Hydrogen is easily released by annealing at high temperatures and in vacuum.

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Photoelectron spectroscopy and magnetism of U hydrides

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Uranium hydrides have both fundamental importance and practical relevance for nuclear energy and devices. This fact provides a continuous input of effort directed to understanding U-H formation and properties [1]. Unlike all other actinides and lanthanides, which have both di- and trihydride, only UH_3 was known so far. UH_2 phase has been stabilized only in a thin film form recently, obtained by reactive sputter deposition [2]. Parameters of the sputtering process, yielding either UH_3 or UH_2, are still explored.

A new experimental run focused on determining the impact of deposition rates on the structure of hydrides. Initial analysis was performed using XPS. We followed an empirical approach based on a gradual increase of H_2 partial pressure in the working gas (Ar) while monitoring changes of the U-4*f* core-level spectra [3]. Such complication is caused by the fact that the H-1*s* spectral intensity is a part of the valence band and cannot be simply used to quantify the H concentration in the film.

Details of electronic states in the vicinity of the Fermi level are explored by UPS, surpassing XPS both by intensity and energy resolution (about 70 meV). Fig. 1 compares the UPS spectra (40.81 eV photon energy - HeII) of U and UH_3.

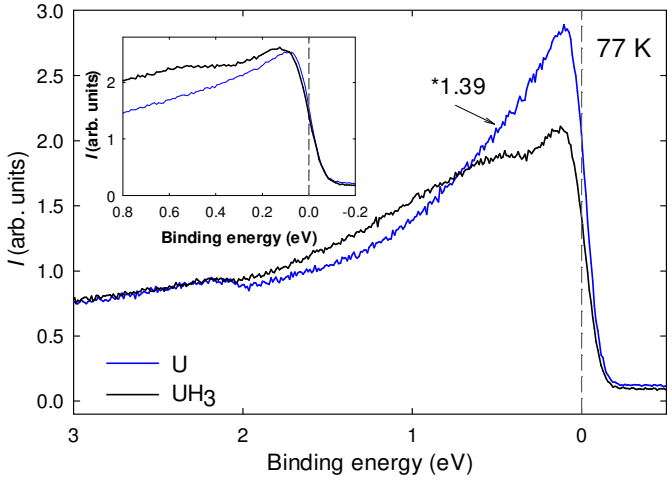

Fig. 1. Valence-band UPS spectra (hv = 40.81 eV) of U metal and UH_3, taken at T = 77 K. The inset shows details around the Fermi level marked by the dashed line.

The figure demonstrates that the spectra are quite similar at the Fermi level (if properly normalized), the maximum for UH_3 is slightly displaced from the Fermi level to ≈140 meV binding energy. It can be compared with pure U metal with DOS increasing up to the Fermi level and the Fermi-Dirac cutoff forming the maximum at 90 meV. Another prominent feature of UH_3 (UH_2 is very similar) is the broad shoulder at 0.5 eV.

Details of the valence-band spectra close to the Fermi level resist to a quantitative description using the DFT or DFT+*U* calculations [1]. However, spectral density obtained from DMFT calculations captures both the maximum just below E_F and the 0.5 eV shoulder. This stresses the importance of electron correlations for the description of U hydrides.

As the photoelectron spectra of UH_3 and UH_2 are so similar, it is challenging to distinguish which species was deposited as a film. Besides XRD, magnetization measurements turned particularly useful. Fig. 2 shows that while both species are ferromagnets, their T_C values are different.

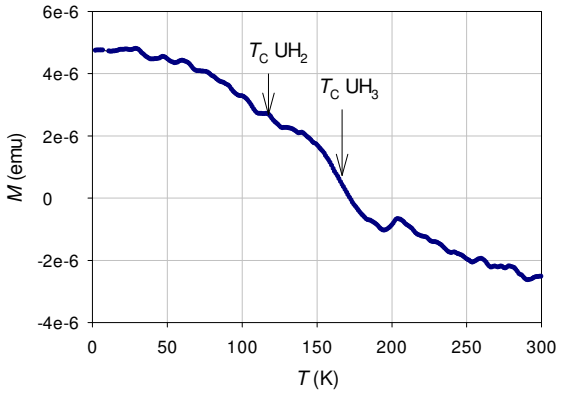

Fig. 2. Temperature dependence of magnetization of the film with mixed UH_2 and UH_3 structure in the field of 0.05 T (field cooled mode). Arrows mark the Curie temperatures of the two phases. The signal is low and noisy due to a small mass of the film.

UH_3 has its T_C ≈ 165 K, whereas UH_2 T_C ≈ 120 K [2]. Using the $M(T)$ dependence, we can assess the phase composition (pure UH_2, UH_3 or mixed-phase) of the samples. It turns out that UH_2 is formed predominantly when the substrate is self-heated during deposition.

Acknowledgments

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Magnetism and superconductivity in complex noncentrosymmetric $M_4Be_{33}Pt_{16}$ (M = Y, La-Nd, Sm-Lu, Th, and U) compounds

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The intrinsic properties of complex solid-state compounds are typically difficult to unveil due to (i) a large number of crystallographic positions, (ii) a large number of atoms in the unit cell, (iii) quantitative limitations of the computational methods, as well as (iv) crystallographic defects. One method of tackling this problem is to synthesize and compare a series of alloys differing by a single element – this also gives an opportunity to tune their physical properties.

