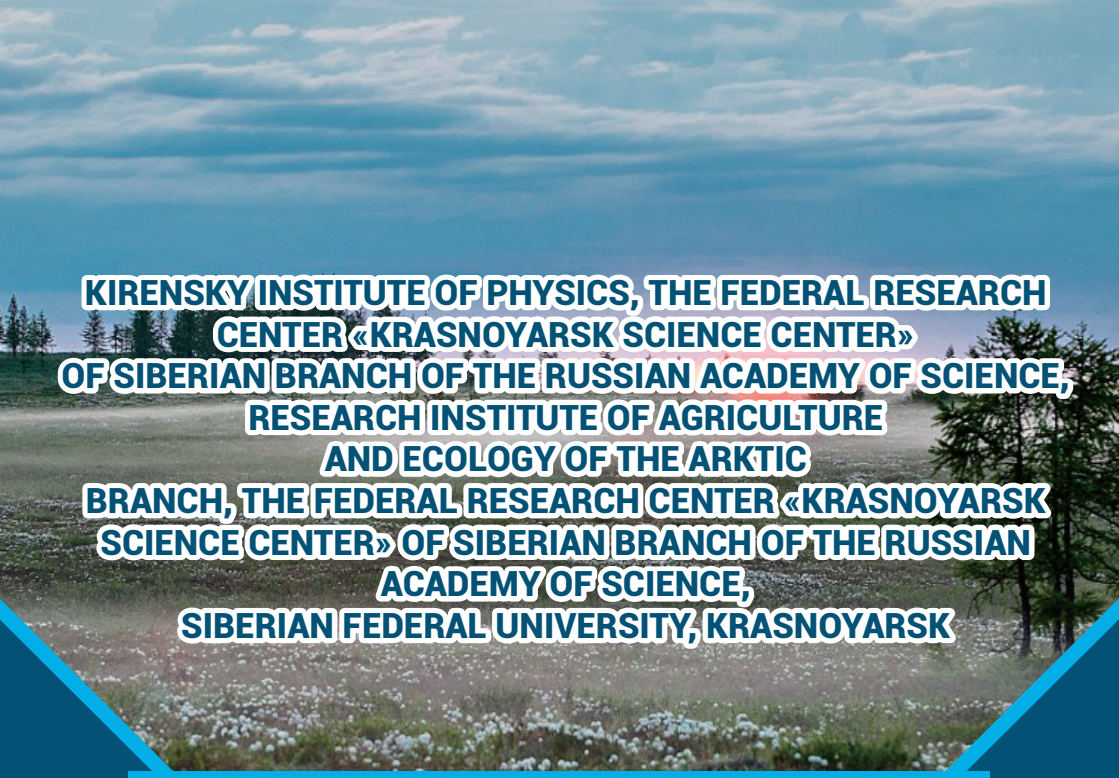


KIRENSKY INSTITUTE OF PHYSICS, THE FEDERAL RESEARCH CENTER «KRASNOYARSK SCIENCE CENTER» OF SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCE,
RESEARCH INSTITUTE OF AGRICULTURE AND ECOLOGY OF THE ARKTIC BRANCH, THE FEDERAL RESEARCH CENTER «KRASNOYARSK SCIENCE CENTER» OF SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCE,
SIBERIAN FEDERAL UNIVERSITY, KRASNOYARSK

THE INTERNATIONAL SCHOOL-WORKSHOP ON ACTUAL PROBLEMS OF CONDENSED MATTER PHYSICS IWCMP-2018

PROGRAM
BOOK OF ABSTRACTS

Norilsk,
12.03-16.03.2018




THE INTERNATIONAL SCHOOL-WORKSHOP ON ACTUAL PROBLEMS OF CONDENSED MATTER PHYSICS IWCMP-2018

KIRENSKY INSTITUTE OF PHYSICS, THE FEDERAL RESEARCH CENTER «KRASNOYARSK SCIENCE CENTER» OF SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCE,

RESEARCH INSTITUTE OF AGRICULTURE AND ECOLOGY OF THE ARKTIC BRANCH, THE FEDERAL RESEARCH CENTER «KRASNOYARSK SCIENCE CENTER» OF SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCE,

SIBERIAN FEDERAL UNIVERSITY, KRASNOYARSK

PROGRAM
BOOK OF ABSTRACTS

The workshop IWCMP-2018 is supported by
The Russian Foundation for Basic Research,
project 18-02-20017, by Siberian Federal University,
program 5-100,
and by Public Joint Stock Company
«Mining and Metallurgical Company «NORILSK NICKEL»

Norilsk , 12.03-16.03.2018

PROGRAM OF THE INTERNATIONAL SCHOOL-WORKSHOP IWCMP-2018
ON ACTUAL PROBLEMS OF CONDENSED MATTER PHYSICS

Date: 12.04.2018 arrival to Norilsk, welcome party

Date: 13.04.2018

8-55-9:00		Opening of the workshop	*Volkov Nikita, Ovchinnikov Sergei*
9:00-9:30	I*	*Balaev Dmitrii* Peculiarities of magnetic properties of antiferromagnetic nanoparticles	
9:30-10:00	I	*Buergler Daniel* Spin-transfer torque (STT): From basics to STT-induced dynamics in nano-oscillators with two stacked and dynamically coupled vortices	
10:00-10:30	I	*Avramov Pavel* Ab initio DFT consideration of electronic structure and magnetic properties of prospective 1D and 2D graphene-based heterostructures	
10:30-10:45		**Coffee break**	
10:45-11:00	O*	*Dubrovskiy Andrey* Possibility of forming of ε-Fe2O3-phase in the xerogel matrix.	
11:00-11:30	I	*Popkov Sergei* Nanoparticles in pulse magnetic fields: techniques and experiment	
11:30-12:00	I	*Tarasov Ivan* A way for targeted synthesis of higher manganese silicides: a new $Mn_{17}Si_{30}$ phase and its distinctive features	
11:45-12:00	O	*Yakushkin Stas* ε -Fe_2O_3/SiO_2 nanoparticles formation; spatial stabilization and the ε -$Fe_2O_3 \rightarrow \alpha$-$Fe_2O_3$ phase transition	

* *Type of talk invited (I) 30 min, oral (O) 15 min*

		Bondarev Ilya
12:00-12:15	**O**	Photovoltaic Phenomena in the Mn/SiO_2/n-Si Hybrid Structure
		Fedorov Alexandr
12:15-12:45	**I**	Ab initio investigations of nanostructures for their application as nanostructured thermoelectric materials
		Yih Jaan Tsai
12:45-13:00	**O**	Discussion of Upconversion Nanoparticles in Raman Spectroscopy
13:00-14:30		**Lunch**
		Schleicher Sebastian
14:30-14:45	**O**	Deposition of pyrene molecules on metal surfaces under ultra-high vacuum conditions for molecular spintronics
		Nikolaev Sergei
14:45-15:00	**O**	Anomalous Spectral Properties of High-Tc Cuprates: Influence of Short-Range Correlations
		Choi Cheol Ho
15:00-15:30	**I**	Understanding Nonadiabatic Processes by Quantum Mechanical Spin Flip Nonadiabatic Dynamics
		Sokolov Alexey
15:30-16:00	**I**	The influence of production regimes on the magnetic properties of nanoparticles for nanomedicine
16:00-16:20		**Coffee break**
		Tarasov Anton
16:20-16:50	**I**	Spin accumulation effect in fabricated planar device based on epitaxial Fe_3Si/p-Si structure
		Ovchinnikov Sergei
16:50-17:20	**I**	Temperature dependent band structure of La_2CuO_4
		Nekrasov Igor
17:20-17:50	**I**	Hidden Fermi surface in $KxFe_2{-}ySe_2$ superconductor
17:50		**Session closing** *Volkov Nikita, Ovchinnikov Sergei*

