IWAMO
2nd International Workshop
on Advanced Magnetic Oxides
2021

Workshop Book

24-26 November 2021
Aveiro, Portugal

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Sara Martins Vieira *Physics Department, University of Aveiro, Portugal*

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IWAMO 2021 – 2nd International Workshop on Advanced Magnetic Oxides

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Welcome

Dear participants, it is my pleasure to welcome you – on behalf of all the organisers – to the 2021 edition of the *IWAMO*!

I hope everyone is doing well and staying safe.

The time after *IWAMO 2019* was overshadowed by the Corona pandemic and made international cooperation unusually difficult. It is all the more important to sustain and develop scientific communication, even if for the most part in the online format.

The workshop continues the exchange of ideas and expertise in the area of magnetic double perovskites, especially, strontium ferromolybdate, but the scope of the workshop is much wider than this topic. New fantastic results were obtained in the past two years in the field of oxides, and we hope to learn a lot of new information from the keynote and contributed presentations included in the program of our workshop.

We hope you'll have many opportunities to meet old friends and research partners and make new ones in cyberspace and discuss the hottest topics of your research. We are convinced new sparkling ideas and fruitful collaborations will result from our gathering.

Finally, we'd like to thank each of you for attending this workshop and bringing your expertise to our meeting.

On behalf of the *IWAMO 2021* organisers,

Nikolai A. Sobolev

(Workshop Chairman)

The Workshop

IWAMO 2021 – 2nd International Workshop on Advanced Magnetic Oxides will be held online during 24-26 November 2021.

As a joint organisation between the University of Aveiro, the Physics Department of the University of Aveiro and the Associate Laboratory i3N/FSCOSD - Institute of Nanostructures, Nanomodelling and Nanofabrication (Aveiro unit), the event will be an excellent opportunity to acquire new knowledge and exchange ideas on state-of-the-art research and the latest advancements regarding magnetic oxides and related subjects. The topics to address will be:

A. *Theory and modelling*
B. *Single crystals, thin films, nanoparticles, 2D and hybrid systems - growth and structure, doping*
C. *Perovskites and double perovskites, diluted magnetic oxides, other functional materials*
D. *Composites, heterostructures and interfaces*
E. *Novel characterization techniques and equipment*
F. *Magnetic resonance, including imaging*
G. *Nanofluids, biomedical applications*
H. *Devices*
I. *New trends and applications in magnetocalorics, photocatalysis, magnonics, multiferroics*

Authors that present their work at **IWAMO 2021** will be invited to contribute with an original paper or feature article (after double reviewing) in a special issue/topical section in *physica status solidi (b)* (Wiley-VCH).

IWAMO 2021 is a networking event included in the planning framework for **Project SPINMULTIFILM – Physical principles of the creation of novel SPINtronic materials on the base of MULTIlayered metal-oxide FILMs for magnetic sensors and MRAM**.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 778308

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Full Programme

Wednesday, 24 November

9:00 – 9:30		**Opening Session** *In memoriam:* **Eliezer Adar**
9:40 – 10:40	Session 01 Chairperson: **N. Sobolev**	Keynote Talk 01: **Elvira Fortunato** *A new era of semiconductors: metal oxides* Oral 01: **M. Batista** *Spectroscopic investigations on Cr doped zinc gallogermanate persistent phosphor*
10:50		*BREAK*
11:00 – 12:20	Session 02 Chairperson: **V. Shur**	Keynote Talk 02: **Gunnar Suchaneck** *Resistivity and tunnel magnetoresistance in double perovskite strontium ferromolybdate ceramics* Oral 02: **O. Toulemonde** *From magnetic cluster glass state to giant vertical magnetization shift induced by ferromagnetic cluster growth in SrFe0.25Co0.75O2.63* Oral 03: **M. Varghese** *Is there any dynamic magnetic dimer in Sr2CrNbO6 ordered double perovskite?*
12:30 – 14:00		*BREAK*
14:00 – 15:20	Session 03 Chairperson: **M. Andrulevicius**	Keynote Talk 03: **Mikalai Kalanda** *Electric transport characteristics of Sr2FeMoO6-δ ceramics with structurally inhomogeneous surfaces* Oral 04: **P.R. Nadig** *The monovalent Ag-substituted La0.67Ca0.33MnO3 manganites: The prediction of magnetocaloric effect by means of various models* Oral 05: **R. Lanovsky** *The structure, magnetic and magnetotransport properties of layered cobaltites Sr1-xYxCoO3-δ*
15:30		*BREAK*
15:40 – 17:00	Session 04 Chairperson: **O. Toulemonde**	Keynote Talk 04: **Shengqiang Zhou** *Tailoring oxide thin films by ion beam* Oral 06: **M. Andrulevicius** *XPS analysis of Mo and Sr oxides thin films* Oral 07: **J. Fedotova** *Local atomic order and magnetic properties in (FeCo)x(SiO2)100-x core-shell nanoparticles for theranostics*
17:10 – 17:25	Session P01 Chairperson: **L. Rino**	Poster Session 01: **Y. Samoshkina** *Magneto-optics of Hydrogenated ZnO, ZnO:Co, and ZnO:(Co+Al) Films* **A. Nikolskaya** *Synthesis and Ion Doping of Gallium Oxide*
17:30		*End of day 1*

Thursday, 25 November

9:00 – 10:30	Session 05 Chairperson: **H. Raebiger**	Keynote Talk 05: **Nerija Žurauskienė** *Engineering of lanthanum perovskite thin films for magnetic sensors applications* Keynote Talk 06: **Peter K. Petrov** *Transition metal nitride and oxide thin films: Growth and properties*
10:40 – 10:50		*BREAK*
11:00 – 12:20	Session 06 Chairperson: **G. Suchaneck**	Keynote Talk 07: **Vladimir Ya. Shur** *Micro- and nano-domain engineering of ferroelectrics crystals* Oral 08: **N.M. Ferreira** *Application of a magnetic field in laser floating zone for processing thermoelectric ceramics* Oral 09: **J. Zanoni** *Spectroscopic studies on doped and proton irradiated ß-Ga2O3*
12:30 – 14:00		*BREAK*
14:00 – 15:20	Session 07 Chairperson: **N. Žurauskienė**	Keynote Talk 08: **Herman Terryn** *New experimental and modelling approaches to understand electrodeposition of metals* Oral 10: **C. Keßler** *Magnetic functionalization of poly(N-isopropylacrylamide) hydrogels for sensor applications* Oral 11: **A. Mieting** *In-situ prepared ferrogels with stimuli-responsive properties for sensing applications*
15:30		*BREAK*
15:40 – 16:40	Session 08 Chairperson: **E. Kotomin**	Keynote Talk 09: **Dmitry Karpinsky** *Phase transitions in magnetoelectric BiMnO3-based ceramics* Oral 12: **A. Batista** *Visualization of PVDF/Fe3O4 composite by MRI: contribution of homopolymer*
16:50 – 17:20	Session P02 Chairperson: **N.M. Ferreira**	Poster Session 02: **S.M. Konoplyuk** *Magnetic and magnetocaloric properties of Sr2FeMoO6-d double perovskites with different degrees of superstructural ordering* **V.A. Safina** *Chemical solution deposition of BiFeO3 films with layer-by-layer control of the coverage and composition* **N. Grevtsov** *Porous Silicon Surface Treatment Effect on the Structure of Nickel-Porous Silicon Magnetic Composites* **E. Lazareva** *Structural and magnetic properties interplay in optimizing functionality of magnetocaloric ferrite's fine particles*
17:25		*End of day 2*

Friday, 26 November

9:00 – 10:30	Session 09 Chairperson: **P.K. Petrov**	Keynote Talk 10: **Eugene Kotomin** *First principles calculations of the electronic and magnetic properties for defects in oxide crystals* Keynote Talk 11: **Hannes Raebiger** *Control of magnetism in transition metal doped oxides*
10:40 – 10:50		*BREAK*
11:00 – 12:20	Session 10 Chairperson: **V. Amaral**	Keynote Talk 12: **Andrii Korostil** *Features of electrically induced spin torque effect in multilayer magnetic nanostructures* Oral 14: **K. Sharma** *A DFT+U study of point defects in spinel ferrites* Oral 15: **K. Tsysar** *Ab initio study of magnetic and optical properties of Co oxide nanowires on vicinal Pt surfaces*
12:30 – 14:00		*BREAK*
14:00 – 15:20	Session 11 Chairperson: **S. Zhou**	Keynote Talk 13: **Aleksandr Kislyuk** *Electrophysical properties, morphology and memristive behavior of completely charged domain walls in reduced bidomain lithium niobate* Oral 16: **A. Trukhanov** *Impact of the nanocarbon (CNT/CNF) on magnetic properties of the "polymer/hexaferrite" composites* Oral 17: **D. Mastrippolito** *Effects of oxidation and chlorine defects on ferromagnetic CrCl3 monolayer*
15:30		*BREAK*
15:40 – 16:20	Session 12 Chairperson: **A. Trukhanov**	Keynote Talk 14: **Nikolai Sobolev** *Energy harvesting and magnetic field sensing with bidomain LiNbO3-based composites*
16:30 – 16:40		**Closing Session**

Keynote Speakers

Elvira Fortunato

Universidade NOVA de Lisboa,
Portugal

A new era of semiconductors: metal oxides

Electric transport characteristics of $Sr_2FeMoO_{6-\delta}$ ceramics with structurally inhomogeneous surfaces

Mikalai Kalanda

SSPA Scientific and Practical Materials Research Centre of the NAS of Belarus,
Belarus

Dmitry Karpinsky

National Research University of Electronic Technology “MIET”,
Russia

Phase transitions in magnetoelectric $BiMnO_3$-based ceramics

Electrophysical properties, morphology and memristive behavior of completely charged domain walls in reduced bidomain lithium niobate

Aleksandr Kislyuk

National University of Science and Technology “MISiS”,
Russia

Andrii Korostil

Institute of Magnetism of the NAS of Ukraine and the MES of Ukraine,
Ukraine

Features of electrically induced spin torque effect in multilayer magnetic nanostructures

First principles calculations of the electronic and magnetic properties for defects in oxide crystals

Eugene Kotomin

Latvijas Universitāte,
Latvia

Peter K. Petrov

Imperial College London,
United Kingdom

Transition metal nitride and oxide thin films: growth and properties

Control of magnetism in transition metal doped oxides

Hannes Raebiger

Yokohama National University, Japan

Vladimir Ya. Shur

Ural Federal University, Russia

Micro- and nano-domain engineering of ferroelectrics crystals

Resistivity and tunnel magnetoresistance in double perovskite strontium ferromolybdate ceramics

Gunnar Suchaneck

Technische Universität Dresden, Germany

Herman Terryn

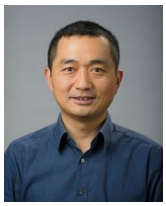
Vrije Universiteit Brussel, Belgium

New experimental and modelling approaches to understand electrodeposition of metals

Tailoring oxide thin films by ion beam

Shengqiang Zhou

Helmholtz-Zentrum Dresden-Rossendorf, Germany



Nerija Žurauskienė

Centre for Physical Sciences and Technology, Lithuania

Engineering of lanthanum perovskite thin films for magnetic sensors applications

Energy harvesting and magnetic field sensing with bidomain $LiNbO_3$-based composites

Nikolai Sobolev

Universidade de Aveiro, Portugal

Presentation Guidelines

In order to ensure a successful and trouble free presentation, kindly follow the instructions given below

Workshop Time Zone

Western European Time - WET. Please consider the Lisbon time zone: UTC/GMT (+0h).

Language

The Workshop's official language is English.

Duration of Presentations

Each speaker must ensure that their presentation, including the period for questions and answers that follows the presentation, takes no longer than the time stipulated in the Scientific Programme:

- **Keynotes**: 40 minutes, followed by 10 minutes for Q&A;
- **Orals**: 15 minutes, followed by 5 minutes for Q&A;
- **Posters**: pitch of 5 minutes, followed by 2 minutes for Q&A.

Workshop Programme

The Workshop will be broadcasted using the *Zoom* meetings platform. The event's live stream will be carried out in accordance with the Workshop's final Programme and speakers must join their respective session at least 15 minutes before it starts. Speakers were free to pre-record their respective presentation and send the video to the Workshop's Secretariat until 17 November 2021. For those who sent it and do not wish to make a live presentation, or in case there are difficulties related to poor internet connections or different time zones, the pre-recorded video will be played during the live stream on the presentation's established schedule and the speaker can follow it. Once the presentation ends, the speaker must be online and available for the Q&A.

Public Display and Privacy Procedures: Presentations, Posters and Videos

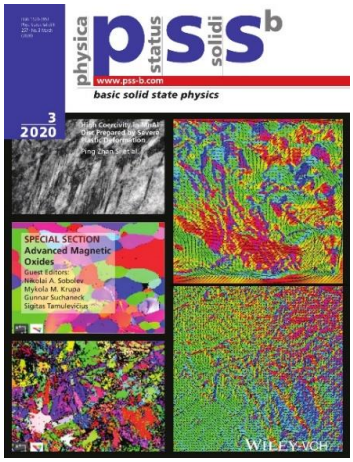
Authors/presenters are encouraged to share with the general public their presentation slides and their poster, after the Workshop is over. To do so, please send a PowerPoint or PDF file (max. size: **20 Mb**) with the slides/poster (and additional presentation material, if relevant) to iwamo2021@ua.pt. The files will be made available on the Workshop's webpage. **Pre-recorded presentation videos sent to the Workshop's Secretariat and broadcasted during the event will not be provided to anyone else outside the organising team and the files will be deleted once the Workshop ends. *IWAMO 2021* will not be recorded.**

pss (b) Call for Papers

Invitation to Authors that present their work at **IWAMO 2021**:

Special Issue / Topical Section in *physica status solidi (b)* - **Advanced Magnetic Oxides**

Submission Deadline: 15 January 2022



Guest Editors: Nikolai A. Sobolev, Mykola M. Krupa,
Gunnar Suchaneck, Sigitas Tamulevičius

Submission at: www.editorialmanager.com/pssb-journal

Special category: **Advanced Magnetic Oxides (IWAMO 2021)**

Dear Speaker,

Related to the forthcoming *IWAMO 2021* event in Aveiro, it is planned to publish once again a special issue/topical section in 'pss (b) – basic solid state physics'. In collaboration with the Guest Editors and the pss Editorial Office, we cordially invite you to submit a **Review Article** (topical review) or a **Research Article** based on, or related to, your presentation.