In this talk, we will present chemical and physical properties of the new $M_4Be_{33}Pt_{16}$ (M = Y, La–Nd, Sm–Lu, Th, and U) series of compounds. All seventeen systems are isostructural (space group $I\bar{4}3d$), exhibiting a cage-like crystallographic arrangement with 212 atoms per unit cell [1]. Four compounds – M = Y, La, Lu, Th – are superconducting with transition temperatures of 0.9 K (M = Y and Th), 2.5 K (M = La), and 0.7 K (M = Lu). They appear to be type II superconductors with weak spin-orbit coupling. However, they are the most crystallographically complex noncentrosymmetric superconductors discovered to date. The M = Ce–Nd, Sm–Yb compounds were found to order magnetically with transition temperatures ranging from T = 0.4 K (M = Yb) to T = 40 K (M = Pr). On the other hand, no ordering was found in the M = U system down to T = 0.35 K. A moderately enhanced electronic mass in this system is evidenced by the Sommerfeld coefficient $\gamma = 175$ mJ/mol$_U$K^2.

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^{57}Fe Mössbauer studies of 122-iron arsenides

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Mössbauer spectroscopy is a useful technique to investigate the microscopic properties of iron-based systems. This method enables determining the ionic state of the investigated isotopes, site-occupancy, shape of the spin-density-wave (SDW) and values of the transferred hyperfine field on the investigated nucleus from the neighbouring magnetic ions [1].

One of the most thoroughly investigated families of the iron-based superconductors is 122-family. MFe_2As_2 (where M = Ca, Sr, Ba, Eu) are unconventional superconductors. For the M elements being rare earths with non-zero localized 4f magnetic moments one observes antiferromagnetic order of these moments at much lower temperatures [2]. Superconductivity of these compounds can be achieved upon suppression of the SDW transition by partial chemical substitutions [3] or by application of an external pressure [4]. The principal structure of these materials are FeAs-layers with tetragonally coordinated Fe^{2+} ions. These layers are the electronically active structures for the competing magnetic and superconducting ground states.

Although "122" systems do not demonstrate as high critical temperatures, they are of a great interest since large single crystals can be grown for this family. This gives the opportunity to investigate not only superconductivity of materials containing "magnetic" ion (iron), but also anisotropy effects in such systems. To detailed investigation of the magnetic structure, the measurements were performed in the temperature range 4.2-300 K by using Mössbauer spectroscopy of the 14.41-keV line in ^{57}Fe.

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A typical heavy fermion system $CeRh_2As_2$

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Recently discovered heavy fermion $CeRh_2As_2$ compound crystallizes in the nonsymmorphic P4/nmm symmetry, which allows unexpected behavior associated with topological protection. Experimental results show that this material exhibits unusual behavior, which is manifested by the appearance of two superconducting phases.

In this work, we uncover and discuss a role of Rh_2As_2 layers and their impact on the electronic and dynamical properties of the system [1]. The location of Ce atoms between two non-equivalent layers allows for the realization of hidden orbital order. We point out that the electronic band structure around the Fermi level is associated with d orbital electrons and suggest the occurrence of the magnetic Lifshitz transition induced by the external magnetic field.

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Origin of large low-temperature specific heat in topological Kondo insulator SmB_6

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SmB_6 exhibits anomalous magnetic and electronic properties and recently it becomes widely studied as a topological Kondo insulator. The difficulty in understanding electronic and magnetic properties caused that SmB_6 is loosely regarded as a mixed-valence system in which the Sm ions rapidly fluctuate between non-magnetic Sm^{2+} ($4f^6$) and magnetic Sm^{3+} ($4f^5$ $5d^1$) ions, resulting in an average intermediate valence of 2.5-2.7. Moreover this valence can change with temperature.

The experimentally derived specific heat of SmB_6 exhibits a large extra heat compared with that of isostructural nonmagnetic LaB_6. This excess heat in SmB_6 is enormous because the entropy related to this excess, up to 300 K, amounts to 19-23 J/(K mol f.u.) [1,2]. It corresponds to 2.3-2.9 R, where R is the gas constant R=8.314 J/(K mol f.u.). This extra entropy would point to a number of involved localized states from 10 to 16. Such big numbers are not expected for the Sm^{2+} and Sm^{3+} ions.

According to us, this large low-temperature specific heat, with a maximum of 10J/K at 50 K is related to localized CEF-like states associated with the Sm^{2+} ion [3]. These states can be theoretically revealed by calculations within the spin-orbital $|LSL_zS_z>$ space, with L=3 and S=3, i.e making calculations beyond the usually-accepted $|LSJJ_z>$ space with J=0. Within the spin-orbital $|LSL_zS_z>$ space, with L=3 and S=3, there is 49 states related to the largely-degenerated quasi-atomic term ^7F ($4f^6$). This term becomes split by the cubic crystal-field (CEF) and the finite spin-orbit interactions. Success of our calculations is related with considering much weaker spin-orbit interactions as up-to-now were considered and with taking into account higher-order CEF interactions (B_6^4 CEF parameter). The derived CEF and spin-orbit parameters produce the lowest singlet state at 0 K with an excited triplet at 89 K and a next triplet at 215 K. These 7 states are within the energy of the 20 meV (= 232 K) and they are responsible for the large low-temperature specific heat.

Our approach is very similar to the one used by us in description of 3*d* compounds (CoO, NiO) [4,5]. This similarity is due to a fact that the orbital quantum number L=3 for the Sm^{2+} ion is the same as for the Co^{2+} or Ni^{2+} ions.

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Intermediate Valence Behavior of $Yb_2Cu_9Al_8$

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Intermediate valence behavior is frequently observed in compounds containing Ce, Yb, Eu, Sm, or Tm. In the current talk, I will discuss synthesis and characterization of an intermetallic compound $Yb_2Cu_9Al_8$ which crystallizes in the Th_2Zn_{17} structure type.