Date: 14.04.2018 excursion in Tukhard to the local holiday		
Date: 15.04.2018		
10:00-11:00	**Round table 1**	*Ovchinnikov Sergei* ***MODERATOR*** New physics of magnetic materials
11:00-12:00	**Round table 2**	*Avramov Pavel* ***MODERATOR*** Magnetic nanoparticles and biomedical applications
12:00-12:30	**Conference closing**	*Ovchinnikov Sergei*
12:30-14:00	**Lunch**	
14:00-18:30	**Excursion**	
18:30-22:00	**Conference dinner**	
Date: 16.04.201 Departure		
		Ovchinnikov Sergei ***DEPUTY CHAIRMAN***

Peculiarities of magnetic properties of antiferromagnetic nanoparticles

***Dmitry A. Balaev*[1]**

[1]*Kirensky Institute of Physics, Federal Research Center KSC SB RAS, 660036, Krasnoyarsk, Russia*

keywords: *: antiferromagnetic nanoparticles, uncompensated magnetic moment, superparamagnetic behavior, exchange bias.*

The materials containing magnetic nanoparticles are interesting both for fundamental research concerning the drastic difference of their magnetic properties from those of bulk analogs and for application in various fields.

In the antiferromagnetically (AFM) ordered nanoparticles, the surface effects and defects in the bulk of particles play a fundamentally different role: these particles acquire uncompensated magnetic moment μ_{unc}, ($\mu^P = \mu_{unc}$), the value of which depends on the particle size and defect type. Based on the statistical considerations, Néel proposed the interrelation between number of atoms N in a particle (obviously, N~V), uncompensated magnetic moment μunc, and defect type [6]

$$\mu_{unc} \sim \mu_{at} N^{b}. \quad (1)$$

Here, μat is the magnetic moment of a magnetically active atom and *b* is the exponent that takes the values of 1/3, 1/2, or 2/3 for defects on the surface and in the bulk of a particle or the odd number of ferromagnetically ordered planes in a particle. Indeed, according to the data reported in literature, equality (1) is valid for AFM nanoparticles of different compositions. This gives grounds for studying the fundamental properties of AFM nanoparticles and opens the opportunities for their application, e.g., in medicine, due to the fact that an AFM particle of a few nanometers in size can have a magnetic moment comparable with that of a ferro- or ferrimagnetic particle.

I will present a brief review of the investigations of the magnetic properties of AFM nanoparticles of different compositions. This involves superparamagnetic behavior, origin of uncompensated magnetic moment in various materials, peculiarities of magnetization curve, and shift of magnetic hysteresis loops after field cooling of AFM systems.

Special attention will be paid to nanoparticles of ferrihydrite with the nominal formula $5Fe_2O_3 \cdot 9H_2O$ and its biogenic analog horse spleen ferritin exhibit the AF ordering. We studied magnetic properties of both, so called, biogenic and chemical ferrihydrite samples[1-3]. Also, special attention is focused on the aspects of possible biomedical applications of this material, i.e., the particle elimination, toxicity, and possible use for targeted drug delivery.

1 D.A. Balaev, A.A. Krasikov, et al, JMMM 410, 71 (2016).
2 D.A. Balaev, A.A. Krasikov, et al, J. Exp. Theor. Phys. 119 (3), 479 (2014).
3 D.A. Balaev, A.A. Krasikov, A.A. Dubrovskiy, et al, J. Appl. Phys. 120, 183903 (2016).

Spin-transfer torque (STT): From basics to STT-induced dynamics in nano-oscillators with two stacked and dynamically coupled vortices

Daniel E. Bürgler[1]

[1]*Peter Grünberg Institute (PGI-6) & Jülich-Aachen Research Alliance, Fundamentals of Future Information Technology (JARA-FIT), Forschungszentrum Jülich, D-52425 Jülich, Germany*

keywords: *: spin-transfer torque, magnetic vortex, spin-torque oscillator.*

A spin-polarized current entering into a ferromagnetic material exerts a torque on the magnetization by transferring spin angular momentum from the current to the ferromagnet. This so-called spin-transfer torque (STT) gives rise to current-driven magnetization dynamics with unprecedented properties like magnetization switching without applying an external field or ex-citation of persistent large-angle precessions of the magnetization with frequencies in the GHz range, which are the basis of the so-called spin-transfer oscillators (STOs). In the first part, I will give an introduction to STT in magnetic multilayers with emphasis on developing a physical picture of the microscopic processes.

In the second part, I will present measurements and simulations of STOs formed by two stacked magnetic nanodisks that both contain a magnetic vortex. For an isolated nanodisk, the rotation of the vortex around the disk center is the fundamental magnetic excitation. The frequency of this gyrotropic mode varies with material and aspect ratio of the disk, but is independent of the vortex' vorticity and core polarity. I will show that this degeneracy can be lifted in double-vortex STOs due to STT-induced dynamic coupling of the two vortices[1]. The experimental system is a nanopillar with a diameter of 150 nm comprising two 15 and 30 nm thick Fe layers separated by a 6 nm thick Ag spacer. Suitable sequences of DC current-induced Oersted fields and external magnetic fields are used to prepare specific combinations of vorticities and polarities of the vortices in the top and bottom disks. STT acting on the two nanomagnets due to a DC current (e.g. 5.7×10^7 A/cm^2) excite a set of dynamic modes with discretely split frequencies. Micromagnetic simulations reveal that each mode with its characteristic frequency corresponds to a specific combination of vorticities and relative core polarities. A first splitting arises from the DC current-induced Oersted field that leads to a higher frequency when it is parallel to the magnetization circulation of the vortex in the thinner Fe disk. A "hyperfine"-splitting results from vortex-vortex interaction and depends on the relative alignment of the core polarizations with higher excitation frequencies for antiparallel polarities. The fine-splitting exists in zero field, demonstrating that such devices can function as zero-field, multi-channel STOs for communication technologies. It also facilitates the detection of the relative core polarization enabling multi-state memory devices based on double-vortex STOs.

1 V. Sluka, A. Kákay, A.M. Deac, D.E. Bürgler, C.M. Schneider, and R. Hertel, Nat. Commun. 6, 6409 (2015)

Ab initio DFT consideration of electronic structure and magnetic properties of prospective 1D and 2D graphene-based heterostructures

Pavel Avramov[1], Cheol Choi[1], Woohyeon Baek[1], Artem Kuklin[1]

[1]Kyungpook National University, Daegu, Republic of Korea

keywords: *graphene, graphene nanoribbons, carbon nanotubes, fullerenes, Buchkov-Rashba interfaces, induced spin polarization, magnetic supports, half-metallic states.*

The progress in developing of low-dimensional magnetic heterostructures for spin-related applications is based on weak spin-orbital interactions of light B atoms[1] and predictions of low-dimensional nanomaterials with unique magnetic properties. The effectiveness of spin injection in low-dimensional carbon nanostructures by ferromagnetic supports has already been discovered experimentally and interpreted theoretically[2]. The atomic and electronic structure, spin states and spin-dependent mechanisms of surface chemical reactions of a set of key spin-polarized low-dimensional pristine nanomaterials and heterostructures were studied using PBC ab initio DFT+U approach.