In 2021 'physica status solidi (pss)' has reached its 60th year of publishing high-quality materials physics and condensed-matter research! Over the last six decades we have seen fantastic progress in many areas of physical and materials science, and pss has been honoured to witness these advances, publishing, distributing and archiving countless important papers.

The publication will be a regular special issue, not a conference proceedings. Articles must fulfil the typical standards and requirements of the journal. Submitted manuscripts will undergo editorial evaluation and, if considered appropriate, subsequent **peer review**. According to the editorial policy of pss, two positive recommendations by independent referees are a prerequisite of acceptance. Published in Wiley Online Library **Accepted Articles** and **Early View** shortly after acceptance, your article is **citable with DOI** or article number immediately; hence there is **no waiting for the remainder of the contributions**. When all articles are complete, they will be assigned to the monthly issue of pss (b).

Please refer to the author instructions available on our homepage http://www.pss-b.com (including optional Word template and LaTeX style files and the link to online submission to pss (b) through Editorial Manager). Please **mention the conference** in your cover letter and select the appropriate section/category Advanced Magnetic Oxides (IWAMO 2021) during online submission to expedite handling).

We look forward to receiving your contributions!

Nikolai A. Sobolev, Mykola M. Krupa, Gunnar Suchaneck and Sigitas Tamulevičius (Guest Editors), Marc Zastrow (pss Editor) and Stefan Hildebrandt (pss Editor-in-Chief)

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Information on submissions

Research Articles expose original and previously unpublished work of general interest to the community. Manuscripts do not have a strict length limit (typical lengths vary from 6 to 10 journal pages). Articles must fulfil the standards and requirements of the journal. Main criteria for consideration by pss (b) are:

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Reviews should provide an overview of a current topic in the format of a topical review of about 10-12 (max. 15) journal pages. Due to this length restriction, a complete bibliographic overview on the existing literature cannot be expected but referencing should be well-balanced. The manuscript should represent a snapshot of most recent progress, the state of research and particularly relevant aspects, with focus on the highlights and possibly open or controversially discussed questions. They are intended to inform an audience not immediately familiar with the specific topic. Original, previously unpublished results may also be included to a certain extent.

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IWAMO
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Abstracts

Wednesday, 24 November 2021

SESSION 01

Chairperson: **Nikolai Sobolev**

- Keynote Talk -

SESSION 02

Chairperson: **Vladimir Ya. Shur**

- Keynote Talk -

SESSION 03

Chairperson: **Mindaugas Andrulevicius**

- Keynote Talk -

SESSION 05

Chairperson: **Olivier Toulemonde**

SESSION P01

Chairperson: **Luis Rino**

A new era of semiconductors: metal oxides

Elvira Fortunato *, Emanuel Carlos, Rita Branquinho, Pedro Barquinha and Rodrigo Martins

CENIMAT/i3N, Department of Materials Science, NOVA School of Science and Technology (FCT-NOVA) and CEMOP/UNINOVA, NOVA University Lisbon, Campus de Caparica, 2829-516 Caparica, Portugal
** emf@fct.unl.pt*

Oxide electronic materials is one of the most promising technologies for electronic devices, as distinct from the traditional silicon technology. The fact that circuits based on conventional semiconductors such as silicon and conductors such as copper can be made transparent by using different materials, the so-called transparent semiconducting and conducting oxides (TSOs and TCOs, respectively), is of great importance and allows for the definition of innovative fields of application with high added value.

Oxide electronic materials are becoming increasingly important in a wide range of applications including transparent electronics, optoelectronics, magnetoelectronics, photonics, spintronics, thermoelectrics, piezoelectrics, power harvesting, hydrogen storage and environmental waste management. Synthesis and fabrication of these materials, as well as processing into particular device structures to suit a specific application is still a challenge. Further, characterization of these materials to understand the tunability of their properties and the novel properties that evolve due to their nanostructured nature is another facet of the challenge.

In this presentation we will present the most important landmarks achieved by these stimulating scientific area as well as some insights to emerging applications.

Spectroscopic investigations on Cr doped zinc gallogermanate persistent phosphor

Batista M [1*], Rodrigues J[1], Relvas M S[1], Zanoni J[1], Girão A V[2], Rino L[1], Sobolev N[1], Costa F M[1], Pereira S O[1*], Monteiro T[1*]

[1] *i3N, Departamento de Física, Universidade de Aveiro, 3810-193 Portugal*
[2] *CICECO, Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*

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Persistent luminescence materials can store energy from light irradiation and release it after for a certain afterglow time (from seconds to minutes, hours and days) upon the removal of the excitation light. Nowadays, these materials are of particular importance for anti-counterfeiting, optical information, night vision surveillance, photocatalysis and optical probes in bioimaging, among other applications.

With bandgap energies of 4.4-5.0 eV, zinc gallate (ZGO) and zinc gallogermanate (ZGGO) are suitable hosts for the incorporation of a wide range of electronic levels of emitting centres, such as the trivalent chromium ions levels leading to the $^2E \rightarrow {}^4A_2$ red/NIR emission [1]. Additionally, the observation of persistent luminescence due to Cr^{3+} requires the presence of traps that store the excitation energy and release it to the ion levels, which is discussed in this work.

The purpose of this study is to investigate the optical properties of sintered ZGGO:Cr ($Zn_{1+x}Ga_{2-2x}Ge_xO_4$:Cr with x=0.1) using temperature, time and excitation energy dependence of the photoluminescence (PL). Indeed, persistent PL was observed for about 8 h after ceasing the excitation light.

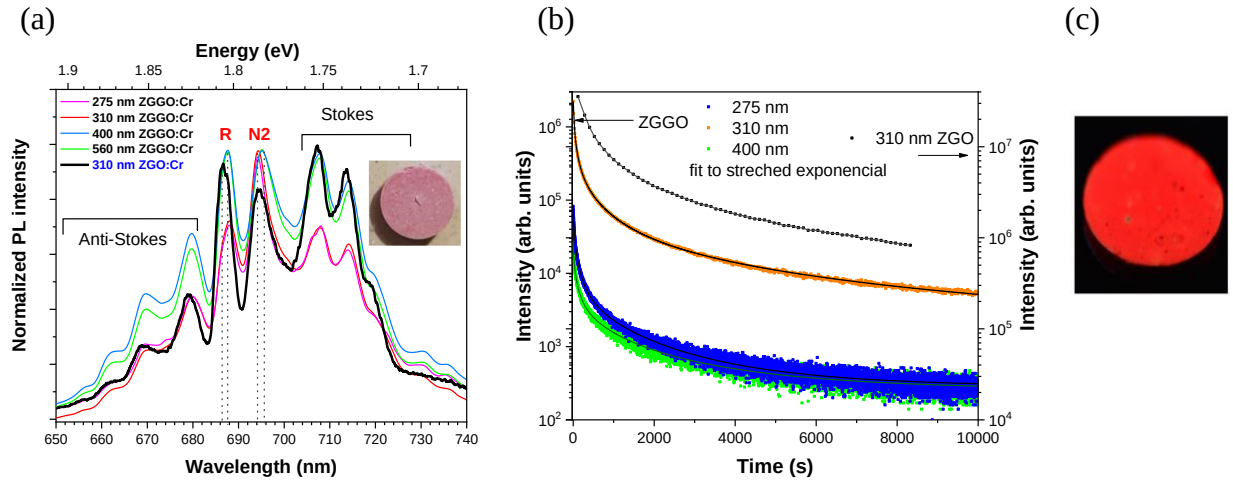

Figure 1. (a) RT PL spectra of ZGGO:Cr (inset: visual appearance of the sintered pellet); (b) selective excited afterglow time of ZGO:Cr and ZGGO:Cr; and (c) persistent luminescence of ZGGO:Cr pellets.

[1] M. S. Relvas, M. R. N. Soares, S. O. Pereira, A. V. Girão, F.M. Costa, T. Monteiro, Trends in Cr^{3+} red emissions from $ZnGa_2O_4$ nanostructures produced by pulsed laser ablation in a liquid medium, J. Phys. Chem. Solids, 129 413 (2019).

Resistivity and tunnel magnetoresistance in double perovskite strontium ferromolybdate ceramics

Suchaneck G [1]*, Artiukh E [2], Gerlach G [1]

[1] *TU Dresden, Solid State Electronics Laboratory, 01062 Dresden, Germany*
[2] *SSPA "Scientific-Practical Materials Research Centre of NAS of Belarus", 220072 Minsk, Belarus*
** Corresponding author: gunnar.suchaneck@tu-dresden.de*

$Sr_2FeMoO_{6-\delta}$ (SFMO) double perovskite is a promising candidate for room-temperature spintronic applications since it possesses a half-metallic character (with theoretically 100% spin polarization), a high Curie temperature of about 415 K, and a low-field magnetoresistance (LFMR) [1]. However, due to different synthesis conditions of ceramics as well as thin films, different mechanisms of electrical conductivity and magnetoresistance prevail.

The intrinsic resistivity of SFMO obeys a temperature dependence $\rho_0 = \rho_D + AT^{\nu}$, where ρ_D is the inverse of the Drude conductivity, A a constant defined by the mean free path of spin waves in SFMO [2], and $\nu \approx 2.5$. Ceramic grain boundary oxidation leads to the appearance of spin-polarized tunneling via an oxide barrier. Increasing the barrier width beyond the limit of thin tunneling barriers, inelastic hopping occurs via localized states within the barrier. Here, second and third order hopping conductances are characterized by $T^{4/3}$ and $T^{5/2}$ conductivity terms, respectively. With further increase of the barrier width, the metallic-like conductivity disappears totally accompanied by an increase of the resistivity by about six orders of magnitude. The samples now exhibit a negative temperature coefficient of resistivity in the whole temperature region. Its resistivity behavior can be described in terms of the fluctuation-induced tunneling model, which converts near room temperature to a variable-range hopping conductivity mechanism [4]. Here, the electron transport occurs through a thick barrier via more conductive chains of localized states in series with nanosized tunnel barriers between the grains. In the bulk limit and at high temperatures, inelastic hopping changes to variable range hopping [3] as obtained experimentally [4].

The magnetic flux dependence of the tunneling barrier height was modeled by a series expansion, with empirical coefficients determined up to the second order.

The different mechanisms of magnetoresistance in SFMO are: (i) tunneling resistance across intergrain barriers in granular ceramics [6], (ii) tunnel resistance across intergrain nanocontacts in cold pressed and intermediate temperature annealed, granular ceramics [5], and (iii) intragrain tunneling across antiphase boundaries [7]. The magnetoresistance due to inelastic tunneling is not suitable for application.

We discuss consequences for a controlled SFMO ceramic fabrication and thin film deposition for the purpose of designing spintronic devices with advantageous magnetic properties, in particular, magnetic field sensors and magnetoresistive random access memories.

References:
[1] G. Suchaneck, N. Kalanda, E. Artiukh, and G. Gerlach, Phys. Status Solidi B 257 (2019) 1900312.
[2] F. J. Dyson, Phys. Rev. 102 (1956) 1217-1230.
[3] Y. Xu, D. Ephron, and M. R. Beasley, Phys. Rev. B 52 (1995) 2843-2859.
[4] G. Suchaneck, N. Kalanda, E. Artsiukh, M. Yarmolich and N. A. Sobolev, J. Alloys Comp. 860 (2020) 158526.
[5] G. Suchaneck, E. Artiukh, Phys. Status Solidi B 258 (2021) 2000629.
[6] G. Suchaneck, E. Artiukh, Open Ceram 7 (2021) 100171.
[7] G. Suchaneck, E. Artiukh, Phys. Status Solidi B (2021) (in print).

From magnetic cluster glass state to giant vertical magnetization shift induced by ferromagnetic cluster growth in $SrFe_{0.25}Co_{0.75}O_{2.63}$

Madhu Chennabasappa [1, 2], Alain Pautrat [3], Olivier Toulemonde [1, *]

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[2] *Department of Physics, Siddaganga Institute of Technology, BH Road, Tumakur – 572103, India*
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Transition metal oxides with ABO_3 and A_2BO_4 are known as perovskite-type and K_2NiF_4 type structures respectively. Their ability to undergo reversible oxydo-reductions chemical reaction are technologically very attractive as electrodes in fuel cells (SOFC), as oxygen storage materials in anaerobic processes and as three way catalysts (TWC's). That is why, it is the control of oxygen released and/or up taken that opens ways towards huge change of their physical properties such as metal / insulator transition and/or antiferromagnetic to ferromagnetic transition.
When a single transition metal is introduced on the B crystallographic site, its oxidation state is indeed in direct relationship with the oxygen content. However, when two transition metal cations are introduced on the B crystallographic site, our recent results highlight that their relative oxidation states are closely related to a metal to metal charge transfer giving unexpected oxidation states distribution. Especially, in $SrFe_{1-x}Co_xO_{3-\delta}$ materials, we highlight that the distribution of cobalt and iron oxidation states is heterogeneous [1], indicating that oxidation of cobalt cation requires higher oxidation potential than for the iron ones. Recently, the correlation in between the exhibited paramagnetic to ferromagnetic transition around room temperature and oxidation state distributions has been done [2]. It allow us to better analyse the giant exchange bias like properties exhibited by the $SrFe_{0.25}Co_{0.75}O_{2.63}$ material [3] as seen in the proposed figure.