An excitation energy E_{ex}/k_B of 319 K and a spin fluctuations temperature T_{sf} of 60 K are characteristic of its intermediate valence behavior, whereas the valence state of Yb is estimated to be close to 2.04 for the low-temperature region. The valence gradually evolves to the value of 2.80 at T = 400 K. The Sommerfeld coefficient of γ_{exp} = 59 mJ/mol_{Yb} K^2 indicates a moderate effective mass enhancement, together with a finite density of states at the Fermi level. The latter is also confirmed by the band structure calculations.

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The interplay of 4*f* states and superconductivity in $CeIr_3$: DMFT study

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$CeIr_3$ has caught the attention over the past few years. It grows in trigonal structure and is superconducting below T_c=3.1K. The muon spin rotation and relaxation measurement shows its superconductivity to be of nearly BCS character [1] and multiband character of this effect has been deduced from temperature dependence of critical magnetic field [2].

In our first work [3] we have shown, that its electronic band structure, including multiband Fermi surface, is dominated by Ir 5*d* states, thus they are suggested to be crucial for superconductivity of $CeIr_3$.

However, the role of 4*f* states of cerium is still unclear. If nearly BCS character of superconductivity is a case in $CeIr_3$, the McMillan formula for electron-phonon coupling (EPC) constant λ should be proper and resulted value should agree with the EPC constant calculated as a renormalization of electronic part of heat capacity, $\lambda=\gamma_{expt}/\gamma_{calc}-1$, where γ_{expt}, γ_{calc} are Sommerfeld constants determined on the basis of measured heat capacity and calculated electronic structure respectively. However, McMillan formula gives the value 0.67, while the result of latter formula is strongly dependent of a treatment of *f* states in calculations, being equal to 1.47 in the case of GGA approximation of electronic correlation and 3.40 in the case of GGA+U approximation. Both values are in strong disagreement with McMillan value, suggesting, that both approximations of electronic band structure of $CeIr_3$ fail and a role of 4*f* states is more subtle.

Here we are presenting the new approach to the band structure of $CeIr_3$ with help of embedded dynamical mean field theory (eDMFT) [4], which allows to treat *f* states properly and has been shown to describe band structure of Ce succesfully. We show, that in the band structure of $CeIr_3$ the 4*f* states of Ce are present around the Fermi level more than previous study show, leading to smaller renormalization of heat capacity and a better agreement with McMillan value of EPC constant.

This study show, that even if Ir 5*d* states are crucial for superconductivity of $CeIr_3$, Ce 4*f* states are also important, as they are present around Fermi level and are weakening the electron-phonon interactions.

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Posters

EXAFS as a Probe of Actinide Oxide Formation in the Tender X-Ray Regime

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Recent developments in Resonant Inelastic X-Ray Scattering Experiments have vastly improved the resolution in X-ray Spectroscopies such as X-ray Absorption [1]. However, the use of Tender X-rays (~3keV) and the reactivity of actinides such as uranium have given rise to new questions about bulk and surface sensitivity, what constitutes a surface and how to characterize the formation of an oxide. It will be shown that the *in situ* electron scattering features that are part of the RIXS spectrum can be used to quantify the uranium oxide formation and determine cleanliness, independently of the near edge features that provide information about the unoccupied electronic density of states.

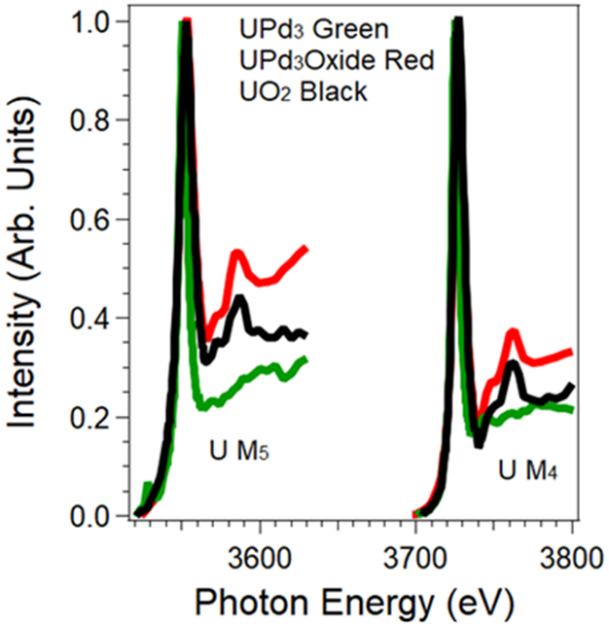

Figure 1. Shown here are the UM_4 and UM_5 Total Fluorescence Yield (TFY) measurements for UO_2 (black), cast UPd_3 (green) and oxide contaminated UPd_3 (red). All of the spectra were normalized to unity. Note the signature peak of the oxide near hv = 3580 eV and hv = 3760 eV.

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Observation of c-f hybridization gap in heavy-fermion system $EuNi_2P_2$ by using Point-contact spectroscopy

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The research on heavy-fermion (HF) system is an important topic in condensed matter physics [1] because the novel phenomena, such as unconventional superconductivity, non-fermi liquid, have been observed in HF systems. These characteristics of HF systems originate from the hybridization between conduction band and *f*-electron band (*c-f* hybridization). According to the theoretical calculation on the HF systems, when the temperature decreases below the Kondo temperature (T_K), a conduction band composed of *s*-, *p*-, *d*-electron band splits into two bands due to *c-f* hybridization, which leads to formation of the flat band (heavy band) near the fermi energy [1]. Hence, the direct observation of *c-f* hybridization gap is crucial for a deeper understanding of the HF system.