In particular, it was found that pi-conjugated carbon nanofragments and nanoclusters (2D graphene, zigzag nanoribbons, carbon nanotubes and C60 fullerene and pentacene molecule) are bounded with half-metallic LSMO(001) surface by weak disperse interactions. The types of coordination of the fragments, the strength of bonding and the rate of spin polarization are determined by the nature of the fragments. The direct and indirect exchange interactions with with Mn ions of LSMO ferromagnetic support and interface-induced structural asymmetry lead to the lift of the spin degeneracy and strong spin-polarization. Spin polarization changes the semiconducting nature of infinite graphene nanoribbons to half-metallic state with visible spin-up density of states at the Fermi level.

It was found that strong electron correlation effects in 2D VX2 (X=S,Se) monolayers and graphene/VX2 heterostructures are responsible for stability of 1T phases of VX2 monolayers. The study of vertical junctions comprising of graphene and VX2 monolayers demonstrated that interlayer interactions leads to formation of strong induced spin polarization of both graphene and VX2 fragments with keeping the linear dispersion of partial graphene band structure.

The work was supported by National Research Foundation of Republic of Korea under the grant NRF-2017R1A2B4004440

1 Marrows C. H., Hickey B. J., New directions in spintronics. Philos. Trans. A. 2011, 369, 3027–3036.

2 Tombros N., Jozsa C., Popinciuc M., et. al., Electronic spin transport and spin precession in single graphene layers at room temperature. Nature, 2007, 448, 571–574.

Possibility of forming of ε-Fe_2O_3-phase in the xerogel matrix.

Andrey Dubrovskiy[1]

[1]*Kirensky Institute of Physics, Federal Research Center KSC Siberian Branch Russian Academy of Sciences, Krasnoyarsk, Russia*

keywords: *nanoparticles, magnetic metamaterial.*

Magnetic metamaterials are widely used as magnetic recording media and magneto-optical devices. In this study we draw our attention to epsilon-iron oxide (ε-Fe_2O_3). ε-Fe_2O_3 is known to be unique among other iron oxide polymorphs due to its extremely high coercive field and high frequency millimeter wave adsorption. ε-Fe2O3 is a metastable phase, it can be obtained only in the form of particles with the size less than a particular nanometer threshold. Therefore to obtain the ε-Fe_2O_3 nanoparticles without admixture of other iron oxide polymorphs, one has to control the particle size and prevent the agglomeration process. There are different approaches for ε-Fe_2O_3 synthesis, for example sol-gel method. In this method iron-containing nanoparticles are coated by tetraethoxysilane (TEOS) and are sintered to obtain ε-Fe_2O_3 in SiO_2 matrix. Another synthesis method uses porous silica, which is firstly impregnated by the Fe ions and then sintered at high temperatures. The main problem then creating ε-Fe_2O_3 nanoparticles is to control size of nanoparticles to get ε-Fe_2O_3 without admixtures of other iron oxides. For the sol-gel method one's ability to obtain pure ε-Fe_2O_3 phase depends from the obtainability of stable sol of iron-containing nanoparticles with narrow size distribution. For the mesoporous silica impregnation method this problem falls onto the controlling the size distribution of the pores into the silica. Sometimes it is difficult to obtain narrow size distribution of the pores, since the drying of the silica may alter the pores size distribution. In this situation it is always difficult to create materials with high concentration of ε-Fe_2O_3 nanoparticles in it, since increasing of the content of precursors always leads to the narrowing of the stable zone of synthesis.

Considering a metamaterial based on supported magnetic nanoparticles, the density of the material and the interparticle magnetic interaction becomes paramount. At the same time transition to 3-dimensioanl systems may significantly complicate and alter investigations of the role of interparticle interactions. That is why it is important to study well characterized samples of concentrated magnetic nanoparticles with controllable fill-factor, density and the magnetic nanoparticles size distribution.

In the present work we report a novel synthesis method, to obtain a silica-gel material with combination of sol-gel and impregnation method. Using this technique we have succeeded creating ε-Fe_2O_3 nanoparticles in silica matrix with high iron oxide content, without admixture of other iron oxide polymorphs and with nanoparticles narrow size distribution.

The work was supported by the Russian Science Foundation grant № 17-12-01111.

Nanoparticles in pulse magnetic fields techniques and experiment

Dmitry Balaev[1], Alexander Krasikov[1], Alexander Balaev[1], Andrey Dubrovsky[1], Sergey Popkov[1]

[1]Kirensky Institute of Physics, FRC KSC SB RAS, 660036, Krasnoyarsk, Russia

keywords: *: nanoparticles, pulse magnetic fields.*

Pulsed magnetic fields are widely used in research laboratories. In most cases, the attention of researchers is not focused on the maximum magnetic field, but rather on research techniques implemented with the use of pulsed magnetic fields. In addition, using an alternating pulsed magnetic field of low frequency in experiments, it is possible to observe effects that depend on the rate of change of external magnetic field [1,2].

Installation of pulsed magnetic fields build at the Kirensky Institute of Physics makes it possible to conduct studies of magnetization and electrical resistivity in fields up to 45T with the possibility of changing the frequency of the applied external magnetic field.

The magnetization dynamics of e-Fe_2O_3 nanoparticles with an average size of about 9nm is investigated. From comparison of the hysteresis loops obtained in quasi-static conditions and under pulse fields with amplitudes up to 200 kOe and pulse lengths 8–32ms, it follows that the effective coercivity increases considerably with the variation rate of the imposed magnetic field.

A theoretical explanation of this behavior is proposed[3]. The model takes into account the superparamagnetic effects as well as the fact that magnetic anisotropy of the nanoparticles, along with the bulk term, includes a surface contribution. The latter, being of minor importance for the observed magnetic behavior of 25–50 nm particles, becomes essential when the particle size is below 10 nm. From the experimental data, a reference value of the surface anisotropy of nanodisperse e-Fe_2O_3 is established, and evidence is presented to the effect that below 300K this contribution does not significantly depend on temperature.

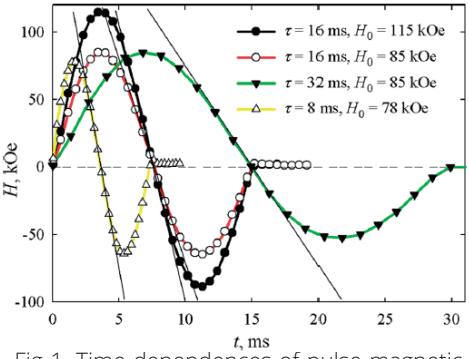


Fig 1. Time dependences of pulse magnetic field with various duration. Lines illustrate the determination of the rate of magnetic field change.