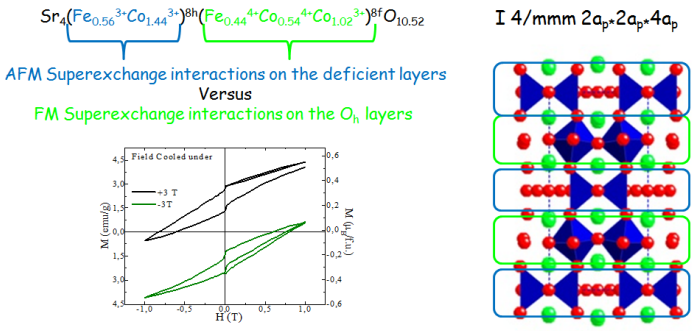

Figure 1 Super-exchange competition shown in the natural layered material resulting giant vertical magnetization shift at 15K

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Is There Any Dynamic Magnetic Dimer In Sr_2CrNbO_6 Ordered Double Perovskite?

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Competing magnetic interactions in materials had always given rise to fascinating phenomena in the field of condensed matter.[1] Geometric magnetic frustration induced by the edge shared tetrahedra had been the reason behind the observance of exotic magnetic properties like spin liquid, spin ice, spin glass, valence bond solid, valence bond glass etc. in double perovskites.[2,3]

The main objective of our study on ordered double perovskite Sr_2CrNbO_6 is to investigate if these systems behave like a valence bond glass (VBG). Room temperature powder X-ray diffraction (PXRD) pattern showed that Sr_2CrNbO_6 crystallizes in the cubic space group, $Fm\bar{3}m$ with cell parameter, a = 7.8(1) Å with 44% ordering of Cr^{3+}/Nb^{5+}. This poor degree of ordering likely results from a metal-metal charge transfer observed from UV-vis-NIR spectroscopy. Temperature dependent Neutron Diffraction measurement showed no magnetic peak in Sr_2CrNbO_6 at 1.8K and a quadratic distortion of the octahedra increase with charges localization with temperature decrease. The magnetization measurements in zero field cooled/field cooled (ZFC/FCC) mode under 1T have been carried out. It shows two different regions at high and intermediate temperature suggesting a valence bond glass behavior in the intermediate temperature range along with a spin glass transition at low temperature.

In this presentation, complementary temperature Electron Paramagnetic Resonance and specific heat will be presented aiming to characterize this exotic intermediate state prior to spin glass in Sr_2CrNbO_6.

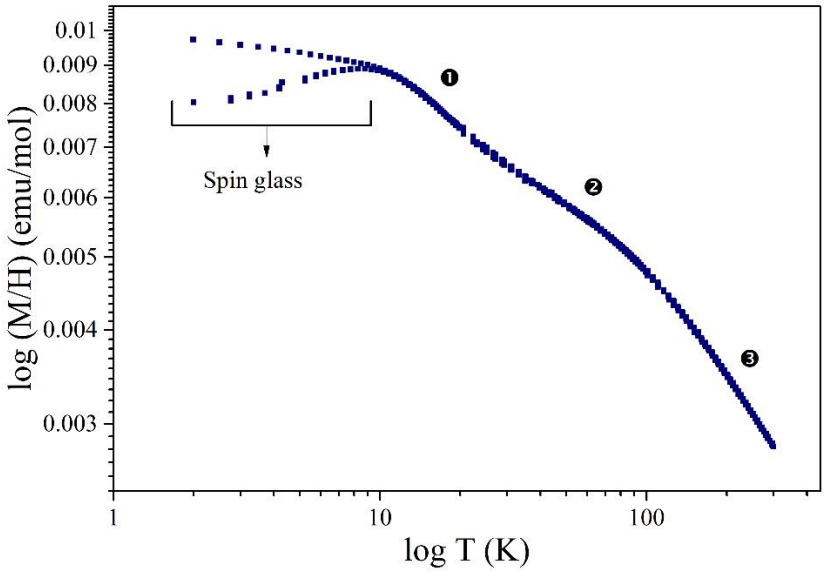

Figure 1: M/H vs T (logarithmic scale) plot of Sr_2CrNbO_6 double perovskite.

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ELECTRIC TRANSPORT CHARACTERISTICS OF $Sr_2FeMoO_{6-\delta}$ CERAMICS WITH STRUCTURALLY INHOMOGENEOUS SURFACES

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One of the most important properties for applications of half-metals $Sr_2FeMoO_{6-\delta}$ with a double perovskite structure as spintronic devices is the electric charge transport there. In this way, an important task is to study the features of the mechanisms of electric transport in such structures. To investigate these properties, two series of samples of strontium ferromolybdate powder obtained by the citrate-gel method and pressed at a pressure of 4 GPa and T = 800 K were prepared: an unannealed series (SFMO – I) annealed at T = 700 K and $p(O_2)$ = 10 Pa for t = 3 h (SFMO – II) (Fig. 1).

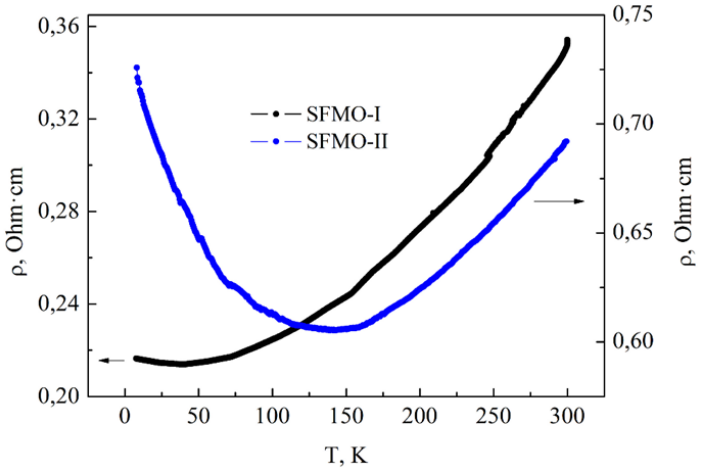

Figure 1: Temperature dependence of the resistivity for the SFMO–I and SFMO–II samples

The temperature dependence of the SFMO-I resistivity exhibits metallic behavior at temperatures above 36 K and a slight increase in the resistivity at T ≤ 36 K. The SFMO-II sample at T = 300 K has a higher electrical resistivity ρ = 0.692 Ohm·cm, which decreases with a decreasing temperature to 133 K with its subsequent increase to 4.2 K (Fig. 1). Despite the fact that the sample exhibits a change in the sign of dρ/dT from positive to negative, it can be assumed that there is a metallic type of conductivity in SFMO – II near the metal – insulator transition. The expression for the electrical resistivity in the temperature range 4.2-300K was written in the form: $\rho(T) = \frac{1}{\sigma_0 + A_w T^{k/2}} + A_p T^n$. When approximated by this function, good agreement was found between the experimental data and the theoretically calculated values.

Resistivity is determined by various mechanisms of electric charge scattering on structural inhomogeneities located both in the bulk of the grain and on its surface. The reason for this is the inhomogeneity of the electron density distribution due to the presence of different valence Mo/Fe cations, anti-structural defects, etc. In this case, charge transfer occurs under conditions of the presence of various kinds of structural disorder. This indicates the need to take into account the processes of weak localization caused by the quantum interference of conduction electrons. In the disordered magnet $Sr_2FeMoO_{6-\delta}$ in the low-temperature region, the probability of electron-electron interaction increases due to diffusion rather than ballistic motion of electrons with multiple elastic scattering by structural inhomogeneities.

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The monovalent Ag-substituted $La_{0.67}Ca_{0.33}MnO_3$ manganites: The prediction of magnetocaloric effect by means of various models

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In this work, we address various effective field theories to predict magnetocaloric effect in monovalent Ag-substituted $La_{0.67}Ca_{0.33-x}Ag_xMnO_3$ (x=0.05) perovskite manganite. The sample is prepared by solid state reaction method. The room temperature powder X-ray diffraction patterns were subjected to Rietveld refinement, result confirms that our compound is mixed phase containing orthorhombic and rhombohedral perovskite symmetry. The sample undergoes a second order magnetic phase transition from ferromagnetic (FM)-paramagnetic (PM) at Curie temperature, T_C ~ 275K. The isothermal magnetization data M (H, T) taken across this transition is used to estimate magnetic entropy change. The maximum magnetic entropy change (ΔS_M) determined from Maxwell-thermodynamic equation (MI) is 7.91 J/kg K under the field change of 5 T. The obtained result was compared to ones calculated based on phenomenological model (PM), Landau theory of phase transitions (LT) and Arrott-Noakes equation of state (ANEOS) and good concordance is observed. Moreover, a phenomenological construction of master curve based on Scaling relation, intrinsic to second order phase transition is used in order to estimate magnetocaloric properties. This opens up the predictions, as it allows extrapolations to any magnetic fields or temperature ranges.

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The Structure, Magnetic and Magnetotransport Properties of Layered Cobaltites $Sr_{1-x}Y_xCoO_{3-\delta}$

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The structure and the magnetic and magnetotransport properties of the perovskite $Sr_{0.9}Y_{0.1}CoO_{2.63}$ have been studied using different diffraction methods and magnetization and conductivity measurements. Synchrotron X-ray diffraction shows that the sample is structurally two-phase. The majority phase has a tetragonally distorted unit cell and is described by the space group *I4/mmm*. The large broadening of the diffraction peaks with *hkl* indices corresponding to a doubling of the unit cell parameter *c* indicates that there is no strict translational symmetry along the *c* axis. A very strongly broadened superstructure peak observed at small angles in X-ray diffraction patterns at temperatures below 400 K are explained by the existence of a monoclinic phase with large unit cell whose phase fraction is much smaller than that of the tetragonal phase, but which is dominant in $Sr_{0.8}Y_{0.2}CoO_{2.65}$.

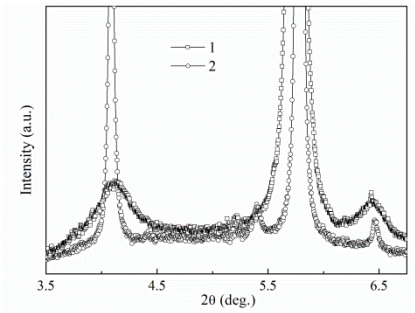

Figure 1: X-ray powder diffraction patterns for samples $Sr_{0.9}Y_{0.1}CoO_{2.63}$ (space group *I4/mmm+ A2/m*) (1) and $Sr_{0.8}Y_{0.2}CoO_{2.65}$ (*A2/m)* (2) at 100 K over the range of angles 3.5-6.5

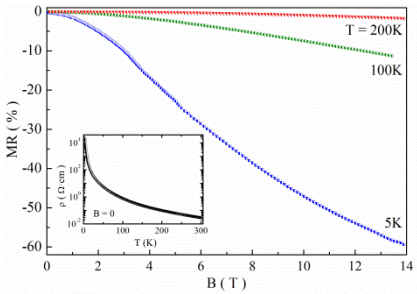

Figure 2: Dependence of the magnetoresistance for composition $Sr_{0.9}Y_{0.1}CoO_{2.63}$ at 5K, 100K and 200K (the inset shows temperature dependence of electrical conductivity without an applied field)

The spontaneous magnetization strongly increases with increasing the Y content up to 20% due to formation of the monoclinic phase. The magnetic structure is predominantly an antiferromagnetic G-type. Magnetic moments are 1.5 μ_B for $Sr_{0.9}Y_{0.1}CoO_{2.63}$ and 1.7 μ_B for $Sr_{0.8}Y_{0.2}CoO_{2.65}$ in the layers of CoO_6 octahedra and 2 μ_B for $Sr_{0.9}Y_{0.1}CoO_{2.63}$ and 2.7 μ_B for $Sr_{0.8}Y_{0.2}CoO_{2.65}$ in the anion-deficient $CoO_{4+\gamma}$ layers. The electrical conductivity of $Sr_{0.9}Y_{0.1}CoO_{2.63}$ has a semiconductor character. The magnetoresistance reaches 58% in a field of 14 T at 5 K and decreases strongly with increasing temperature and Y content (Fig.2).

Tailoring oxide thin films by ion beam

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Complex oxides host a multitude of novel phenomena in condensed matter physics, such as various forms of multiferroicity, colossal magnetoresistance, quantum magnetism and superconductivity. Defect engineering via ion irradiation can be a useful knob to control these physical properties for future practical applications. Two prominent effects are disorder and uniaxial strain. Particularly, the uniaxial strain, manifesting as the elongation of the out-of-plane lattice spacing, is not limited to available substrates, the conventional and well-known strain engineering approach. In this talk, I will introduce the basics of ion irradiation and its applications to oxide thin films, including the modification of magnetic properties of $NiCo_2O_4$ [1], $SrRuO_3$ [2], the magneto-transport properties of rare-earth nickelates [3] and $SrRuO_3$ [4] and the structural properties of $BiFeO_3$ [5]. It is worth to note that ion beam technology has been well developed for microelectronics. Once the principle of concept is approved, the approach can be easily scaled up and integrated to the industry production line.