The scanning tunneling spectroscopy (STS) is an effective technique to directly observe the electronic density of state (DOS) near the Fermi energy. STS technique has been utilized to reveal the DOS on strongly correlated systems, such as unconventional superconductor, topological materials. The technique is also utilized to observe the DOS on HF systems; however, the literature is limited, which may come from the difficulty of the tip electron tunneling into heavy band formed in HF system due to the localization of the wave function of *f* electron near atomic nucleus. In the point-contact spectroscopy (PCS) measurements on HF system URu_2Si_2 by Park *et al.*[2], on the other hand, the hybridization gap can be observed clearly in the differential conductance *dI/dV* spectra. This is understood by the increase of the tunneling probability from a probe tip to heavy bands in the PCS measurements compared to the STS due to the direct contact between the probe tip and the sample surface (Fig. 1(a)).

The U-based compound is classed as 5*f* electron systems, meaning that the wave function of 5*f* electron is more itinerant than that of 4*f* electron. To compare the theoretical study, it is important to investigate the electronic DOS in 4*f* electron systems with a well-localized wave function. Hence, we have carried out PCS measurements on a 4*f* electron system $EuNi_2P_2$ in the present study. From the various measurements, $EuNi_2P_2$ is confirmed to exhibit the typical HF behavior at low temperatures, where the Kondo temperature (T_K) is evaluated to be 80 K [3].

The *dI/dV* spectra of $EuNi_2P_2$ using W probe tip show asymmetric double peak structure around the zero bias voltage, as shown in Fig. 1(b). The double peak structure becomes broad with increasing temperature, and merges into a single broad peak above T_K as shown in Fig. 1(c). First, we reproduce the spectra by a Fano curve, which is the theoretical model explaining the spectrum of the single impurity Kondo effect observed in the STS measurement for a magnetic ad-atom on metal substrate [4]. Above T_K ~ 80 K, the spectra are well fitted by the Fano curve as shown in Fig. 1(c)

(black solid line), indicating that the electronic DOS is understood by the single impurity Kondo picture. In contrast, below T_K, the spectra cannot be reproduced by the Fano curve because of the emergence of the double peak structure. To reproduce the spectra, we employ the MDC model, which is proposed to fit the spectra from a probe tip to HF system in STS and PCS measurements [5]. The spectra can be well fitted by the MDC model as shown in Fig. 1(c)(red solid line). The results indicate that the c-f hybridization gap opens near the fermi energy on $EuNi_2P_2$ at low temperatures. The gap is estimated to be 16 meV at the lowest temperature, which is in good agreement with the previous optical conductivity measurements [6].

As shown above, changing the spectra with decreasing temperature is well understood by the evolution of the electronic DOS from a localized Kondo state to HF state [7]. In the presentation, we also show the results of PCS measurement on valence-ordered YbPd [8], and discuss the difference of the spectral shape observed in $EuNi_2P_2$ and YbPd.

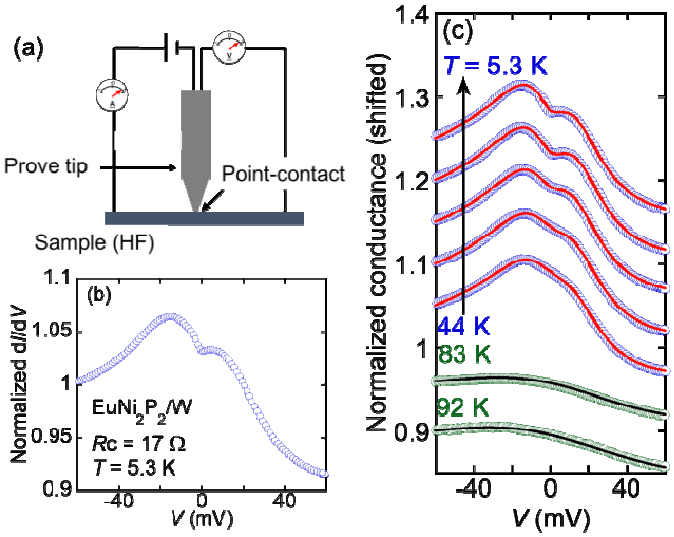

Fig 1. (a) The schematic diagram of PCS measurement. (b) The dI/dV spectra of $EuNi_2P_2$ with W probe tip. (c) Temperature dependence of dI/dV spectra. The symbols correspond to the experimental data. Black and red solid line correspond to the theoretical calculation using Fano model and MDC model, respectively.

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Magnetism of $TmFe_4CoAl_7$ single crystal

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The ternary intermetallic compound $TmFe_5Al_7$ (tetragonal crystal structure of the $ThMn_{12}$ type) was recently investigated within a systematic study of RFe_5Al_7 series (R = rare-earth metal) [1]. It is a highly anisotropic ferrimagnet below the Curie temperature T_C = 193 K. In the ground state, the magnetic moment of the Fe sublattice is slightly higher than that of the Tm one, the spontaneous magnetic moment is M_s = 0.5 μ_B at 2 K. The Fe sublattice dominates in whole range of the ordered state. It was found for the compounds with R = Dy and Ho that Fe can be partially substituted by Co (Co does not form isostructural compounds RCo_5Al_7) which leads to interesting changes in the magnetic properties, in particular, to an unexpected strong reduction of T_C [2,3]. In the present work, we studied effects of the 20% Co substitution for Fe on the magnetism of $TmFe_5Al_7$ on a single crystal.

Single crystal was prepared by arc melting the pure elements in a tri-arc furnace by the Czochralski method. Phase purity and lattice parameters were determined by standard X-ray diffractometry on powders prepared from the single crystals. The magnetization was measured at 2-300 K in static fields up to 14 T using PPMS-14 magnet and in pulsed fields up to 58 T (pulse duration 20 ms) by the induction method using a coaxial pick-up coil system.