1 Balaev D.A., Dubrovsky A.A., Krasikov A.A. et al. Phys. solid state, 59-8, 1547-1552, 2017.
2 Balaev D.A., Popkov S.I., Krasikov A.A. et. al. Phys. solid state, 59-10, 1940-1946, 2017.
3 Balaev D.A., Poperechny I.S., Krasikov A.A. et al. J. Appl. Phys. 117, 063908, 2015.

A way for targeted synthesis of higher manganese silicides: a new $Mn_{17}Si_30$ phase and its distinctive features

I.A. Tarasov*[*1], M.A.Visotin[1,2], T. V. Kuznetzova[3,4], L.A. Solovyov[5], A.S. Fedorov[1,2], I.A. Yakovlev[1], A.S. Tarasov[1,2], S.N.Varnakov[1], S.G.Ovchinnikov[1].

[1]*Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Krasnoyarsk, 660036, Russia*

[2]*Siberian Federal University, 660041, Krasnoyarsk, Russia*

[3]*M.N. Miheev Institute of Metal Physics of the UB RAS, Yekaterinburg, 620108, Russia*

[4]*Institute of Physics and Technology, Ural Federal University, 620002, Yekaterinburg, Russia*

[5]*Institute of Chemistry and Chemical Technology, Federal Research Center KSC SB RAS, 660036, Krasnoyarsk, Russia*

keywords: *: Higher manganese silicides; Solid-state reaction; Optical properties; DFT calculations; Thermoelectrics; Electronic structure;*

Higher manganese silicides (HMSs) are attractive materials that can be utilised for thermoelectric[1] and photovoltaic power generation, light emittance and detection[2] In spite of a great number of works on HMS synthesis and investigation of their physical properties, both in bulk and 1D and 2D nanostructure forms, several technological and scientifically important issues remain not fully explored. The HMS family includes several homologous phases with Nowotny chimney ladder (NCL) tetragonal crystal structure that is composed of tetragonal manganese *ß*-Sn-like chimney subcell and double-helically arranged silicon subcell. Five different commensurate HMS compounds in chemical composition range $MnSi_{1.72-1.75}$ have been reported with the atomic position determined by X-ray diffraction (XRD) on bulk samples[3]. Along with these well–known HMS phases other HMS compounds such as have been described in XRD and electron diffraction studies on nanosized samples, thin films, nanowires, nanorods[4]. Nevertheless, the list of possible homologous HMS phases may be not fully determined because there is evidence of existing other NCL commensurate phases in other systems and incommensurate HMS phases.

Formation of $Mn_{17}Si_{30}$ HMS compound and its crystal structure is reported for the first time. Absorption measurements show that both samples prepared demonstrate direct transition around 0.9 eV, while the lowest indirect transitions are observed close to 0.4 eV. Accord ing to *ab inito* calculations, $Mn_{17}Si_{30}$ is a degenerated n-type semiconductor. The role of intrinsic lattice defects such as silicon, manganese vacancies on the electronic properties is analysed. It is asserted that silicon vacancies in Mn_4Si_7 lead to metallisation of the density of electronic states and in case of $Mn_{17}Si_{30}$ result in non-degeneracy. Introduction of manganese vacancy in HMS lattice leads to strong metallicity. Hall measurements on the samples indicate their p-type conductivity and degenerated nature which along with optical characteristics in low photon energy range (0.076 – 0.4 eV) argues for a high density of silicon vacancies. The hall mobility for $Mn_{17}Si_{30}$ thin film was found to be 25 $cm^2/V*s$ at room temperature.

We also present experimental permittivity spectra for the Mn_4Si_7 and $Mn_{17}Si_{30}$ compounds in a wide range (0.076 – 6.54 eV), which also indicate degenerated nature of both samples and put more emphasis upon the intrinsic relationship between lattice defects and optical properties. X-ray photoelectron spectroscopy discloses a presence of plasmon satellites in the Mn_4Si_7 and $Mn_{17}Si_{30}$ valence band spectra. This work was supported by the Russian Science Foundation, project no. 16-13-00060.

[1] S. A. Barczak, R. A. Downie, S. R. Popuri, et al, J. Solid State Chem. **227**, 55 (2015).
[2] J. E. Mahan, Thin Solid Films **461**, 152 (2004).
[3] D. Migas, V. Shaposhnikov, a. Filonov, at al. Phys. Rev. B **77**, 1 (2008).

ε-Fe2O_3/SiO_2 nanoparticles formation; spatial stabilization and the ε-Fe_2O3 → α-Fe_2O_3 phase transition

S.S. Yakushkin[1], D.A. Balaev[2], K.A. Shaikhutdinov[2], A.A. Dubrovskiy[2], G.A. Bukhtiyarova[1] and O.N. Martyanov[1]

[1]Boreskov Institute of Catalysis, 5 Lavrentieva pr., 630090, Novosibirsk, Russia,
[2]Kirensky Institute of Physics, Federal Research Center KSC Siberian Branch Russian Academy of Sciences, Krasnoyarsk, Russia

keywords: *εFe_2O_3 nanoparticles, superparamagnetic nanoparticles, size effect, phase transition.*

The iron-oxide based systems are one of the most available, cheap and nontoxic magnetic materials, which can be used in various applications, e.g. magnetic memory, controlled drug delivery, catalysis etc. The systems based on εFe_2O_3 nanoparticles among those materials attract particular and growing attention during the last decades. The εFe_2O_3 phase, is the intermediate between α- and γ-Fe_2O_3; it was characterized just recently, e.g. in 1998[1]. εFe_2O_3 nanoparticles display high (up to 20 kOe) coercivity at room temperature, which makes them a promising material for application in magnetic recording.

In the Boreskov Institute of Catalysis the εFe_2O_3/SiO_2 system based on few nanometers εFe_2O_3 supported nanoparticles was created for the first time that has no other detectable iron-oxide polymorphs[2]. The system displays superparamagnetic behavior at room temperature[3]. FMR method *in situ* in comparison with HR TEM, XRD, Mossbauer spectroscopy, and magnetization measurements data were applied to investigate the magnetic structure of εFe_2O_3/SiO_2 nanoparticles formed[4].

It was shown that the stabilization of the nanoparticles precursor on the silica support is the key factor to obtain the system free of admixture of other iron oxide polymorphs.

Samples with different iron contents were investigated in order to establish the conditions for obtaining the εFe_2O_3/SiO_2 samples without impurities of other iron oxide polymorphs[5]. It was demonstrated that the increase in the iron content leads to the formation of larger particles and gradual changes of the Fe^{3+} ion local environment during the phase transition ε-Fe_2O_3 → α-Fe_2O_3[6].

Support by Russian Science Foundation (Grant No. 17-12-01111)

1 Tronc E., Chaneac C., Jolivet J.P. (1998), J Sol. Stat. Chem. 139(1), 93-104
2 Bukhtiyarova G.A.,Shuvaeva M.A., Bujukov O.A. , Yakishkin S.S. , Martyanov O.N. (2011), J. Nanoparticle Res., 13(10), 5527-5534
3 Yakushkin S.S., Dubrovskiy A.A., Balaev D.A, Shaykhutdinov K.A., Bukhtiyarova G.A., Martyanov O.N. (2012), J. Appl. Phys., 111(4), 044312
4 Balaev D.A., Dubrovskij A.A., Shajkhutdinov K.A., Bayukov O.A., Yakushkin S.S., Bukhtiyarova G.A., Martyanov O.N. (2013), J. Appl. Phys., 114(16), 163911
5 Balaev, D.A., Yakushkin, S.S., Dubrovskii, A.A., Bukhtiyarova, G.A., Shaikhutdinov, K.A., Martyanov, O.N. (2016) Tech. Phys. Lett. 42, 347
6 Yakushkin, S.S., Balaev, D.A., Dubrovskiy, A.A., Semenov, S. V., Shaikhutdinov, K.A., Kazakova, M.A., Bukhtiyarova, G.A., Martyanov, O.N., Bayukov, O.A. J. Supercond. Nov. Magn. (2017).