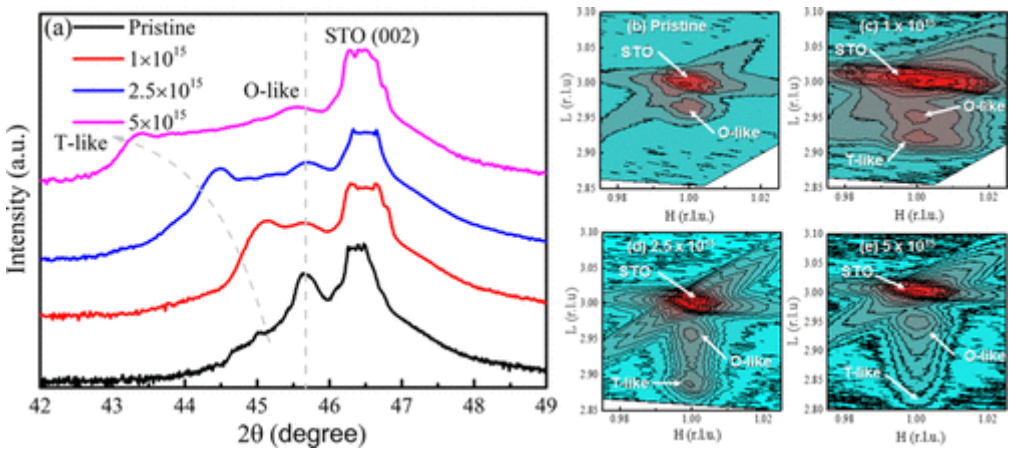

Figure 1. Ion irradiation induced lattice expansion in SrRuO3 films along the out-of-plane direction: (a) θ–2θ scans around the (002) reflection of SRO thin films on STO substrates under different He fluences. (b–e) Corresponding RSMs around the (103) reflections of SRO films.

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XPS Analysis of Mo and Sr Oxides Thin Films

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Strontium molybdate ($SrMoO_4$) demonstrating good chemical and thermal stability is widely used in many areas including magnetic applications [1, 2]. Here we present a surface analysis of thin strontium molybdate films produced by reactive magnetron sputtering of Mo and Sr targets applying the X-ray Photoelectron Spectroscopy (XPS) method. KRATOS XSAM800 spectrometer with nonmonochromatic Al Kα radiation (hν = 1486.6 eV) as an excitation source was used for spectra acquisition. The 20 eV pass energy value of a hemispherical electron energy analyzer was used for survey and high-resolution spectra acquisition. For spectra deconvolution sum of Gaussian- Lorentz functions of 70:30 ratios were used. In Figure 1 both molybdenum and strontium spectra are compared for the samples representing higher (~26%, upper red line) and lower (~12%, bottom blue line) Mo atomic concentration in the film. While strontium spectra for these samples are similar, the molybdenum spectra showed additional peaks representing different Mo oxidation states for lower Mo atomic concentrations.

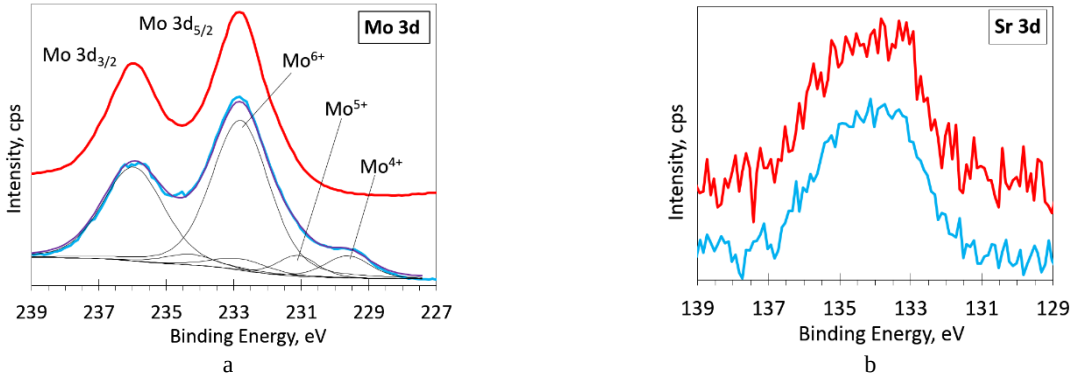

Figure 1 Comparison of Mo 3d and Sr 3d high-resolution XPS spectra for lower higher Mo atomic concentration: a – Mo 3d spectra, b – Sr 3d spectra. The thick red line corresponds to the sample with higher Mo atomic concentration, blue thick line - to lower Mo atomic concentration. Thin black lines – fitted peaks, thick violet line – fitted envelope.

Both Mo and Sr were found only in the oxidized state, no metallic peaks were detected. Molybdenum spectra (Figure 1, a) showed that the Mo 3d core level spectrum consists mainly of a Mo^{6+} peak at 232.7 eV [2, 3]. Low-intensity peaks (Figure 1, a, fitted peaks) at 229.6 eV and 231.1 eV most likely represent molybdenum oxides in Mo^{4+} and Mo^{5+}states, corresponding to reported values of binding energy for Mo^{4+} at 229.6 eV, and for Mo^{5+} at approximately 230.8 eV [2]. Strontium spectra (Figure 1, b) are very similar and show two overlapping peaks at 133.4 eV and 135.3 eV positions. Both peaks are in good agreement with known Sr $3d_{5/2}$ and Sr $3d_{3/2}$ positions for $SrMoO_4$ [3]. Oxygen spectra showed very similar spectra (not shown here) consisting of one peak at approximately 530.5 eV, representing oxygen bounded to molybdenum [3].

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Local Atomic Order and Magnetic Properties in $(FeCo)_x(SiO_2)_{100-x}$ Core-Shell Nanoparticles for Theranostics

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Magnetic nanoparticles (NPs) of $Fe_{25}Co_{75}$ alloy covered with porous SiO_2 shell offering the combination of unique properties (high magnetic moment, high drug-loading capacity, biocompatibility) can be applied for designing of new theranostics agents, that combine both diagnostic process and therapy. Core-shell $(Fe_{25}Co_{75})_x(SiO_2)_{100-x}$ ($90 \le x \le 10$, wt. %) NPs powders are sintered in two stages, first, by preparation of FeCo cores by chemical deposition from aqua solutions with consequent deposition of SiO_2 shell onto FeCo cores by TEOS hydrolysis. Local atomic order in NPs is studied by ^{57}Fe Mossbauer spectrometer system (See Co) with closed-cycle refrigerator (Janis) in transmission geometry at T = 16 K and 300 K using ^{57}Co/Rh source of 30 mCi. Temperature $M(T)$ and magnetic field $M(H)$ dependencies of magnetization are recorded by vibrating sample magnetometry at T between 5-300 K and magnetic fields H up to 9 T. Fitting of Mossbauer spectra (Fig. 1a) reveals that initial FeCo NPs contain 30 % contribution of nonmagnetic Fe(Co)O phase assigned to surface oxidation of NPs and 70 % of magnetically-ordered agglomerations of pure FeCo alloy NPs. Formation of SiO_2 shells draw to the 4 times decrease of non-magnetic surface oxides contribution evidencing suppression of undesirable oxidation of FeCo cores (Fig. 1b). $M(H)$ and $M(T)$ curves (Fig. 1c) recorded under field-cooled (FC) and zero-field-cooled (ZFC) protocols for pure FeCo cores and $(FeCo)_x(SiO_2)_{100-x}$ core-shell NPs with ZFC maximums within 150 K and high irreversibility temperature (around 300 K) between ZFC and FC curves are typical for superferromagnetic long-range ordering [2]. Annealing of $(FeCo)_x(SiO_2)_{100-x}$ NPs at 723 K during 4 h results in total decomposition of undesirable Fe(Co) surface oxides and crystallization of NPs which draw to the enhancement of magnetization up to 120 emu/g (at 5 K).

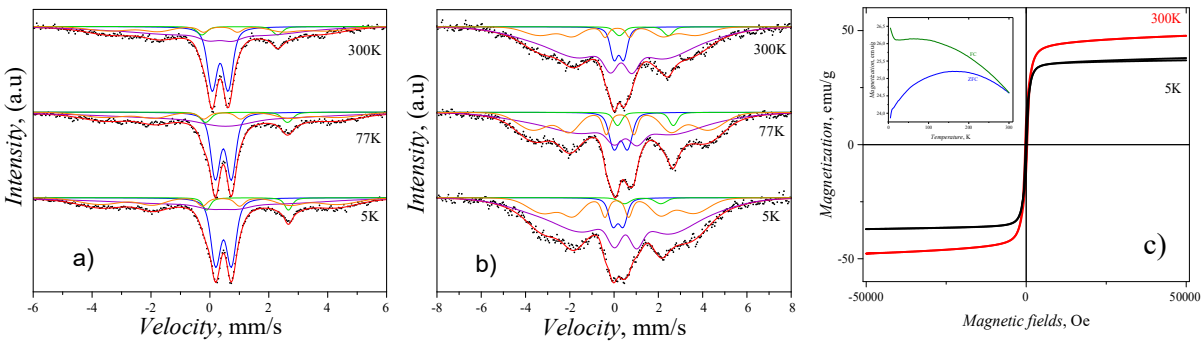

Figure 1 Typical Mossbauer spectra of FeCo cores (a) and FeCo-SiO_2 NPs (b); $M(H)$ curves of FeCo-SiO_2 NPs (c) with the inset showing FC-ZFC $M(T)$ curves.

Therefore, obtained Ns with core-shell structure could be further functionalized by anticancer cisplatin (or doxorubicin substances) to be used as potential nanodevice for effective application in the combined drug delivery and nanochemo-hyperthermia therapy. The experiments on drug loading and hyperthermia are in progress now.

Financial support of BRFFR-VANT project F21V-008 is gratefully acknowledged.

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Magneto-optics of Hydrogenated ZnO, ZnO:Co, and ZnO:(Co+Al) Films

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The origin of ferromagnetism (FM) in diluted magnetic oxides based on ZnO is still under debate, since it critically depends not only on the nature of the doping elements but also on the conditions of the sample synthesis and the post-synthesis treatment. Theoretical and experimental studies (for examples [1, 2]) have led to the conclusions that hydrogenation of the doped ZnO films uniquely induces/enhances FM behavior in the samples. Besides, the unusually large signal of the magnetic circular dichroism (MCD) was observed for the hydrogenated ZnO:Co films [3]. In this work, the spectral and field dependencies of MCD for the hydrogenated films of ZnO, ZnO:Co, and ZnO:(Co+Al) have been studied at room temperature. These films were grown on a glass substrate by the standard RF magnetron sputtering system in mixed atmosphere of Ar+20-50% H_2. The two inches ZnO, $Zn_{0.95}Co_{0.05}$, and $Zn_{0.93}Co_{0.05}Al_{0.02}O$ target were used. The ZnO:(Co+Al) films are first obtained in these conditions. High hydrogen concentration was used together with high enough substrate temperature of 450 ^{0}C.

It was found that the shape of the MCD spectra for the ZnO films differs from those for the doped ZnO films. Herewith, the only ZnO:Co and ZnO:(Co+Al) films exhibit room temperature ferromagnetism. The strong effect of the used technological conditions leads to a large Co content in the samples [4]. The MCD spectra for the ZnO:Co and ZnO:(Co+Al) films were compared with those for the Co film and for Co nanoparticles (Figure 1). The complex nature of magnetism is assumed in the ZnO:Co and ZnO:(Co+Al) films. The spectral MCD features inherent only in the films with internal magnetism are discussed.

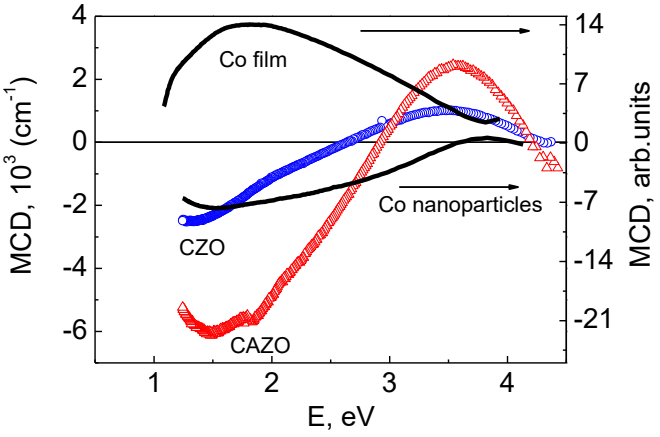

Figure 1 MCD spectra for the ZnO:Co – CZO and ZnO:(Co+Al) – CAZO films with a relative Co content of 25.5% in each sample. A ratio of the MCD signal magnitude to a thickness of the CZO and CAZO films is presented. MCD spectrum for the Co film with a thickness of 30 nm. MCD spectrum for a SiO_2 sample implanted by Co^+ with an ion current density of j = 1 μA and an ion dose of $1.25*10^{17}$ ions/cm^2. The measurements were carried out in a magnetic field of 13 kOe at a temperature of 300 K.