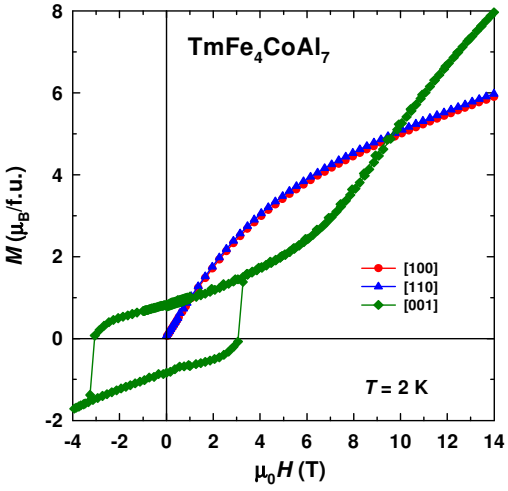

Fig. 1. Magnetization curves along the main axes at 2 K.

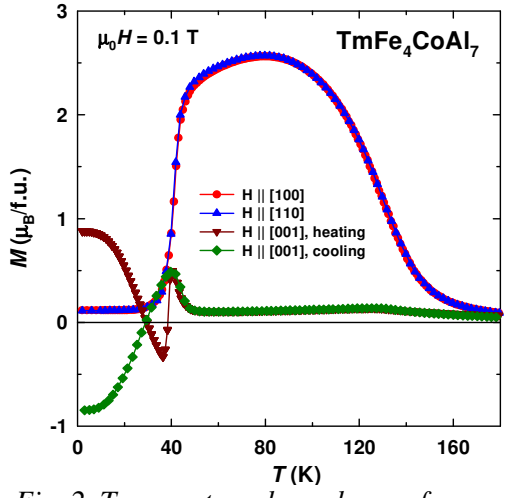

Fig. 2. Temperature dependence of magnetization in 0.1 T field applied along the main axes.

$TmFe_4CoAl_7$ is a ferrimagnet with T_C = 135 K, i.e., the drastic T_C drop observed in the Dy and Ho compounds is confirmed also for R = Tm. In the ground state the

[001] axis is the easy-magnetization direction (Fig. 1). No anisotropy, in contrast to the Dy and Ho systems, is observed within the basal plane. Introduction of Co leads to a decrease of the magnetic moment of the 3d-metal sublattice, the total M_s = 0.5 μ_B (at 2 K) is along the Tm sublattice. It results in the appearance of a compensation point, T_{comp} = 29 K (Fig. 2), with thermal hysteresis characteristic for RFe_5Al_7 (R = Tb, Dy, Ho, Er) ("negative magnetization effect"). The Tm sublattice provides a uniaxial magnetic anisotropy, whereas the Fe sublattice favors an easy-plane anisotropy. A competition between them results in a first-order spin-reorientation transition at 43 K (i.e., only easy axis or easy plane, no easy-cone range). An antiferromagnetic state observed in $TmFe_5Al_7$ just above the spin-reorientation in ~8 K range is, if exists, only at 43 K in $TmFe_4CoAl_7$.

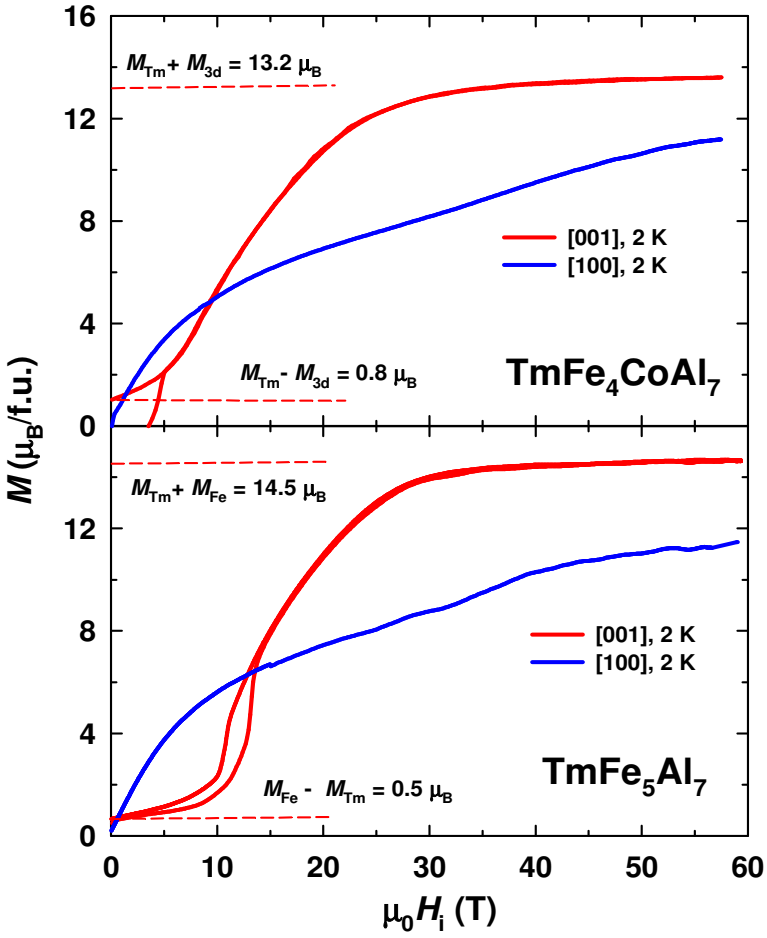

Fig. 3. Magnetization curves along the [100] and [001] axes of $TmFe_4CoAl_7$ and $TmFe_5Al_7$ crystals in pulsed fields at 2 K.