Photovoltaic Phenomena in the Mn/SiO_2/n-Si Hybrid Structure

Ilya Bondarev[1,2], Mikhail Rautskii[1], Lev Shanidze, Anna Lukyanenko [1,2], Ivan Tarasov[1], Sergey Varnakov[1], Sergey Ovchinnikov[1] and Nikita Volkov[1]

[1]Kirensky Institute of Physics, Federal Research Center KSC SBRAS, Krasnoyarsk, 660036 Russia

[2]Siberian Federal University, Krasnoyarsk, 660041 Russia

keywords: *: hybrid structures, lateral photovoltaic effect, photovoltage, transport properties, spintronics.*

Metal-insulator-semiconductor (MIS) hybrid structures have been intensively studied due to some of their physical properties. Combination of semiconductors and magnetic materials allows controlling electron transport via magnetic moment of an electron. Therefore, MIS structures can be used as a basis of magnetic field sensors and different types of spintronic devices.

The lateral photovoltaic effect (LPE) adds a new mechanism of magnetic transport control in hybrid structures. The use of optical irradiation enhances functionality of MIS structures, which allows creating devices sensitive to both optical radiation and magnetic field.

The structure under study was fabricated on a single-crystal *n*-type Si(100) substrate. A SiO_2 layer with a thickness of 1.5 nm was formed on the substrate surface by chemical oxidation. On the top of the oxide layer, a Mn film with a thickness of 15 nm was deposited at room temperature by molecular beam epitaxy (MBE).

The most considerable LPE appears below 40 K. In the diode regime, the temperature dependence of photovolage demonstrates a peak at T ~ 25 K (Fig. 1). This peak originates from the surface states localized at the Si/SiO_2 interface[1].

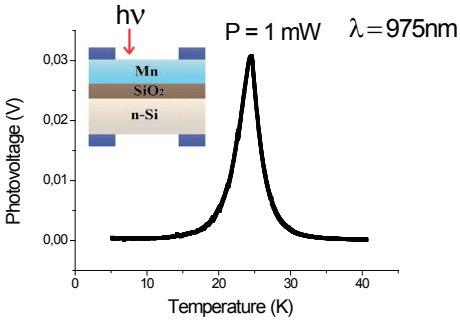


Figure 1. Temperature dependence of photovoltage of the Mn/SiO2/n-Si structure. P and λ are power and wavelength of applied laser, respectively.

The magnetic field influence on the LPE differs, depending on temperature and laser power. The relative change of photovoltage at H = 1T can attain ~30%.

The work was supported by the Russian Foundation for Basic Research, project No. 17-02-00302.

[1] Volkov, N. V., Tarasov, A. S., Rautskii, et. al., Magneto-transport phenomena in metal/SiO 2/n (p)-Si hybrid structures, J. Magn. Magn. Mater. (2017).

Ab initio investigations of nanostructures for their application as nanostructured thermoelectric materials

Aleksandr Fedorov[1], Maxim Visotin[2],
[1]Kirensky Institute of Physics, FRC KSC SBRAS, 660036, Krasnoyarsk, Russia
[2]Siberian Federal University, 660041, Krasnoyarsk, Russia

keywords: *thermoelectric materials, nanowires, Boltzmann's equation solution.*

Direct conversion of heat into electricity through advanced thermoelectric (TE) materials has been one of the most attractive solutions to the severe environmental and energy issues facing humanity. In recent years, great progress has been made in improving their dimensionless figure of merit (ZT), which determines the conversion efficiency of TE devices. ZT is defined as $ZT=S^2\sigma T/k$, where S is Seebeck coefficient, σ is electrical conductivity and k is thermal conductivity[1]. Resent progress in increasing ZT has been mainly driven by a reduction of thermal conductivity via nanostructuring approach. It has been demonstrated that thermal and electrical transport is influenced by crystallite boundary scattering[2].

We report here theoretical investigations of some nanostructures which may have good thermoelectric properties. For that thermoelectric parameters – S and σ were calculated by the semiclassical approach based on the Boltzmann's equation solution (BoltzTraP package)[3].

Specifically, we investigated fullerites which consist of the solid phase of fullerenes or endohedral metallofullerenes (EMF), where the molecules are bound by weak van der Waals forces. It was shown that that although S of some fullerites based on molecules C60, Ti2C2@C78, Sc@C82, Sc2@C82 had high S values (1800 μV/K for C60 and 1200 μV/K for Sc@C82), nevertheless the figure of merit of them were not good enough due to their low electrical conductivity.

For this reason, we investigated also the effects of nanostructuring of the SiGe bulk structure, which is the known thermoelectric material. More precisely, we researched thermoelectric properties of SiGe nanocomposites, consisted of same nanowires connected by a narrow contacts.

It was shown that replacing Si atoms with Ge ones increased the power factor $P=S^2\sigma$ by 40% at T=300 K which was equivalent to appropriate increasing of the figure of merit ZT.

This work was supported by Russian Science Foundation (project No. 16-13-00060)

1 M. Rowe, Thermoelectrics handbook: macro to nano. CRC press. 80, 2005

2 X.W. Wang, H. Lee, Y.C. Lan, G.H. Zhu, G. Joshi, D.Z. Wang, J. Yang, A.J. Muto, M.Y. Tang, J. Klatsky, S. Song, M.S. Dresselhaus, G. Chen, Z.F. Ren, Enhanced thermoelectric figure of merit in nanostructured n -type silicon germanium bulk alloy, Appl. Phys. Lett. **93** (2008) 193121.

3 G.K.H. Madsen, D.J. Singh / Computer Physics Communications **175** (2006) 67–71

Discussion of Upconversion Nanoparticles in the Raman Spectroscopy

Yih-Jaan Tsai[1], Chun-Rong Lin[1], Yu-Lian Yang[1], Sheng-Yuan Lin[2], Ruei-En Tsai[1], Yaw-Teng Tseng[1*]

[1]Department of Applied Physics, National Pingtung University, Pingtung, Taiwan

[2]Department of Applied Chemistry, National Pingtung University, Pingtung, Taiwan

keywords: *: Raman spectra, Upconversion, Nanoparticles*

Scientist found UCNPs (Upconversion Nanoparticles) before ten years ago, then devoted to study the application of UCNPs in biomedicine. Use it unique physical properties to inject inside animals, tried to find the treatment of cancer. The honor attracted many scientists starting the research of UCNPs.

Synthesis of UCNPs could be done by two different ways: one is pyrolysis another is hydrothermal. In this discussion we have chosen pyrolysis, because we can control it very accurate. By using different temperature to control it the Cubic phase (*α*-Phase) or Hexagonal phase(*β*-Phase) can be obtained. Review of the studies shows that when UCNPs is in Hexagonal phase it shows high level of the optical properties. But up to now only the NIR (Near Infrared Laser) measurements have been carried out. That's the subject of this discussion.