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Synthesis and Ion Doping of Gallium Oxide

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Currently, gallium oxide is considered one of the most effective wide bandgap semiconductors for the use in new-generation electronic devices [1]. Due to its wide bandgap, gallium oxide can be used to create high-temperature gas sensors, UV "solar-blind" detectors, power devices, thin-film electroluminescent displays, etc [1]. However, until now, no method has been found for the formation of Ga_2O_3-based materials with the well-controlled defect-impurity composition, which determines the main parameters, such as the type of conductivity and the concentration of charge carriers. One of the possible ways to overcome this problem is the use of non-equilibrium methods for the synthesis of Ga_2O_3-based nanostructures. Here we discuss the formation and modification of Ga_2O_3 layers by ion implantation [2] and magnetron deposition, which allow controlled introduction of defects and impurities of a given type and with a given concentration into the material. The initial samples were β-Ga_2O_3 magnetron films, as well as bulk gallium oxide samples doped with Fe of two orientations (-201) and (010). These samples were implanted by Si ions with energy and dose varying from 85 keV to 120 keV and from $3 \cdot 10^{14}$ to $5 \cdot 10^{15}$ cm^{-2}, respectively. Then, sequential post-implantation annealing was carried out at temperatures from 600 to 950 °C with systematic characterization of the changes in structure, optical and electrical properties of the irradiated Ga_2O_3 layers. Such methods as X-ray and electron diffraction, optical transmission and Raman spectroscopy were used for the characterization of ion-modified layers. Electrical properties were investigated by the Hall Effect measurements with In contacts at room temperature. It is shown for the magnetron-sputtered Ga_2O_3 films that the structure is amorphized at the selected doses of silicon ions with further recovery at annealing. For the bulk β-Ga_2O_3 samples, the difference in the effect of ion implantation on the structure and properties of samples with different orientations is demonstrated, and the possibility of ion doping of semi-insulating (Fe-doped) samples is shown.

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Thursday, 25 November 2021

SESSION 05

Chairperson: **Hannes Raebiger**

- Keynote Talk -

- Keynote Talk -

SESSION 06

Chairperson: **Gunnar Suchaneck**

- Keynote Talk -

SESSION 07

Chairperson: **Nerija Žurauskienė**

- Keynote Talk -

SESSION 08

Chairperson: **Eugene Kotomin**

SESSION P02

Chairperson: **Nuno M. Ferreira**

Engineering of Lanthanum Perovskite Thin Films for Magnetic Sensors Applications

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Increasing demand for magnetic field sensors with high sensitivity in a wide range of magnetic fields and operating temperatures has resulted in numerous investigations of physical phenomena in advanced materials and fabrication techniques of novel magnetoresistive devices. The commercially available magnetoresistive (MR) sensors are based on so-called xMR effects (anisotropic AMR, giant GMR, and tunneling TMR) [1]. Magnetoresistive magnetic sensors are becoming one of the most important components in information technologies, automotive and internet-of-things applications, medical and consumer electronics. Recently it was demonstrated that the colossal magnetoresistance (CMR) effect [2] also can be employed for the development of magnetic field sensors, which can measure high magnetic fields up to megagauss [3]. These sensors are based on nanostructured (polycrystalline with nanosized grains) lanthanum manganite films and are capable to measure the magnetic field magnitude, when field direction is not known in advance (CMR-B-scalar sensors) [4]. Such sensors were used to measure the magnetic field dynamics in railguns [5], non-destructive pulsed-field magnets [3], for monitoring of magnetic pulse welding quality [6], etc. Each application has specific requirements for the sensor fabrication, its specifications, magnetic field and temperature ranges of operation, and sensor accuracy. Therefore, the possibility to tailor magnetoresistive properties of advanced magnetic oxides and their nanostructures for the development of magnetoresistive sensors with increased field and temperature ranges of operation is of great importance.

In this study, the main physical properties of nanostructured lanthanum manganite-cobaltite films grown by pulsed injection MOCVD technique, and examples of their applications for the development of magnetic sensors will be presented. It will be demonstrated that CMR behaviour in such films significantly depends on the chemical composition, structure, and morphology of the films, especially on the properties of nanometer size crystalline grains and intergrain boundary material. The obtained magnetoresistance values, magnetoresistance anisotropy, and relaxation processes will be analyzed to have possibilities to tune the main properties of nanostructured films for the development of magnetic field sensors operating in a wide magnetic field range at the room as well as cryogenic temperatures. Finally, the hybrid manganite-graphene magnetic field sensor which operation is based on negative CMR effect in manganite and Lorentz force induced positive magnetoresistance effect in graphene will be presented. Such hybrid sensor exhibits higher sensitivity to the magnetic field in comparison to individual manganite or graphene sensors.

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Transition Metal Nitride and Oxide Thin Films: Growth and Properties

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Plasmonic materials have a wide range of applications, from energy storage and harvesting to bio-sensing and memory storage devices [1–3]. However, the archetypal plasmonic materials gold and silver are limited in their applicability, displaying poor thermal stability, limited spectral tunability, and incompatibility with standard CMOS fabrication processes.

Consequently, refractory plasmonic materials are capable of with-standing high operating temperatures and can include refractory metal elements (e.g. W, Mo, Ti) in addition to transition metal oxides and nitrides (e.g $SrMoO_3$, $SrNbO_3$, $SrRuO_3$, TiN, NbN).[4] Transition metal oxides (TMOs) and transition metal nitrides (TMNs) are of particular interest as they are capable of delivering tailorable optical properties via deposition-controlled variations in film stoichiometry, morphology and strain.[5] Of the TMNs investigated, titanium nitride (TiN) has been the subject of recent research as its optical constants are comparable to gold and it also displays high temperature stability and a tuneable plasma frequency.[6] However, other binary and ternary TMNs including NbN, TaN, ZrN and TiZrN also hold promise for use within plasmonic applications at varying wave-lengths and operating conditions. [7]

In this paper, the mechanism of formation of transition metal nitride and oxide thin films and their optical properties with tunable epsilon-near-zero (ENZ) behaviour will be discussed. We will present the technological conditions for deposition of thin films with unusual double ENZ frequencies and will show that they can be modified by changing the film deposition conditions. Thus allowing one to fabricate, control and engineer tunable plasmonic and metamaterial devices and surfaces, using CMOS compatible technology.

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Micro- and Nano-domain Engineering of Ferroelectrics Crystals

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The lithium niobate $LiNbO_3$ (LN), lithium tantalate $LiTaO_3$ (LT) and titanyl phosphate $KTiOPO_4$ (KTP) crystals with tailored periodically poled domain structure (PPLN, PPLT, PPKTP) created with nanoscale period reproducibility are used for second harmonic generation (SHG) and optical parametric oscillation (OPO) based on quasi-phase-matched (QPM) nonlinear optical wavelength conversion [1]. The study of the conductivity relaxation of charged domain walls allowed optimization of the poling process [2]. The domain-domain electrostatic interaction has been investigated [3].

Multiply pulse laser irradiation has been used for switching under the action of the pyroelectric field without application of the external field [4]. Formation of the quasi-regular submicron stripe domain structures has been realized in LT by laser beam scanning. Switching at the elevated temperatures opens the way to complicated fractal and dendrite domain shapes. The unique snowflake domains can be created by domain growth at the elevated temperatures in the plates with artificial dielectric layer [5]. The information obtained from the first *in situ* study of the domain kinetics with high temporal resolution allowed to obtain original important information about domain wall motion mechanism and to characterize KTP as the most appropriate crystal for sub-micron periodical poling [6]. The poling process at room and elevated temperatures has been studied by *in situ* optical observation [7].

The domain structure evolution has been studied in lithium-niobate-on-insulator (LNOI) wafers during local switching by the biased tip of the scanning probe microscope. The creation of the stable periodical domain structures with period down to 200 nm was demonstrated.

The obtained knowledge was applied for producing high-fidelity patterns: (1) PPLN:MgO for green and blue light SHG, (2) MgO doped stoichiometric LT for green and yellow light SHG with output power above 14 W for CW, (3) fan-out domain structures in 3 mm-thick MgO:LN for tunable OPO generation from 2,5 to 4,5 μm for 1053 nm pump.

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APPLICATION OF A MAGNETIC FIELD IN LASER FLOATING ZONE FOR PROCESSING THERMOELECTRIC CERAMICS

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The main objective of this work is to evaluate the prospects for processing oxide-based thermoelectric materials, using the Laser Floating Zone (LFZ) technique under an external magnetic field.
Two distinct known thermoelectric oxides, $Bi_2Sr_2Co_{1,8}O_y$ (BSCO) and $Ca_{0.9}Gd_{0.1}MnO_3$ (CGMO) were selected as model materials. During their laser growth, an external magnetic field was applied in the direction of growth (d), opposite to the growth (u) and without magnetic field (s), to study corresponding effects on their properties.
Structural and microstructural, as well as magnetic and thermoelectric analyses were carried out over a wide range of temperatures to assess the effects of the applied magnetic field. The results showed noticeable improvements in the thermoelectric performance. In BSCO samples, the power factor of samples subjected to processing in a magnetic field in the direction of growth, increased 25%, compared to samples without a field. In CGMO samples, the power factor of samples subjected to a magnetic field in the direction of growth decreased by 8.2%. The opposite behaviour was observed in the magnetic measurements (Fig. 1). Based on the results of this study, the application of an external magnetic field during the growth influences the electrical and magnetic properties of the system. It was found that for n-type and p-type semiconductor systems, the direction of the magnetic field during the growth show different behaviour, apparently related to the microstructural changes and evolution of the phase composition.

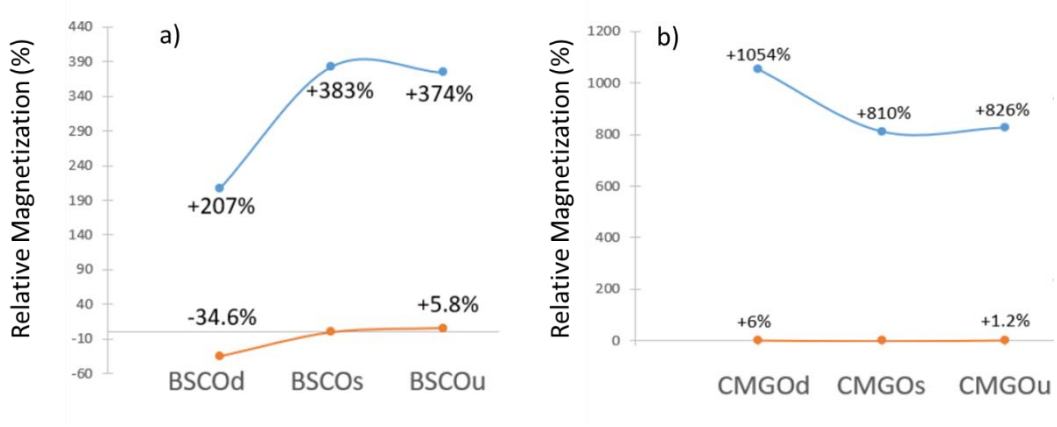

Figure 1 - Effect of external magnetic field on magnetization a) BSCO and b) CMGO systems grown by LFZ

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Spectroscopic studies on doped and proton irradiated β-Ga_2O_3

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Optically active defects in wide and ultrawide bandgap semiconductors pave the way for a myriad of technological applications as is the case of single-photon sources and optical bioprobes. With bandgap energy of ~4.9 eV at room temperature [1], the monoclinic β-Ga_2O_3 is one of the semiconductors capable of accommodating a vast number of defect electronic states within the gap. Under band-to-band excitation, nominally undoped samples typically exhibit broad unstructured bands in the ultraviolet (~370 nm/3.35 eV) and blue (~420 nm/2.95 eV) spectral regions, which have been assigned to the recombination of self-trapped excitons and/or vacancy related defects [1]. Alternatively, the incorporation of Cr^{3+} into the lattice gives rise to a red emission due to $^2E,^4T_2 \rightarrow {}^4A_2$ intraionic transitions [2]. These are responsible for the observation of narrow R-lines (~690 nm/1.8 eV) superimposed on a broad band with a maximum at ~730 nm/1.7 eV.

In this work, we investigate the optical properties of β-Ga_2O_3:Cr grown by a modified edge-defined film-fed method and co-doped with Si and Mg, using the temperature and excitation energy dependence of the photoluminescence (PL). Particle induced X-ray emission indicates that the concentration of Si and Cr are 6.72 and 0.01 at.%, respectively, for the Si co-doped sample, and the concentration of Mg and Cr are 0.29 and 0.03 at.%, respectively, for the Mg co-doped sample. PL excitation was also performed to assess the excitation bands of the optically active defects. Additionally, the Si co-doped sample was irradiated with $1.0x10^{15}$ protons/cm^2 with an energy of 2 MeV. The influence of the dopants, irradiation and annealing on the observed optical centres is evaluated and discussed.

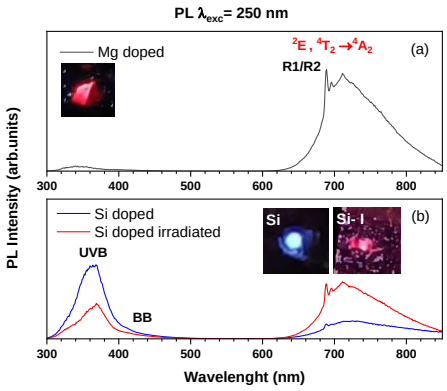

Figure 1. Room temperature PL spectra of (a) Mg and (b) Si co-doped β-Ga_2O_3:Cr before and after irradiation with protons. Inset: A picture of each sample under 325 nm excitation wavelength (He-Cd laser).

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New experimental and modelling approaches to understand electrodeposition of metals

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Recently our research has been focused on understanding better the link between metal microstructure and electrochemistry. While the first part of the talk is on the electron nucleation of particles and related metal microstructural effects, the second parts discusses the electrochemical properties as function of the metal microstructure.