High-field behavior of $TmFe_5Al_7$ and $TmFe_4CoAl_7$ is similar. Both compounds exhibit a field-induced transition in field applied along the [001] axis. In approx. 30 T both compounds reach forced-ferromagnetic state. The field-induced transition in $TmFe_4CoAl_7$, where magnetic moment of the 3d-metal sublattice rotates, is of the second order. Rotation of the Tm-sublattice moment in $TmFe_5Al_7$ goes as the first-order transition.

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Pseudogap state in untwinned $YBa_2Cu_3O_{7-\delta}$ single crystals

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The effect of annealing both in the oxygen atmosphere and at room temperatures on physical properties such as the pseudogap $\Delta^*(T)$ and excess conductivity $\sigma'(T)$ of untwined $YBa_2Cu_3O_{7-\delta}$ (YBCO) single crystal with a small deviation from oxygen stoichiometry is studied [1]. It was revealed that as the charge carrier density, n_f, increases, T_c also slightly increases, whereas the temperature of the pseudogap opening, T*, decreases noticeably, which is consistent with the phase diagram of cuprates [2]. The excess conductivity in the vicinity of T_c is represented by the Aslamazov-Larkin and Hikami-Larkin fluctuation theories, illustrating the three-dimensional to two-dimensional (i.e. 3D-2D) crossover with an increase in temperature [1-3]. The crossover temperature T_0 determines the coherence length along the c axis is $\xi_c(0) = 0.86$ Å, that is 2.6 times larger than for optimally doped YBCO single crystals with defects. Taking into account the short coherence length in high-temperature superconductors, in the model of free charge carriers the phase relaxation time of fluctuating Cooper pairs is determined, $\tau_\phi(100\ K)=(4.55\pm0.4)\cdot10^{-13}$s, which is slightly (1.2 times) larger than in well structured YBCO films, and as in films, does not depend on n_f. It is shown that $\Delta^*(T)$ at different annealing stages practically does not change its shape. As in the well-structured YBCO films, $\Delta^*(T)$ demonstrates maximum at $T_{pair}\sim124$ K which depends weakly on n_f. However, the maximum value of $\Delta^*(T_{pair})$ increases with increasing n_f, as it follows from the phase diagram of cuprates [3]. Comparing the experimental data with the Peters-Bauer theory we estimated the density of local pairs $\langle n_\uparrow n_\downarrow \rangle \approx 0.3$ near T_c that is a common value for high-temperature superconductors.

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Magnetization-Induced Band Shift in Ferromagnetic Weyl Semimetal $Co_3Sn_2S_2$

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The discovery of magnetic Weyl semimetal (magnetic WSM) in $Co_3Sn_2S_2$ has triggered great interest for abundant fascinating phenomena induced by band topology conspiring with the magnetism. Understanding how the magnetization affects the band structure can give us a deeper comprehension of the magnetic WSMs and guide us for the innovation in applications. Here, we systematically study the temperature-dependent optical spectra of ferromagnetic WSM $Co_3Sn_2S_2$ experimentally and simulated by first-principles calculations. Our results indicate that the many-body correlation effect due to Co 3d electrons leads to the renormalization of electronic kinetic energy by a factor about 0.43, which is moderate, and the description within density functional theory is suitable. As the temperature drops down, the magnetic phase transition happens, and the magnetization drives the band shift through exchange splitting. The optical spectra can well detect these changes, including the transitions sensitive and insensitive to the magnetization, and those from the bands around the Weyl nodes. The results support that, in magnetic WSM $Co_3Sn_2S_2$, the bands that contain Weyl nodes can be tuned by magnetization with temperature change.

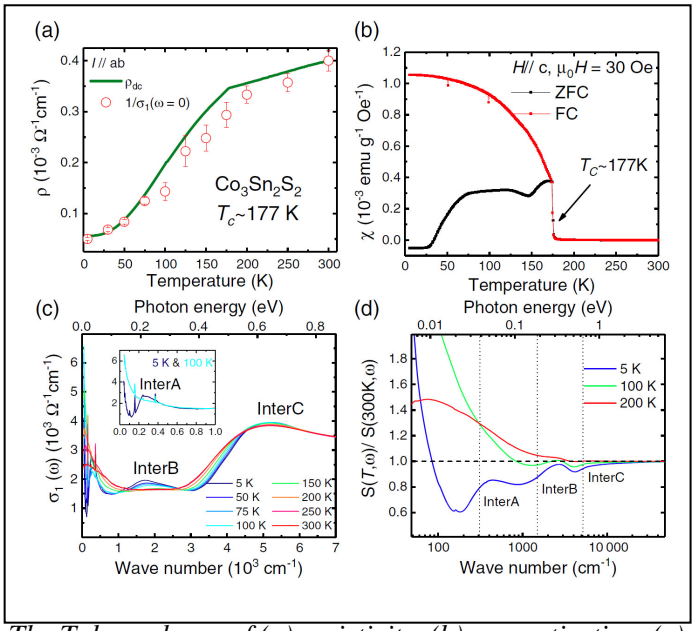

Figure 1: The T dependence of (a) resistivity, (b) magnetization, (c) optical conductivity, (d) specetral weight of $Co_3Sn_2S_2$.

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Influence of strontium atoms substituting on the electronic properties of the $K_{0.5}Bi_{0.5}TiO_3$ studied by *ab initio* methods

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First-principles density functional calculations are performed to calculate the physical properties of a lead-free ferroelectric $K_{0.5}Bi_{0.5}TiO_3$ and $K_{0.25}Sr_{0.25}Bi_{0.5}TiO_3$ systems. Especially, the A-site cation ordering in $K_{0.25}Sr_{0.25}Bi_{0.5}TiO_3$ and its influence on electron density of states are explored. The results suggest that the cation ordering at the A-site in $K_{0.25}Sr_{0.25}Bi_{0.5}TiO_3$ significantly affects its electron density of states spectra. Electron density of states and band structure for these systems were computed to find out the differences of spectra shape with respect to width band gap. It is found that in $K_{0.25}Sr_{0.25}Bi_{0.5}TiO_3$ band gap is bigger than $K_{0.5}Bi_{0.5}TiO_3$ by the value 0.2 eV.