Characteristics of UCNPs was measured by X-Ray diffraction and Raman spectroscopy. X-Ray diffraction shows that the crystal lattice is different for α-phase and *β*-phase. Raman spectroscopy uses a 532 nm laser to irradiate the sample to form Raman scatterings. We will discuss the observed scattering spectrum with analysis of lattice oscillation modes.

Raman spectroscopy shows the reason why the crystal structure is so different between *α*-Phase and *β*-Phase. From Raman Spectra, *β*-Phase UCNPs molecular oscillations can be more clearly observed than in α-Phase. Between 150 cm^{-1} to 850 cm^{-1} the difference in scattering intensity is very large for two phases. The result of the Raman spectra will be discussed in the framework of molecular dynamics and lattice dynamics .

1 Li, Z., LI, Y., Zhang, X., Wang, L., Hu, B., Zhang, Y., . . . Chen, W. Systematic Synthesis and Optical Property Studies of Monodisperse NaYF4: Yb3+, Er3+ Nanocrystals with Pure Hexagonal Phase. *Science of Advanced Material*, (2017) pp. 624-629. doi:10.1166/sam.2017.2352.

2 Xu, X., Wang, Z., Lei, p., Yu, y., Yao, S., Song, S., . . . Zhang, H. αNaYb(Mn)F4:Er3+/Tm3+@ NaYF4 UCNPs as "Band-Shape" Luminescent Nanothermometers over a Wide Temperature Range. *Applied Materia*l, 2015, August 27, pp. 20813-20819.

Deposition of pyrene molecules on metal surfaces under ultra-high vacuum conditions for molecular spintronics

Sebastian Schleicher[1], Bogdana Borca[1,2], Jeff Rawson[1,3], Frank Matthes[1], Daniel E. Bürgler[1], Paul Kögerler[3], Claus M. Schneider[1]

[1]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich, Germany

[2]National Institute of Materials Physics, Bucharest, Romania

[3]Institute of Inorganic Chemistry, RWTH Aachen University, Germany

keywords: *: aromatic molecules, ferromagnetic surfaces, spin-dependent hybridization.*

Interfacial properties of organic adsorbates featuring aromatic π-orbitals on metal surfaces play an important role for organic electronics and molecular spintronics. On ferromagnetic transition metal surfaces the chemisorption of the molecules is governed by strong hybridization of molecular π-orbitals with spin-split *d*-orbitals of the substrate that results in a spin-imbalanced molecular density of states. Pyrene can be considered as a precursor for pyrene-based double-decker molecules that are expected to show exciting magnetic and spintronic properties such as spin-filtering[1] due to spin-polarized hybridization with ferromagnetic surfaces. However, the deposition of single pyrene molecules with a size between ultimately small benzene and extended graphene on clean and reactive surfaces is challenging, since pyrene forms a solid with a high vapor pressure. Hence, it cannot be evaporated from a Knudsen cell, nor dosed from the gas phase. Here, we present a sublimation procedure under ultra-high vacuum (UHV) conditions and image single as well as self-organized pyrene molecules on in-situ prepared Au(111) and Fe/W(110) substrates by means of low temperature scanning tunneling microscopy (LT-STM) at 77 K to ensure low mobility of the molecules. For the Au(111) surface, the molecule-surface interaction is weak such that the Au(111) herringbone reconstruction is not lifted and visible through the self-organized pyrene layer. Pyrene desorption due to the weak intermolecular bonding self-limits growth to a monolayer. Fe films of one to four atomic layers epitaxially grown on W(110) serve as ferromagnetic substrates with well-defined magnetic properties. STM images reveal that in spite of the stronger interaction on Fe compared to Au the pyrene molecules remain intact upon deposition and adsorb in a flat geometry. However, the molecular arrangement sensitively depends on Fe thickness. Irregular configurations occur on the pseudomorphically strained first Fe layer, while self-assembled ordered arrays form on the second Fe layer. On the third and fourth Fe layer the pyrene molecules arrange according to the moiré pattern of the Fe surface.

In the future we plan to realize a spin filter made of a specifically designed single molecule that features two stacked π-systems. Spin-polarized STM (SP-STM) will be used to confirm the molecular spin filter property.

1 K.V. Raman et al., Nature 493, 509 (2013).

Anomalous Spectral Properties of High-Tc Cuprates: Influence of Short-Range Correlations

Sergey Nikolaev[1,2], Valerii Kuz'min[2], Sergey Ovchinnikov[1,2]

[1]Siberian Federal University, Svobodny pr. 79, 660041, Krasnoyarsk, Russia

[2]Kirensky Institute of Physics, Akademgorodok 50/38, 660036, Krasnoyarsk, Russia

keywords: *: electronic structure, strong correlations, cluster perturbation theory, Fermi surface.*

The physics of strongly correlated electron systems is greatly influenced by many-particle correlation effects. A significant contribution to the formation of such effects is introduced by local and short-range correlations as the consequence of Coulomb interaction's local character. One of the manifestations of correlation effects is the presence of different anomalies in the electronic spectrum. Due to the ability to investigate the electronic structure by means of angle-resolved photoemission spectroscopy (ARPES), anomalous properties of high-Tc cuprates, such as the pseudogap and Fermi-arcs, are known. Further ARPES studies of high-Tc cuprates, as well as other strongly correlated compounds, revealed a variety of low-energy and also high-energy kinks along with the so-called waterfalls. Another anomalous property, an electron-like pocket at the Fermi surface at hole doping p=0.1, has been uncovered by the observation of quantum oscillations.

We aim to obtain the fine structure of quasiparticle bands contributing to the electron spectral function within cluster perturbation theory (CPT)[1-3]. CPT provides a possibility to account exactly for local and short-range correlations in the framework of a finite cluster.

In this work CPT has been applied to the Hubbard and Hubbard-Holstein t-t'-t''-U models at low hole doping. Based on full exact diagonalization (ED) of a 3x3 cluster for the Hubbard model and a 2x2 8-phonon cluster for the Hubbard-Holstein model, we have obtained the fine structure of quasiparticle bands of Hubbard fermions and polarons in order to investigate in detail, how different spectral anomalies arise in strongly correlated systems, when short-range correlations from local Coulomb and electron-phonon interactions affect the properties of such quasiparticle bands.

We obtain the Fermi surfaces with a nodal electron pockets similar to the obtained in the mean-field models of charge ordering within the fundamental model of strong correlations, the Hubbard model, without *ad hoc* introducing of density waves, in the same manner as other anomalous features of the electronic structure.

This work is supported by Russian Foundation for Basic Research (grant 16-02-00098), Government of Krasnoyarsk Territory, Krasnoyarsk Region Science and Technology Support Fund to the research projects 18-42-243004.