1) Metal nanocrystals are of great interest due to their unique properties that can be tuned by adjusting their size and shape. When supported on different substrates, they find applications in different fields, such as catalysis or sensing. Electrochemical deposition allows the growth of the nanostructures in one step, directly on the final support. Hence, it has been proven effective to obtain highly electroactive nanostructures with potential for fuel cell or (bio)sensing applications. One of the key issues to benefit from the properties of supported nanostructures is to understand their formation mechanisms to achieve a good control of their morphology. However, the early stages of electrochemical nucleation and growth are still an active field of research and remain unraveled. Although the classical theory predicts that nanocrystals grow irreversibly by atomic addition until the reaction is halted, we have found proof that alternative growth mechanisms are taking place [1]. In our work, we combine Field Emission Scanning Electron Microscopy (FESEM), aberration-corrected Transmission Electron Microscopy (TEM), electron tomography, in-situ Small Angle X-ray Scattering (SAXS) and electrochemical characterization to study the early stages of metal electrodeposition onto carbon substrates from aqueous solutions and Deep Eutectic Solvents (DESs) [2]. As evidenced from an innovative experimental approach, we have identified some key processes that influence the early growth mechanisms and microstructure of metals electrodeposited on carbon substrates.

2) When aiming for an increased and more sustainable use of metals a thorough knowledge of the corrosion phenomenon as function of the local metal microstructure is of crucial importance. In this work, we bring together the information presented in our last publications on pure Cu [3-5] to present an overview of the different local (electrochemical) techniques that proved to be efficient to study the relation between different microstructural variables and their different electrochemical behavior. The Atomic force microscopy (AFM) [3], Scanning electrochemical microscopy (SECM) [4] and Electrochemical scanning tunneling microscopy (EC-STM) [5] were used in combination with Electron backscatter diffraction (EBSD), consequently, correlations between grain orientation and grain boundary characteristics, on the one hand, and the electrochemical behavior on the other hand, could be identified.

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Magnetic functionalization of poly(*N*-isopropylacrylamide) hydrogels for sensor applications

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With respect to future sensoric applications, clay-based poly(*N*-isopropylamide) (PNIPAM) nanocomposite gels [1] were modified with various magnetic nanoparticles. These particles include Fe_3O_4, CrO_2 and $SrFe_{12}O_{19}$ with loads of up to 50 w%. The aim of this modification is the preparation of a hydrogel for future use in a Hall effect sensor system to measure the degree of swelling in real time. [2] It is therefore necessary to synthesize a gel that emits a magnetic field.
Part of the nanoparticles was used without further modification while another part was coated with 3-(trimethoxysilyl)propylmethacrylate to achieve a covalent bonding to the network structure (Fig.1). [3]

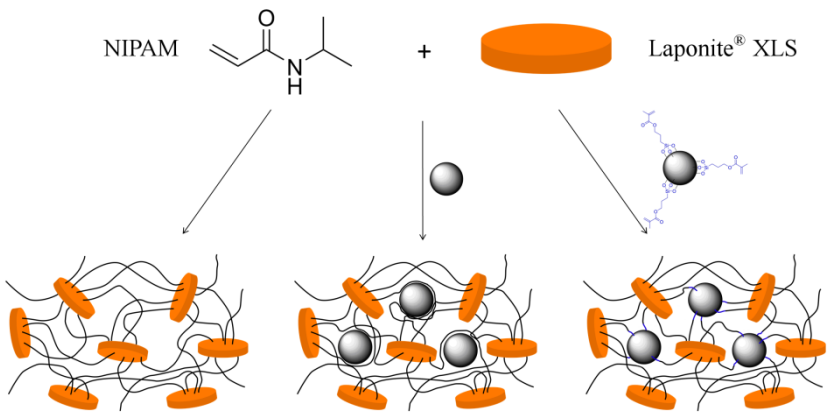

Figure 1: Synthesis of nanocomposite hydrogels based on NIPAM and Laponite® XLS containing coated and uncoated magnetic nanoparticles.

Gels prepared from uncoated particles showed a loss of particles in the outer region of the gel as well as decreased mechanical stability. The use of coated particles drastically reduced the average chain length and degree of swelling while improving the mechanical properties. The consistent temperature response of each gel was tested over a period of two weeks.
Furthermore the gels were synthesized in a magnetic field to achieve a permanent orientation of the magnetic particles inside the network structure. The particles formed rod-like strains parallel to the magnetic field. These structures remained fixed after conditioning of the hydrogels. The influence of these bound structures on swelling and mechanical properties was further investigated.

Acknowledgement: This work was supported by the DFG-GRK 1865.

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In-situ prepared ferrogels with stimuli-responsive properties for sensing applications

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Ferrogels are promising composite materials for sensing applications in aqueous environments. Firstly, they combine the adsorptive properties of iron oxide particles against heavy metals, such as arsenic, with the swelling properties of hydrogels. Therefore, they are designed to work as a stimuli-responsive material in piezoresistive sensors. Secondly, ferrogels can be used for magnetic field-controlled drug delivery in microfluidic and in-vivo systems. Iron oxide obtained by precipitation exhibits the property of releasing thermal energy under high-frequency alternating magnetic fields in case nanometer-sized single-domain particles have been formed. This effect can be used for hyperthermia, a therapeutic tool in medicine for the treatment of cancer, or to induce deswelling of ferrogels based on temperature-sensitive hydrogels.
Aim of this work is the preparation of ferrogels by wet-chemical in-situ precipitation in variously composed hydrogels to investigate the influence of the hydrogel structure on the chemical and physical properties of iron oxide formation.
Thus, Hydrogels of polyacrylamide and their copolymers with carboxylate and sulfonic acid groups as well as porous hydrogels were soaked in iron salt solution under inert gas atmosphere. Iron oxide was then precipitated using alkaline solution. To provide magnetite, the concentrations of the iron salt and alkaline solutions were used in the appropriate stoichiometric ratio. Ionic strength and pH-dependent swelling experiments were performed to characterize the ferrogels. Analytical methods, including SEM and XRD, are used to characterize the morphology and crystalline structure of the precipitated particles. Magnetization measurements were made in order to determine the saturation magnetization and remanence of the ferrogels.
The swelling experiments reveal for all ferrogels a deswelling as a function of ionic strength comparable to the deswelling of ion-sensitive hydrogels. Ferrogels based on polyacrylamide demonstrate the greatest influence of iron oxides on ion-sensitive and pH-dependent swelling. In electron microscopic images, homogeneous, nanometer-sized particle shapes can be detected within the ferrogels compared to iron oxide particles precipitated in solution.
In summary, suitable sensor concepts for the ferrogels in respect to their characterized swelling properties and particle properties, like and magnetism, will be proposed.

Phase Transitions in Magnetoelectric $BiMnO_3$-based Ceramics

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Crystal structure of $BiMnO_{3+\delta}$ ceramics has been studied as a function of nominal oxygen excess using synchrotron and neutron diffraction as well as a magnetometry. Increase in oxygen excess leads to the structural transformations from the monoclinic structure to another monoclinic, and then to the orthorhombic through the two-phase regions. The sequence of the structural transformations is accompanied by a modification of the orbital ordering followed by its destruction.

Analysis of the diffraction data points to the changes of crystal structures from the monoclinic structure (*C2/c*) to another monoclinic ($P2_1/c$) and then to the orthorhombic structure (*Pnma*) with nominal increase in the oxygen content which is consistent with available data [1]. The mentioned series of the structural transformations is accompanied by a gradual decrease in the unit cell volume. The deviation from the stoichiometric cation/anion ratio specific to the $BiMnO_{3.08}$ sample leads to a stabilization of the monoclinic structure having lower symmetry, viz. $P2_1/c$ as compared to the stoichiometric compound - *C2/c*, further decrease in the cations content leads to a stabilization of the non-polar orthorhombic structure *Pnma*. Decrease in the cations content leads to a reduction in magnetization of the compounds as confirmed by our neutron diffraction and magnetization data (Figure 1). The changes in the magnetic structure are mainly caused by two factors - modification in the orbital ordering of the manganese ions and a dilution of magnetic sublattice by the cations vacancies. The first factor is determined by the geometry of the bond lengths Mn – O and angles Mn – O – Mn, the second factor is associated with a character of vacancies distribution over the A- and B- sublattices of the perovskite structure. The both mentioned factors have different impact on the magnetic structure of the compounds. Thus an increase in the amount of the cations vacancies causes a rearrangement of the orbital order (which is accompanied by a change of the dominant superexchange interactions) followed by a disruption of the orbital ordering and the long range spin order removal.

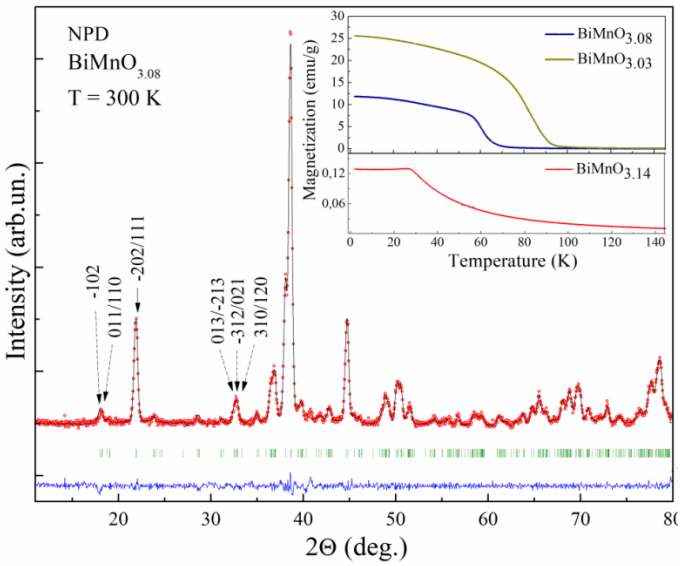

Figure 1. Refined NPD pattern of the compound $BiMnO_{3.08}$ using the space group $P2_1/c$. Inset shows M(T) magnetization curves for the compounds $BiMnO_{3+\delta}$ (δ=0.02, 0.08, 0.14) measured in a field-cooled mode (H~100 Oe).

This work was supported by the RSF (project #21-19-00386).

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Visualization of PVDF/Fe_3O_4 composite by MRI: contribution of homopolymer

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Biomaterials are materials that are used for biomedical applications, being in direct contact with living organisms, such as implants. The study of materials with suitable properties for use as an implant includes the possibility of post-implant visualization using non-invasive imaging techniques such as MRI. In this work we describe the production of a composite based on PVDF, added with Fe_3O_4 to add magnetic properties to the material, enabling its visualization by MRI. The contributions of the PVDF matrix itself in the visualization achieved by MRI, in addition to that conferred by the magnetite itself, were studied. For this, we used the sequence for obtaining MR images called IP-OP (In-Phase and Opposed-Phase). Considered as chemical shift imaging, is a unique tool available to investigate the cellular composition of tissue. By leveraging the inherent difference in resonant frequency between protons configurates in the material that is due to their local chemical environment, chemical shift image acquisition can be timed to image most mobile and rigidous protons when their collective signals are in phase or out of phase, to determine the relative amount of polymer composition protons signal and body simulator protons signal within an individual voxel [1]. It started from the hypothesis that the proton present in the polymer composition would also be used in the production of the image, in addition to those present in the body simulator in which the composite samples are inserted. The result can be seen in Figure 1, where the best delineation of the composite edges is observed, provided by the PVDF signal return. It is concluded that the PVDF matrix also contributes to the visualization of the composite when used as an implant.

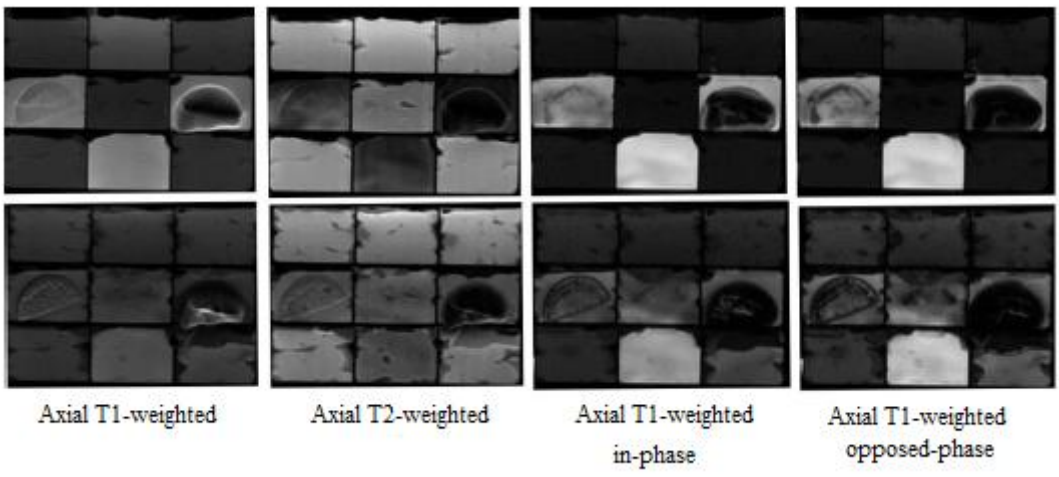

Figure 1 MRI axial sequential slices in weights: a) T1, b) T2, c) in phase and d) out of phase.