The electron density of states and band structures spectra are prospective to provide benchmark first-principles data for further analysis of theoretical considerations and experimental spectra.

The calculations made will also be used in subsequent research on the search for optimal materials employed in photovoltaics.

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The fracture toughness of TiB_2 doped by tungsten measured by the nanoindentation method

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The material's resistance to brittle fracture is a very important parameter for characterization of the PVD coatings. Especially, for the anti-wear coatings, which are used in the environment of cyclically changing external loads. The main goal of shaping the properties of these materials is to achieve high fracture. Consequently, it is also one of the most important criteria for their suitability. The fracture toughness of solid materials is determined by the critical value of the stress concentration coefficient K_{Ic} [1,2]. The literature analysis showed the different models for determining the K_{Ic} coefficient of thin coatings[3,4]. The methods proposed by Niihiara [5] and Laugier [6] is nowadays the most often used.

We presented the way of how the fracture toughness coefficient of ceramic-based coatings doped by metal can be determined by using the nanoindentation method with the Berkovich indenter and Laugier model. For this purpose, the TiB_2 coatings doped by tungsten in the range of 0-10 at.% were deposited by magnetron sputtering in a DC system. The literature information[7-9] indicated that composites with a ceramic matrix are very perspective because they can achieve the resistance to brittle fracture comparable to the metals.

The brittleness of thin ceramic TiB_2 coatings can be improved by doping with tungsten. The tungsten concentration in the range of 0-10 at. % changes the microstructure of the investigated coatings from the columnar structure for TiB_2 coating to the nano-composite structure for TiBW(10%) coating. The analysis of the brittle fractures, which including changes in hardness (H) and Young's modulus (E), plasticity index H/E and resistance to plastic deformation H^3/E^2, enabled microstructure diagrams for the TiB_2 coating and TiBW coatings with different concentration of tungsten (Fig. 1a). Doping the TiB_2 coating with 3at.% of tungsten (TiBW(3%)) reduces columnar grains to a diameter of 30 nm (Fig.1b). The grain fragmentation does not change the cracking mechanism, which still works mainly in a direction perpendicular to the surface. For TiB_2 coating, which contains 6 at.% of tungsten (TiBW(6%)), the column structure with a diameter of grains 30 nm also dominates (Fig. 1c). The cracking mechanism is noticeably changed because the cracking directions parallel and perpendicular to the surface of the coating are equivalent. In the TiB_2 coating with doping 10at.% of tungsten(TiBW(10%)) can be observed a compact columnar structure with the individual columns, which are agglomerates of equiaxed grains with a diameter ≈100 nm (Fig.1e). The cracking process is not oriented but indicates the possibility of energy dissipation during fracture [10].

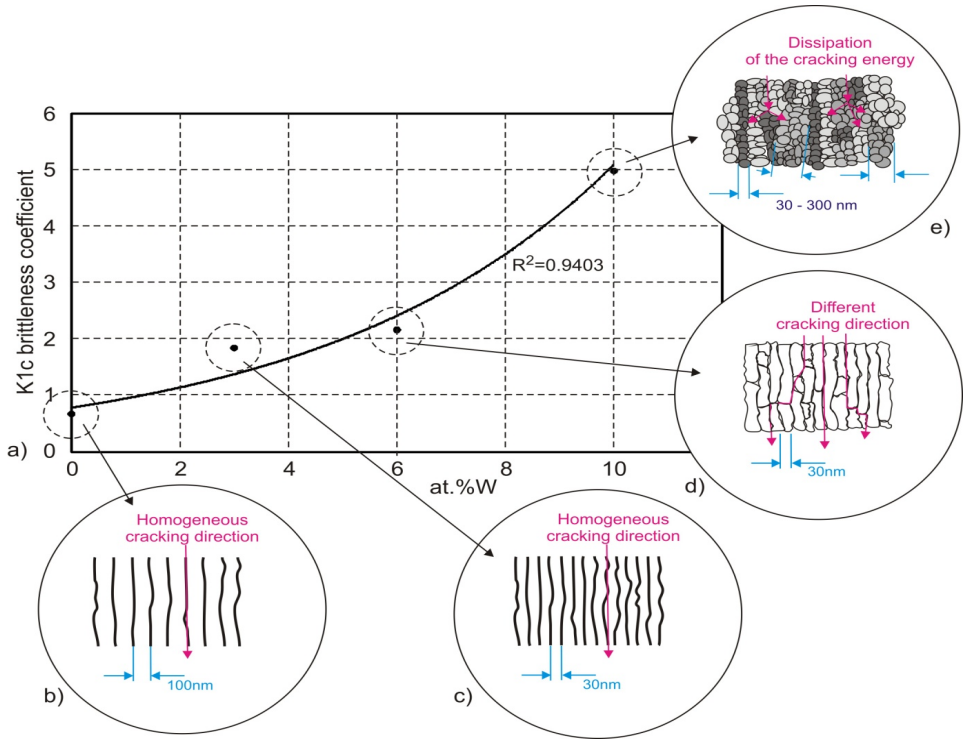

Fig.1. *The results of the K_{Ic} analysis for investigated coatings: a) changes of K_{Ic} values for TiB_2 and TiBW coatings depending on the tungsten concentration (at. % W) and diagrams of microstructure for b)TiB_2 coating, c) TiBW(3%) coating, d) TiBW(6%) coating, e) TiBW(10%) coating [10].*

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Is there a relationship between curvature and inductance in the Josephson junction?