1 Nikolaev S.V. and Ovchinnikov S.G. (2010), JETP 111, 635; (2012) JETP 114, 118.

2 Kuz'min V.I., Nikolaev S.V., Ovchinnikov S.G. (2016), Pis'ma v ZhETF 103 (2), 132.

3 Kuz'min V.I., Nikolaev S.V., Ovchinnikov S.G. (2014), Physical Review B 90, 245104.

Understanding Nonadiabatic Processes by Quantum Mechanical Spin Flip Nonadiabatic Dynamics

Cheol Ho Choi[1]

[1]*Kyungpook National University, Daegu, Republic of Korea*

keywords: *Nonadiabatic dynamics, spin flip, coupling terms, chemical reaction dynamics, conversion of light, photovoltaics, artificial photosynthesis*

Observing chemical reactions in real time is one of the ultimate goals of physical chemistry. Experimentally, a great deal of time-resolved spectroscopies as well as ultrafast X-ray have been developed to observe the events. The interests on such chemical reaction dynamics grow rapidly, since they are also strongly related with the light energy conversion mechanisms of photovoltaics and artificial photosynthesis. In general, they belong to "nonadiabatic processes" with the timescale of ~100 fs. Contrasting to the experimental efforts, easily accessible theoretical tools for them are rare. In this talk, we describe an efficient and practical method for "nonadiabatic processes" by combining MD, QM/MM, NACT (Nonadiabatic Coupling Term) and newly developed FOR-SP-TDDFT (Fractionally Occupied Reference-v-Time Dependent DFT). In addition, we also present its applications on photochemical reactions.

The influence of production regimes on the magnetic properties of nanoparticles for nanomedicine

Alexey Sokolov[1,2], Olesia Solodova[2], Alina Bachal[2], Anna Sherepa[1], Vladimir Zabluda[1], Dmitry Velikanov[1], Ivan Lapin[3], Anastasiia Shabalina[3] and Valery Svetlichnyi[3].

[1]Kirensky Institute of Physics, FRC KSC SBRAS, Akademgorodok 50/38, 660036, Krasnoyarsk, Russia

[2]Siberian Federal University, Svobodny pr., 79, 660041, Krasnoyarsk, Russia,

[3]Tomsk State University, Novosobornaya pl., 1, 634050, Tomsk, Russia

keywords: *Magnetic materials for biomedical applications, magnetic nanoparticles, iron oxides, magnetization, magnetic circular dichroism, pulsed laser ablation*

Currently, there are nanoparticles that are being applied successfully in the diagnosis and therapy of cancer. A huge number of reviews and articles are devoted to use of the magnetic nanoparticles to increase the contrast of MRI, targeted drug delivery, magnetic hyperthermia and mechanical destruction of cancer cells, for instance [1-3]. Nevertheless, it remains an open question about the influence of methods for obtaining magnetic nanoparticles on their magnetic properties and the possibility of using them in the nanomedicine.

This work is devoted to the investigation of the effect of the regimes of obtaining nanoparticles of iron oxides by pulsed laser ablation. Radiation of Nd:YAG laser was used for Fe target ablation (wavelength of 1064 nm, pulse duration of 7 ns, frequency of 20 Hz, pulse energy of 150 mJ). Produced nanoparticles were collecting on the bottom of the reactor (glass tube) using a permanent magnet. To change the phase composition and structure of the product it was annealed at different temperatures (200, 300, 400, and 500°C).

The structure of the nanoparticles obtained was investigated using transmission electron microscopy. The magnetic properties of the obtained nanoparticles were investigated using a direct (SQUID magnetometer in a magnetic field up to ± 20 kOe) and indirect (spectroscopy of magnetic circular dichroism of nanoparticle dispersion) methods.

The relationship of shape, size, magnetic properties of nanoparticles and the possibility of their use for theranostics is discussed

The reported study was funded by Russian Foundation for Basic Research, Government of Krasnoyarsk Territory, Krasnoyarsk Region Science and Technology Support Fund to the research project No.17-42-240080

1 Karkan S.F., Mohammadhosseini M., Panahi Y., et al., Artificial cells, nanomedicine, and biotechnology, **45(1**), 1-5.

2 Belyanina I, Kolovskaya O., Zamay S. et al., Molecules 2017, **22**, 975

3 Belyanina I., Zamay T., Zamay G. et al., Theranostics 2017, Vol. 7, Issue 13, pp. 2956-2967.

Spin accumulation effect in fabricated planar device based on epitaxial Fe_3Si/p-Si structure

Anton Tarasov[1], Mikhail Rautskii[1], Ilya Bondarev[1], Anna Lukyanenko[1], Ivan Tarasov[1], Ivan Yakovlev[1], Sergey Ovchinnikov[1], Nikita Volkov[1]

[1]Kirensky Institute of Physics, FRC KSC SB RAS, 660036, Krasnoyarsk, Russia

keywords: *: epitaxial magnetic films, iron silicide, wet etching, spin accumulation, Schottky barrier, interface states.*

Efficient spin injection and detection of charge carriers in ferromagnetic metal/insulator/ semiconductor (MIS) structures requires high interface quality, because various defects and imperfections cause scattering of spin-polarized electrons. However, epitaxial growth of insulating layer is a non-trivial technological task. This significantly complicates fabrication of MIS structures for spintronics. Nevertheless several groups had demonstrated spin transport in ferromagnetic metal/ semiconductor (MS) structures, where the role of an insulator is played by the Shottky barrier [1]. In this work we represent fabrication process of planar microdevices based on epitaxial $Fe_{1-x}Si_x$ films grown on Si(111) and spin accumulation effect in Fe_3Si/p-Si MS structure probed by 3-terminal Hanle measurements.

The $Fe_{1-x}Si_x$ films were formed on *p*-doped Si(111) substrate (ρ = 7.5 Ω·cm) at 400 K by molecular beam epitaxy (MBE) under ultrahigh vacuum conditions. Structural characterization of the films was performed by X-ray diffraction, reflective high-energy electron diffraction, Rutherford backscattering spectrometry and transmission electron microscopy, which confirmed single crystallinity and interface abruptness for all films[1]. To create planar microdevices standard photolithography and wet etching with solution of hydrofluoric acid and nitric acid (HF: HNO3: H_2O = 1: 2: 400) were used. For the films with various chemical composition etching rates were obtained, the etching speed of Fe3Si film was about 50 Å/sec. To study spin-dependent transport phenomena in Fe_3Si/p-Si structures we fabricated 3-terminal planar microdevices and metal/semiconductor diode using developed fabrication process.

I-V curve diode shape indicates the presence of Schottky barrier at Fe_3Si/p-Si interface. Calculated Schottky barrier height is 0.57 eV, which can provide necessary conditions for spin accumulation in p-Si. Indeed, in Fe3Si/ p-Si 3-terminal planar device spin accumulation effect was observed. Calculated spin lifetime and spin diffusion length in p-Si are 145 ps and 405 nm, respectively (at T=300K). Spin lifetime strongly depends on temperature which can be related to the fact that spin-dependent transport in our device is realized via the surface states.

The work was supported by the RFBR, Government of Krasnoyarsk Territory, Krasnoyarsk Regional Fund of Science (grant Nos. 18-42-243022, 17-02-00302).