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Magnetic and magnetocaloric properties of $Sr_2FeMoO_{6-\delta}$ double perovskites with different degrees of superstructural ordering

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The double perovskite Sr_2FeMoO_6 (SFMO) magnetic oxide is known as prospective giant magnetoresistance material with high value of spin polarization [1, 2]. Its properties can be improved by composition tuning and employment of suitable preparation techniques.
The $Sr_2FeMoO_{6-\delta}$ samples with different degree of the occupational (superstructural) order in Mo - Fe cation sublattice were fabricated by the solid-state reaction method to investigate their magnetic and magnetocaloric properties. The XRD data analysis confirmed the influence of the number of oxygen vacancies on the degree of the superstructural ordering and allowed to calculate it.
Magnetic measurements demonstrated correlation between the number of oxygen vacancies and value of magnetic moment per formula unit in the low-temperature tetragonal phase. The phase transitions registered in the strontium ferromolybdate compounds were established to be the second order. The samples with higher superstructural ordering showed higher Curie temperatures and saturation magnetizations. The magnetocaloric effect calculated from the set of isothermal magnetization curves using the Maxwell relation revealed that SFMO is a promising material for magnetic cooling.

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Chemical solution deposition of $BiFeO_3$ films with layer-by-layer control of the coverage and composition

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$BiFeO_3$ is a unique multiferroic material with high spontaneous polarization and anti-ferromagnetic properties at room temperature [1,2]. The coexistence of these properties allows to consider it in the applications to the different ferroelectric memory devices with combined electric-magnetic writing/readout and in the sensors and actuators compatible to the micro- and nanoelectronics. The most expensive part of the technological processing of the $BiFeO_3$ films is epitaxial growth demanding specific equipment and challenging to scale properties uniformly.

The chemical solution deposition makes it possible to cover large-scale wafers with thickness from a few to few hundred nanometers. To achieve the films with thicknesses larger than 100 nm, the layer-by-layer deposition method is usually used. It makes possible to increase the thickness of the film and keep the stoichiometry of the initial solution, which excludes aggregation of reagents in the initial solution. Nevertheless, the surface coverage and microstructure of the films are often imperfect. As a result, the pores and micro-breaks can act as leakage channels in the material.

In our work, we study the role of the deposition and gelation steps of the sol-gel process to the quality of the films' microstructure and leakage current in the material. The local approach based on the piezoresponse force and conductive atomic force microscopies combination was used to evaluate the functional properties of $BiFeO_3$ thin films obtained by layer-by-layer deposition. The morphology, distribution of local piezoelectric properties, and leakage current were analyzed depending on the number of deposited film layers. It was found that the final properties of the obtained thin films are determined not only by the heat-treatment conditions at the crystallization stage but also by the morphology of the film formed at the gelation stage. The film coverage quality was demonstrated to strongly affect further crystallization kinetics, the final morphology of the films, and their electromechanical properties.

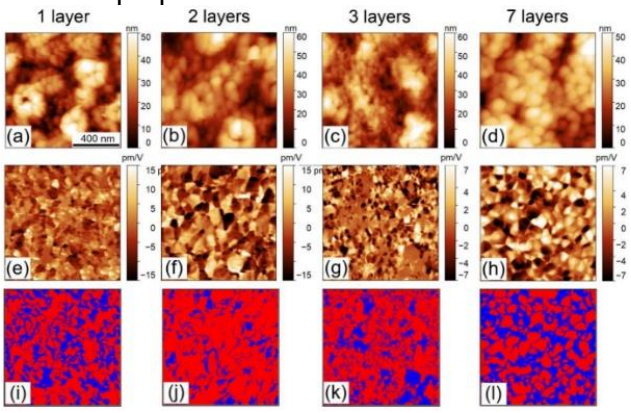

Figure 1 – (a)-(d) Topography, (e)-(h) piezoelectric response and (i)-(l) distribution of the polar (red)/non-polar (blue) phase in polycrystalline $BiFeO_3$ films obtained by the sol-gel method with the various number of the layers.

The investigations were made possible by the Russian Science Foundation (grant 19-72-10076). The equipment of the Ural Center for Shared Use "Modern nanotechnology" UrFU was used.

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Porous Silicon Surface Treatment Effect on the Structure of Nickel-Porous Silicon Magnetic Composites

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Nanocomposites of ferromagnetic metals and nonmagnetic porous matrices have been the subject of thorough investigations over the last years. Structures such as these are primarily attractive for their highly-promising applications in magnetoelectronics and biomedicine and can be fabricated on Si wafers by depositing ferromagnetic metals into porous silicon (PS) host matrices. Up to now, Ni-containing PS matrices have been the most intensively studied nanocomposites of this type from technological and characterization points of view [1, 2].

One of the main problems preventing the formation of uniform Ni nanowires inside PS is the bottleneck effect caused by the narrowing of the pore channels in their topmost subsurface areas. In order to reduce or outright eliminate it, various approaches to PS's pre-treatment prior to depositing the metal can be utilized. The present work aims to investigate the effect of a selection of these techniques on the structure of the resulting Ni-PS nanocomposites.

Ni-PS nanocomposites were produced in three stages. On the first stage, a PS layer was fabricated on n+-type highly doped Si (100) wafers with a volume resistivity of 0.01 Ohm·cm by anodization in aqueous hydrofluoric acid. As a result, a 10 μm-thick PS layer with a porosity value of 72% was formed, consisting of vertically oriented pores roughly 100 nm in diameter. The details of the aforementioned anodization process and an in-depth structural analysis of its results were published as part of our previous work [3].

On the second processing stage, PS's surface was treated with one of two methods: (1) chemical etching in an aqueous KOH solution and (2) ion etching in argon plasma. Another examined approach involved gradually decreasing the current density value in the first processing stage in order to increase the porosity on the surface and in the subsurface areas of the PS layer.

On the third stage, Ni was electrodeposited inside the pores in galvanostatic regime at constant current density from a modified Watts bath at room temperature. The corresponding Ni deposition parameters and the results of the samples' structural characterization were previously described in detail elsewhere [3].

The structure of the resulting samples was studied using scanning electron microscopy and subsequently compared to that of the previously obtained PS-based composites formed by depositing nonmagnetic metals such as indium [4]. The results would indicate that the highest quality samples were acquired on PS layers pre-treated by ion etching. This method, however, is rather complicated and requires the use of expensive equipment. On the other hand, nanocomposites obtained on PS layers anodized with gradually varying current density – the simplest of the three approaches and the one not requiring any additional surface treatments – were also found to be of ample quality. Finally, the nanocomposite of the worst quality was procured on layers of PS pre-treated by chemical etching.

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Structural and magnetic properties interplay in optimizing functionality of magnetocaloric ferrite's fine particles

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Iron containing oxides are the most important functional particles, which finds tremendous applications. A modern attractive application is their use in biomedical technologies as components in systems for imaging, drug delivery, magnetically mediated hyperthermia et al. Particles with spinel and garnet structures possessing the highest performance in techniques where magnetically excited heating provide functionality. Specific important magnetic properties of ferrites used for these purposes may be modulated by the shape, size so as by substituting metals, included in their composition as by creating defects influencing the magnetic structure by cationic distribution and exchange interaction.

In this work we report the results of investigation of polycrystalline ferrite particles based on spinel $MgFe_2O_4$ and $Y_3Fe_5O_{12}$ garnet structure synthesized by different chemical route with and without substitution with various dimensions. Complex study including Mössbauer and Raman spectroscopy accompanied by X-ray diffractometry, SEM and measurements of field and temperature magnetic properties FORC allowed to reveal peculiarities of the structural and magnetic state of the samples and its influence on the heat generation performance. The experimental measurements were complementary supported by modern theoretical study based on the density functional theory (DFT) calculations.

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Friday, 26 November 2021

SESSION 09

Chairperson: **Peter K. Petrov**

SESSION 10

Chairperson: **Vitor Amaral**

SESSION 11

Chairperson: **Shengqiang Zhou**

SESSION 12

Chairperson: **Aleksei Trukhanov**

First principles Calculations of the Electronic and Magnetic properties for Defects in Oxide Crystals

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The radiation-resistant oxide insulators (Al_2O_3, $Y_3Al_5O_{12}$, $MgAl_2O_4$) are important materials for application in fusion reactors, e.g. as optical windows. It is very important to predict/simulate a long-time defect structure formation and evolution including thermal defect annealing after irradiation. For further prediction of the radiation stability of materials, it is also necessary to determine main kinetic parameters - interstitial migration energy E_a and diffusion pre-exponent D_0.

In this talk, we discuss the latest results of the defect computer simulations combining the first principles calculation of the atomic, electronic, magnetic structure and optical properties of advanced defective oxides with the kinetics of defect recombination upon annealing. Primary radiation defects in ionic solids consist of Frenkel defects—pairs of anion vacancies with trapped electrons (*F*-type centers) and interstitial ions. Many of these defects are paramagnetic and observed in ESR. Their thermal annealing is controlled by the interstitial ion migration, whose mobility is much higher than that of the *F* centers.

The basic theory (how to extract from experimental data the *migration energy* of interstitials and *pre-exponential factor* of diffusion) was developed and applied to irradiated insulators in our recent study [1,2]. It was showed that the correlation of these two parameters in strongly irradiated oxides satisfies the so-called *Meyer–Neldel rule* (MNR) [2] observed more than once earlier in glasses, liquids, and disordered materials**,** but not in radiation physics.

We performed large scale computer calculations of basic defects and analyzed available experimental kinetics of the *F*-type electronic and V-type hole center annealing for three different ionic solids: neutron/ion-irradiated Al_2O_3 (sapphire) [1-3], ion-irradiated $Y_3Al_5O_{12}$ (YAG) [4,5] and $MgAl_2O_4$ spinel [6] -- all three wide gap insulating materials but with different crystalline structures. We demonstrated that in sapphire upon an increase of radiation fluence, *both* the migration energy and pre-exponent are *decreasin*g, irrespective of the type of irradiation. This is MNR with *normal* dose dependence. For YAG and spinel we have confirmed MNR, but the dose dependence is *inverse*. We discuss the cause of this phenomenon.

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Control of magnetism in transition metal doped oxides

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Transition metal doping of oxides may or may not make the system ferromagnetic. Both theory and experiment suffer of poor reproducibility [1,2,3]. In this talk, I will outline the typical pitfalls of first principles calculations for transition metal doped oxides [1]. At dilute defect concentrations, long-range magnetic interactions need to be mediated by charge carriers in the oxide host, but conventional density-functionals fail to correctly describe carrier localization properties. I will discuss systematic correction schemes that correctly capture the carrier localization properties for various magnetic semiconductor/oxide systems [4-6]. Finally, I will discuss strategies how to control the onset of ferromagnetism by external stimuli, such as electrical gating and mechanical strain [7].

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Features of Electrically Induced Spin Torque Effect in Multilayer Magnetic Nanostructures

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The exchange interaction between the spin polarized states of conductivity electrons and localized spin states in multilayer magnetic nanostructures underlies the effects of electric field-controlled change of localized magnetic states and the spin dependent electron scattering which depends on the configuration of the localized magnetic states. The efficiency of the first effect characterizes by the threshold spin current density which is sufficient to overcome the magnetic anisotropy forces. In this context, the most favorable is the generation of spin current and spin polarization through the spin-orbit interaction when, in contrast to the generation through an effective magnetic field of an magnetic polarizer, the spin current is not accompanied by charge transfer and power consumption. These effects are related to the effect of so-called spin torque exerting on the vector of magnetic order corresponding to both ferromagnetic and antiferromagnetic exchange interaction [1].
For the ferromagnetic multilayer nanostructures, the mentioned two effects are associated with electric controlled magnetization dynamics and switching and also the magnetoresistance effect that are related to processes of magnetic writing and reading information. In the antiferromagnetic case (possessing zero magnetization) the mentioned spin interaction results in the controlled dynamics of antiferromagnetic order vector that is currently a completely unsolved problem. Due to the strong antiferromagnetic exchange interaction and, accordingly, the high frequency of remagnetization, it is important modeling and description of both ferromagnetic and antiferromagnetic dynamics [2].
The microscopic description of the electric-controlled dynamics in the tunnel multilayer ferromagnetic nanostructures is based on the modified for magnetic system theory of non-equilibrium Green functions with the real-time propagation of the embedded Kadanof-Baym equations which are quantum-kinetic equations for the one-particle propagator. It is shown, that these equation in the tight-binding representation systematically describe features of the spin current-induced spin torque effect accompanied by the remagnetization and the inverse effect of the influence of the magnetic configuration on the conductivity of the magnetic nanostructures.

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A DFT+*U* study of point defects in spinel ferrites

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Spinel ferrites MFe_2O_4 (M = Co, Ni) are insulating ferrimagnets with high saturation magnetizations and Curie temperatures well above room temperature, making these materials suitable for various spintronic applications [1-3]. These compounds possess a so-called inverse spinel structure, in which half of the Fe^{3+} cations are located in tetrahedral sites, while the remaining cations are located in octahedral sites formed by the distorted face-centered cubic lattice of oxygen atoms. Manipulating the cation distribution in these compounds could help to tune the magnetic and electronic conduction properties [4] and even lead to the appearance of a multiferroic ordering for perfectly ordered structures [5].

We performed *ab initio* density functional theory calculations, to investigate the changes induced in the Co and Ni spinel ferrite's properties, due to the presence of structural defects, ranging from cation disorder to oxygen and cation vacancies. The obtained results will be discussed in regard to their bulk thermodynamical stability, which will then be extended to surface reconstructions and supported by nudged elastic band calculations of the energy barrier separating two metastable defective structures. We will finally describe in detail the resulting variations of the magnetic moments and orderings, band gap and the possible appearance of gap states at the Fermi level, which would undoubtedly modify the electronic conductivity. Such a study will pave the way for a general understanding of the magnetoelectric and resistive behavior of spinel ferrites.