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A Josephson junction is a device made of two superconducting electrodes separated by a very thin layer of isolator or normal metal. This relatively simple device has found a variety of technical applications in the form of Superconducting Quantum Interference Devices (SQUIDs) and Single Electron Transistors (SETs). One can expect that in the near future the Josephson junction will find applications in digital electronics technology RSFQ (Rapid Single Flux Quantum) and in the more distant future in construction of quantum computers.

Here I concentrate on the relation of the curvature of the Josephson junction with its inductance. I apply a simple Capacitively Shunted Junction (CSJ) model in order to find condition which guarantees consistency of this model with prediction based on the Maxwell and London equations with Landau-Ginzburg current of Cooper pairs. This condition can find direct experimental verification [1].

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Electrical properties of sodium bismuth titanate $Na_{0.5}Bi_{0.5}TiO_3$ ceramics under various sintering conditions

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Sodium bismuth titanate $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) ceramics were prepared by a conventional solid-state reaction method and by a hot-pressing route. The influence of sintering conditions on structural, dielectric and electrical properties of these ceramics was investigated. The obtained samples exhibited a single perovskite phase [1]. Dielectric properties, AC and DC conductivity, Seebeck coefficient and electrical modulus for four samples with different sintering conditions were examined. Dielectric measurements have shown that the sintering conditions affect both the values of electric permittivity as well as the characteristic temperatures of NBT. The depolarization temperature T_d practically does not change the value. However, the value of the temperature of the maximum of electric permittivity T_m differs for the samples for which increased the sintered number [1]. Direct current (DC) studies have shown that the DC conductivity curve consists of 5 linear sections, regardless of the sintering conditions, however, these conditions affect on the activation energy value [2]. The analysis of the electric modulus showed that, depending on the sintering conditions, the spectra of the module consist of one or two semicircles. The relaxation times for the studied samples were determined, and then the activation energies were calculated, which correspond to the energies obtained from the measurements of direct current conductivity [2]. The obtained values of the Seebeck coefficient for the measured samples have a similar nature. Visible anomalies on the obtained curves occur at temperatures that correspond to the T_d and T_m obtained from the dielectric properties measurements. Also the curves obtained for the mobility and concentration of charge carriers have similar nature for studied samples [2].

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Effect of Fe dopping electric properties of $Na_{0.5}Bi_{0.5}TiO_3$ ceramics in unpoled and poled state

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Properties of Fe doped $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) ceramics in two case, NBT doped 0.5 mol% Fe and second 0.1 mol% Fe. In both samples increases the electric conductivity, dielectric loss and depolarization temperature Td, Tm, compared to pure NBT. X-ray diffraction demonstrated the perovskite structure with rhombohedral symmetry. Dielectric study of these ceramics were taken in temperature range from room temperature to 873 K and in the frequency range from 10 kHz to 1 MH.

It was shown that a prior electric field poling process change character of ε(T) and tanδ(T) plots, slightly changes the Raman spectra and shifts Td and Tm. The Raman spectra are similar for both unpoled and poled states. Its means that electric field do not significantly disturbs crystal structure. This effects generally arises reinforcement of polarization and domain ordering and by the partial transformation of tetragonal regions into rhombohedral phase by electric field [1].

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Influence of E-poling on the structural, dielectric, vibrational and ferroelectric properties of $Na_{0.5}Bi_{0.5}TiO_3$ single crystals

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High quality lead-free $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) single crystals grown by the Czochralski method were investigated for both unpoled and poled samples. Raman scattering, structural, thermal, dielectric and second harmonic generation (SHG) studies were performed on this compound. The X-Ray Diffraction patterns indicate the perovskite-type structure of rhombohedral symmetry with small quantity of tetragonal phase even if at room temperature. These crystals are characterised by insignificant optical absorption in the visible light range and by high electric resistivity. Observed decreases of electric permittivity (approximately 10%) and dielectric dispersion (slight) for poled samples indicates the expected increase of the monodomain-like state in NBT single crystals under applied electric field. Dielectric dispersion was smaller than in NBT ceramics [1].

Results of these studies allowed for the designation of three characteristic temperatures: the depolarization temperature T_d near 190^{o}C and temperatures of two diffused rhombohedral - tetragonal (~280^{o}C) and tetragonal - cubic (~530^{o}C) phase transitions, and additionally to the coexistence of the particular phases in the broad vicinities of these transitions. E-poling action results in increase of degree of local order, transformation of the tetragonal regions into the rhombohedral phase and development in monodomain-like state [2].

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The electrocaloric effect in $BaTiO_3$:Eu ceramics determined by an indirect method

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The electrocaloric effect in $BaTiO_3$:Eu ceramics was determined by an indirect method. The temperature and electric field dependences of electrocaloric effect (ECE) of $BaTiO_3$ ceramics, pure and doped with 2% of Eu^{3+} ions, were investigated by the indirect method using the Maxwell relationship. Based on a Maxwell relation, the ECE was characterized via P–T curves under different electric fields.

The ECE experiments have been carried out from room temperature through the Curie region and in the paraelectric phase. A normal positive ECE was found around the phase transition point and is of the order of 0.6 K for pure $BaTiO_3$ and 0.15 K for the BT doped with Eu ions. The abnormal negative ECE was detected for the $BaTiO_3$ ceramic doped with Eu ions above the temperature of the phase transition. This phenomenon was related to the existence of defects that originates from the fixed local polarization of defect dipoles.

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