1 Y. Fujita, S. Yamada, Y. Ando et al., J. Appl. Phys., **113(1)**, 013916 (2013).

2 A.S. Tarasov, A.V. Lukyanenko, I.A. Tarasov, et al. Thin Solid Films **642**, pp. 20-24 (2017).

Temperature dependent band structure of La_2CuO_4

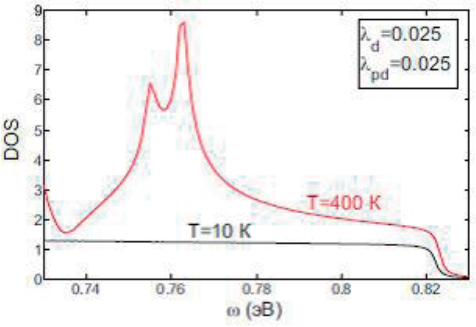
Sergey Ovchinnikov[1,2], Elena Snheyder[1], Ilua Makarov[1], Maria Zotova[2]

[1]Kirensky Institute of Physics, FRC KSC SBRAS Akademgorodok 50/38, 660036, Krasnoyarsk, Russia

[2]Siberian Federal University, av.Svobodnii 89, 660041, Krasnoyarsk, Russia

keywords: *: high temperature superconductivity, strong electron correlations, band structure*

The multielectron generalized tight binding (GTB) method to calculate the electronic structure of strongly correlated electrons in cuprates is modified to incorporate also strong electron-phonon interaction[1]. By exact diagonalization of the p-d- Holstain model Hamiltonian for a separate CuO_6 unit cell we find the multelectron and multiphonon local eigenstates that are used to construct a set of local Hubbard operators. Then we treat the intercell electron hopping t by the perturbation approach over small ratio t/U, where U is the charge transfer excitation energy. Without electron-phonon interaction we obtain the band of spin polaron and a set of local multiphonon Franck-Condon excitations. The electron-phonon interaction results in the hybridization of spin polaron and Franck-Condon excitations that forms the polaronic band structure with strong temperature dependence[2]. Here the temperature dependence of the polaronic band structure in La_2CuO_4 is discussed. We have obtained smooth evolution of the band structure from the polaron in antiferromagnetic low temperature insulator to paramagnetic high temperature Mott-Hubbard insulator at high temperature 600K. At intermediate temperatures 300-400K we found a flat band at the top of the valence band forming peaks in the density of states (fig.1). We discuss the effect of this flat band on the pseudogap formation at the intermediate temperatures.



1 Makarov I.A., Shneyder E.I., Kozlov P.A and Ovchinnikov S.G, (2015) Phys. Rev. B. **92**, 155143.

2 Makarov I.A., Shneyder E.I., Kozlov P.A and Ovchinnikov S.G, (2016) Journal of Superconductivity and Novel Magnetism, **29**, 1063.

3 Shneyder E.I., Makarov I.A., Zotova M.V. and Ovchinnikov S.G (2018). JETP 653, 012095.

Hidden Fermi surface in $K_xFe_2-_ySe_2$ superconductor

Nekrasov I.A.[1], Pavlov N.S.[1], Sadovskii M.V.[1,2]

[1]Institute for Electrophysics UB RAS, Russia, Ekaterinburg

[2]Institute of Metal Physics UB RAS, Russia, Ekaterinburg

keywords: *: iron-based superconductors, electronic structure, Fermi surface, LDA+DMFT.*

Investigation of the superconductivity in recently discovered iron-based superconductors is one of the main trends in modern condensed matter physics. Some of iron chalcogenide superconductors[1] have qualitatively different electronic properties from other iron-based superconductors (e.g. iron pnictides). Among them, the $K_xFe_2-_ySe_2$ compound and the FeSe monolayer on the $SrTiO_3$ substrate take quite a special place. Early days angular resolved photoemission spectra (ARPES) experiments showed that for these compounds there are absent or practically can not be resolved hole-like Fermi surface sheets near the Γ-point of the Brillouin zone. While for the iron pnictides and some iron chalcogenides (e.g. bulk FeSe) these hole-like Fermi surface sheets near the Γ-point were clearly observed by ARPES. The absence of the hole-like Fermi surface sheets near the Γ-point indicates that for $K_xFe_2-_ySe_2$ series there is no possibility of nesting between the hole sheets of the Fermi surface near the Γ-point and electronic sheets near the M-point. Thus a spin-fluctuation mechanism of superconducting pairing (assumed for iron pnictides[2]) is not applicable here.

Recently in the work[3] was reported ARPES observation of a hidden hole-like band approaching the Fermi level near the Γ-point for the $K_{0.62}2Fe_{1.7}Se_2$ system. Also in the work[3] on the basis of the ARPES data analysis there was proposed a presence of a hidden hole-like Fermi surface near the Γ-point. The authors of [3] provide some reasons why the Fermi surfaces near the Γ-point previously were not observed due to the geometry of the experiment.

In the work[4], we already reported theoretical LDA+DMFT[5,6] study of $K_xFe_2-_ySe_2$ material. Here on the basis of the work [4] and inspired by the work[3] we show that for $K_{0.62}Fe_{1.7}Se_2$ system near the Γ-point there are two hole-like bands crossing the Fermi level. One band has the Fe-$3d_{xy}$ orbital character, the second - Fe-$3d_{yz,xz}$. These bands form the hidden Fermi surface near the Γ-point. Its appearance can justify spin-fluctuation mechanism of superconductivity in this class of systems with a rather high critical temperature T_c~30K. Good qualitative and even quantitative agreement of the calculated and ARPES Fermi surfaces is obtained.

This work is supported by RFBR grant №17-02-00015.

1 M.V. Sadovskii. Phys. Usp. **59**, 947 (2016).

2 P.J. Hirshfeld, M.M. Korshunov, I.I. Mazin. Rep. Prog. Phys. **74**, 124508 (2011).

3 M. Sunagawa et al., J. Phys. Soc. Jpn. **85**, 073704 (2016).

4 I.A. Nekrasov, N.S. Pavlov, M.V. Sadovskii. JETP Letters **97**, 15 (2013); ibid. JETP 117, 926 (2013).

5 K. Held et al. Int. J. Mod. Phys. B **15**, 2611 (2001).

6 G. Kotliar et al. Rev. Mod. Phys. **78**, 865 (2006).

Name	e-mail	page
Avramov Pavel	paul.avramov@gmail.com	9
Balaev Dmitrii	dabalaev@iph.krasn.ru	7, 11, 13
Buergler Daniel	d.buergler@fz-juelich.de	8, 17
Bondareva Elena	mainoffice@iph.krasn.ru	
Bondarev Ilia	fbi1993@mail.ru	14, 21
Choi Cheol Ho	cheolho.choi@gmail.com	9, 19
Dubrovskiy Andrey	stas-yk@catalysis.ru	10, 11, 13
Fedorov Alexandr	alex99@iph.krasn.ru	12, 15
Nikolaev Sergei	25sergeyn@mail.ru	18
Nekrasov Igor	nekrasov@iep.uran.ru	23
Ovchinnikov Sergei	sgo@iph.krasn.ru	12, 14, 18, 21, 22
Popkov Sergei	dir@iph.krasn.ru	11
Schleicher Sebastian	s.schleicher@fz-juelich.de	17
Sokolov Alexey	alexeys@iph.krasn.ru	20
Tarasov Anton	taras@iph.krasn.ru	12, 21
Tarasov Ivan	tia@iph.krasn.ru	12, 14, 21
Tsai Yih-Jaan	ytt@mail.nptu.edu.tw	16
Volkov Nikita	volk@iph.krasn.ru	14, 21
Yakushkin Stas	stas-yk@catalysis.ru	13