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Ab initio study of magnetic and optical properties of Co oxide nanowires on vicinal Pt surfaces

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Recent experiments revealed the formation of novel 1D metal oxide wires on step edges of a vicinal metal surfaces [1,2]. These experimental evidences made these fascinating nanostructures very attractive for further investigations of their electronic and magnetic properties. Since 1D oxides, like many molecular systems, can exhibit unusual optical properties, they can be used for tailoring magnetic properties using electromagnetic radiation [3]. In this work we studied the magnetic and optical properties of cobalt nanowires (NWs) built up at the step edges of vicinal platinum surfaces (Pt(322) and Pt(332)) in the presence of oxygen impurities. Our main goal is to expose the role of oxygen on the magnetic behaviour and its relation to optical characteristics of Co NWs in low- (0.1 monolayer (ML) oxygen coverage) and high- (0.4 ML oxygen coverage) oxidized states.

The magnetic and optical properties of Co oxide nanowires have been explored in two stages. At the first stage, the ground state magnetic behavior of Co oxides were studied in the framework of density functional theory (DFT) as implemented in VASP code [4], at the second stage, the optical behavior were exposed by means of the numerical scheme proposed by Gajdos et al. using the VASP code and LOPTICS method [5].

The DFT calculations have shown that Co oxides (CoO and CoO_2) related to low- and high-oxidized states exhibit magnetic behaviour. However, their magnetic ground state depends on the step edge geometry. For instance, CoO NW at step edge of Pt(332) demonstrates ferromagnetic (FM) coupling between Co atomic spins with the large value of local magnetic moment (~ $1.5\mu_B$), while in CoO NW at Pt(322) surface these atomic spins reveal the antiferromagnetic (AFM) solution for spin coupling with the same value of local magnetic moment (~$1.5\mu_B$,-$1.5\mu_B$) per each Co spin. However, we found the significant decrease of the magnetic behavior in CoO_2 NW at high-oxidized state. The local magnetic moment per Co atom within CoO_2 NW decreased strongly up to $0.6\mu_B$ and $0.2\mu_B$ at the step edges of Pt(332) and Pt(322) surfaces, respectively. Besides that, CoO_2 NW revealed FM and AFM solutions for spin coupling for these vicinal surfaces. Having obtained the magnetic spin configurations for Co oxides, we have carried out the calculations of their optical characteristics. For this purpose, the reflectance difference spectra (RDS) and also surface dielectric anisotropy (SDA) spectra has been calculated [6]. We observed the formation of a singular peak at energy 6eV for clean Pt surface in SDA spectra, the position and polarity of this peak are not specific and do not differ for two types of step edges. The formation of this peak we associated with the optical response of the step edges as heterogeneities of Pt surface. This peak was observed also for pure Co NW. However we found the peak displacement on Pt(332) surface on 0.1eV to the low-energy region relative to a clean Pt(332) surface (for Co NW-Pt(322) system, no peak shift was observed). Low-oxidized state led to small changes in RDS and SDA spectra. We observed a significant changes in the RD and SDA spectra at high-oxidized state of Co NW on Pt(322) surface. We found the reverse of the polarity of the SDA peak in this system and its position does not change in compare to low-oxidized state. We did not observe the significant changes in spectral characteristics for CoO_2 NW on Pt(332) surface. The band structure analysis of Co oxide nanowires has shown that the change of polarity of singular peak in SDA spectra can be associated with magnetic transition in CoO_2 NW on the Pt(322) surface.

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Electrophysical Properties, Morphology and Memristive Behavior of Completely Charged Domain Walls in Reduced Bidomain Lithium Niobate

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The influence of a charged domain wall (CDW) on the formation of the induced domain structures in congruent x-cut lithium niobate crystals ($LiNbO_3$, LN) was studied. By diffusion annealing in air ambient near Curie temperature, as well as infrared annealing in oxygen-free ambient bi- and multidomain ferroelectric structures containing CDWs head-to-head and tail-to-tail were formed. By Kelvin probe mode of atomic force microscopy (AFM) surface potential near the CDWs was investigated. We studied surface needle-shaped induced microdomains which were formed in a vicinity of the domain boundary and far from it by applying of voltage to the cantilever being in a contact with the surface of the sample. Dependence of morphology of the induced domain structure on the crystal's electric conductivity was demonstrated. Screening effect of charged head-to-head domain wall on a shape and size of the domain, that was induced near the boundary was shown. We described partition of the single needle-shaped domains formed by AFM cantilever to several microdomains having a shape of several beams based in a common nucleation point. We found an influence of the CDW on the topography of the samples, which consisted in the appearance of a long groove corresponding to the domain boundary after the reducing annealing.
It was revealed that the electrical conductivity of head-to-head CDWs in the reduced LN is accessible without super-bandgap photoexcitation, shows memristive behavior and can be tuned by external voltage while tail-to-tail CDWs are insulating. The activation energy of polaron mobility as well as electron localization energy was estimated based on I-V curve measurements. The data obtained for the head-to-head CDWs in bidomain crystals shows comparative or even higher local conductivity relatively to inclined CDWs in $LiNbO_3$:Mg as well as ion-sliced single-crystal LN films. Moreover, domain walls in bidomain crystals are highly reproducible, almost flat and possess maximum interface charge density which is promising for future mass production of CDW-based nano-electronic devices operating at the intersection of electronics, optics and mechanics.

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Impact of the Nanocarbon (CNT/CNF) on Magnetic Properties of the "Polymer/Hexaferrite" Composites

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To establish the impact of the type of nanocarbon (CNT -carbon nanotubes and CNF - carbon nanoflaces) composites based on hexaferrite or HF ($BaFe_{11.7}Al_{0.3}O_{19}$) and polymer (PVDF) were formed with the addition of CNT and CNF. Concentration of the HF in PVDF was fixed 85 mass.%. Concentration of the CNT and CNF was fixed 5 mass. %. The CNT diameter was on the order of 50-100 nm, the length was from 2 to 10 μm. CNF is a thin plate with a thickness of 50-70 nm and planar dimensions from 2 to 30 μm. Investigations of the magnetic characteristics (field dependences of the specific magnetization) were carried out at T = 300K in a wide range of external magnetic fields (up to 2 T). Fig. 1 shows the field dependences of the specific magnetization of the samples.

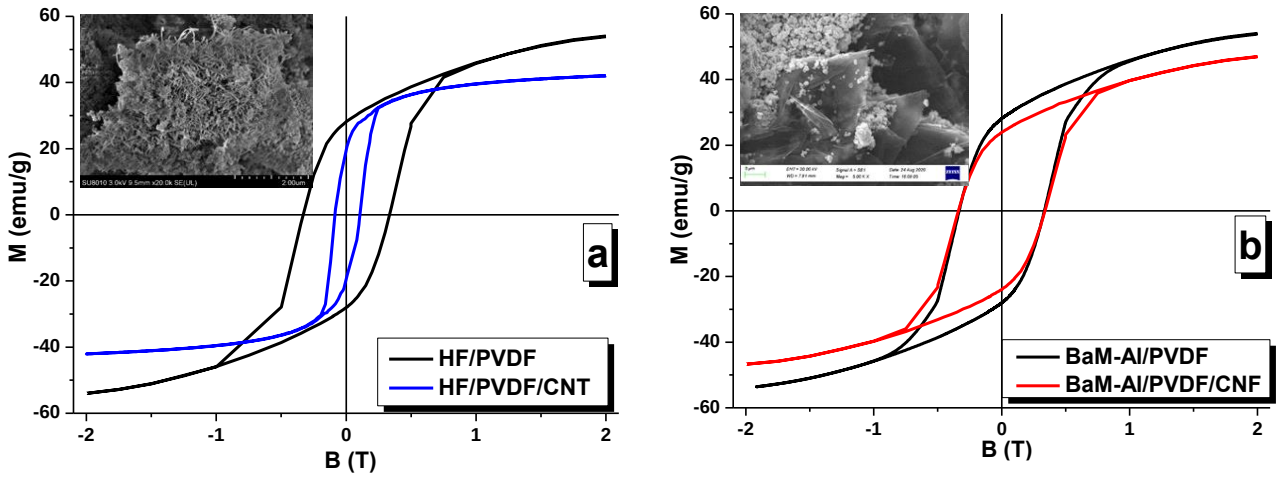

Figure 1 Field dependences of the specific magnetization of the HF/PVDF/CNT (a) and HF/PVDF/CNF (b)

Magnetic characteristics (Ms and Mr) of the HF/PVDF/CNT and HF/PVDF/CNF are lower than for HF/PVDF: for HF/PVDF Ms=54.22 emu/g, Mr=27.79 emu/g and H_C=0.31 T; for HF/PVDF/CNT Ms=42.04 emu/g, Mr=19.35 emu/g and H_C=0.081 T; for HF/PVDF/CNF Ms=48.77 emu/g, Mr=23.90 emu/g and H_C=0.31 T. And magnetic characteristics HF/PVDF/CNT are lower than for HF/PVDF/CNF It should be noted that the sample of CMs with CNT, in contrast to the sample with CNF, goes to the magnetic saturation state at B~0.5 T (Fig. 1a). HF/PVDF/CNT does not saturate even in B up to 2 T (Fig. 1b), which may be due to the weakening of the dipole-dipole exchange interaction due to the influence of the type of nanocarbon. The impact of the type of nanocarbon is critical for H_C and S_q. CNT-based CM values S_q (0.46) and H_C (0.081 T) are significantly lower than when CNF-based CM S_q (0.50) and H_C (0.31 T). This fact may be due to the influence of the shape of nanocarbon. It can be explained by the weakening of the intergranular exchange interaction in CM based on CNF as compared to CNT, as well as the enhancement of the exchange interaction and a decrease in the anisotropy fields in HF/PVDF/CNT.

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Effects of oxidation and chlorine defects on ferromagnetic $CrCl_3$ monolayer

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The van der Waals magnetic chromium trichloride ($CrCl_3$) crystal is the only chromium trihalides to be relatively stable under ambient conditions in reduced dimensionality [1] with the emergence of extrinsic long-range ordered oxidized and Cl-vacancy defective $CrCl_3$ phases [2]. In this work, we study the magnetic properties of such two-dimensional (2D) phases using density functional theory (DFT) calculations and Monte Carlo simulations, including the electron-electron (U) repulsion interactions. The results indicate that pristine $CrCl_3$ monolayer is a 2D ferromagnet with magnetic moment stemming mainly from Cr atoms, which is enhanced linearly by Cl vacancies (up to 3.14 μ_B) in the low vacancy concentration range (1-10 \%), determining a strengthening of ferromagnetic state and a two-fold increase of the Curie temperature (up to 146 K). More interestingly, the oxygen impurities hybridize the monolayer structure allocating on the Cr atomic layer in the center of the honeycomb ring formed by Cr atoms. The ordered oxidized O-$CrCl_3$ phase has magnetic moments localized on both Cr and O atoms, with oxygen which is antiferromagnetically coupled with chromium, resulting in a 2D ferrimagnetic triangular lattice system with high Curie temperature (110 K) and a total magnetic moment of 4.27 μ_B per unit cell. Thus, the oxygen functionalization of metal trihalides can lead the way to the realization of novel 2D ferrimagnetic systems. Besides, the observed enhancement of the critical temperature by Cl vacancies can represent an alternative route to enhance the operation temperature of this class of 2D magnets.

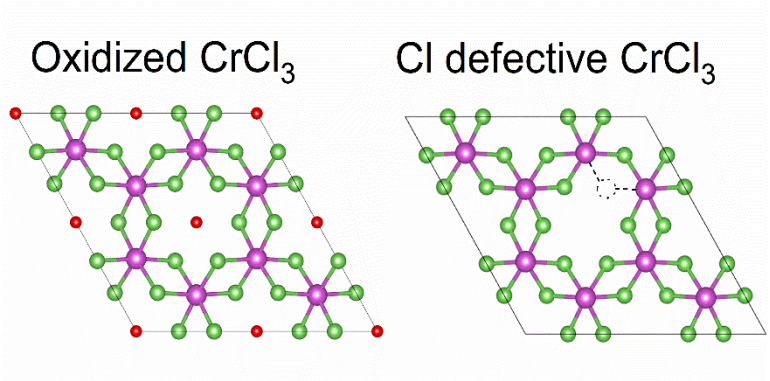

Figure 1: Model structures of ordered oxidized (left) and Cl-vacancy defective (right) $CrCl_3$ phases.

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Energy Harvesting and Magnetic Field Sensing with Bidomain $LiNbO_3$-Based Composites

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With the recent thriving of low-power electronic microdevices and sensors, the development of components capable of scavenging environmental energy has become imperative. We have developed a laminar composite based on bidomain LiNbO3 (b-LN) / metglas. This low-frequency, lead-free, and high-temperature MME system can scavenge power simultaneously from both low-level ambient vibration and magnetic field sources. With an appropriate storage circuit, it should thus be able to support ultralow-power electronic components. Due to its very large voltage transduction ratio, an attractive option could be a self-powered sensor used simultaneously as a vibration / magnetic sensor and a power generator when inactive.
At the same time, b-LN metglas composites can detect low magnetic fields at room temperature with a record value of sensitivity to the magnetic field as low as 200 fT at a frequency of ca. 7 kHz. Furthermore, ME tuning-fork-shaped composite structure based on a b-LN / metglas has shown a sensitivity down to 3 pT under real-life conditions at a low resonance frequency of ca. 300 Hz.
Importantly, the lead-free nature of LN meets the demands of the RoHS directive which assumes the restriction of the use of certain hazardous substances in electrical and electronic equipment. Thus, applications based on LN can substitute commonly used PZT ceramics. The b-LN crystals demonstrated excellent properties in the application of magnetoelectric magnetic sensors, vibration sensors, energy harvesters, actuators, position and magnetic field sensors.

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