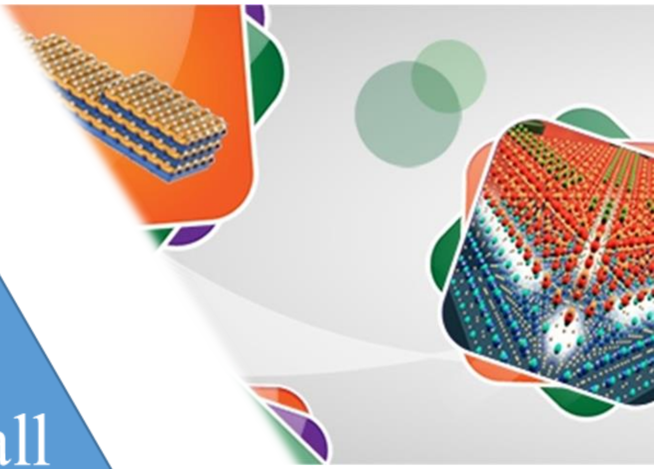

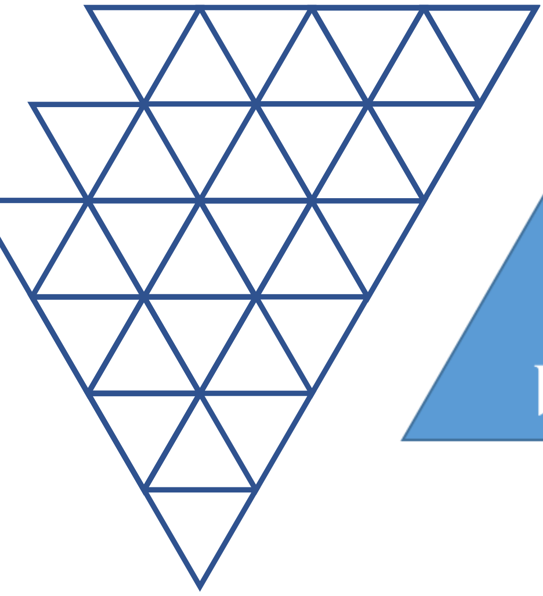

2017
TO-BE Fall Meeting
Towards oxide-based Electronics

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10:30	Management Committee meeting (closed meeting)
12:30-13:30	LUNCH (own expenses)
11:30-13:30	Registration (ISSP, 1st floor)
13:30	OPENING (Martins Rutkis, Juris Purans)

WG2 Oxides Growth and Fabrication Methods		
Chairman:	Gertjan Koster / Carmela Aruta	
14:00	Judith Driscoll	Invited talk: Nanocomposite Films with Strong Room Temperature Converse Magnetoelectric Effect
14:40	Saeedeh Farokhipoor	Invited talk: Mottronics in magnetic domain walls
15:10	Mariona Coll	Compositional tuning of multiferroic $BiFeO_3$ thin films for next generation PV by low-cost chemical deposition methodologies
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WG1 Fundamental Understanding of oxides for electronics: Theory and Experiments		
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16:20	Vladislav Kataev	Insights into the spin-orbital entanglement in complex iridium oxides from high-field ESR spectroscopy
16:35	Pavan Nukala	On the origin of ferroelectricity in HfO_2-ZrO_2 thin films
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WG3 Oxide-based applications and devices		
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17:45	Ana M Sanchez	Exploring oxide boundaries by Scanning Transmission Electron Microscopy

18:00-…	Welcome Party

12th September (TUESDAY)

8:30-9:00	Registration (ISSP, 2nd floor)	
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09:40	Federico Baiutti	Space-charge effects inducing high-temperature superconductivity in La2CuO4 - based heterostructures
09:55	Tony Schenk	The Rayleigh Element – Rayleigh Behavior and its Implications for Impedance Spectra of Ferroelectrics
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11:20	Daniel Khomskii	Invited talk: Orbital-selective effects in transition metal compounds: “molecules” in solids against magnetism
11:50	David Keeble	Point Defect Characterization in Complex Oxides
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12:20	Dennis Christensen	Coexistence of high electron mobility, colossal magnetoresistance and magnetism at the γ-$Al_2O_3/SrTiO_3$ heterointerface
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14:35	Alexis Boileau	Synthesis and characterisation of $SrVO_3$ thin films deposited on varied substrates at low temperature as a new strategic transparent conductive oxide
14:50	Mathieu Mirjolet	Growth and Characterization of Transparent Conducting $SrVO_3$ Thin Films
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09:00	**Bernard Keimer**	**Invited talk: Magnetic order and excitations in metal-oxide heterostructures**
09:40	**Yunzhong Chen**	**Two-Dimensional Electron Gases at Modulation-doped Oxide Interfaces**
09:55	**Alessia Sambri**	**Epitaxial ultra thick LAO/STO films**
10:10	**Roberts Eglitis**	**First principles calculations of ABO_3 perovskite (001), (011) and (111) surfaces, interfaces and defects therein**

10:25-10:50	**COFFEE BREAK**

	WG3 Oxide-based applications and devices	
Chairman:	**Gunnar Niklasson / Daniele Marrè**	
10:50	**Monica Burriel**	**Invited talk: Nano engineering of manganites for miniaturized devices**
11:20	**Lambert Alff**	**Invited talk: Control of Switching Modes and Conductance Quantization in Oxygen Engineered HfO_x based Memristive Devices**
11:50	**Catarina Dias**	**Multi-mode Resistive Switching in Pt/MgO/TaOx/Ta/Ru nanostructures**
12:05	**Sarunas Bagdzevicius**	**Interface-type Resistive Switching in double-perovskite $GdBaCo_2O_{5+\delta}$ thin film devices**
12:20	**Eric Sandana**	**Commercial Perspectives for Ga_2O_3**

12:35-14:05	**LUNCH (own expenses)**	
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14:35	**Qin Wang**	**Applications of photon-induced phenomena in ZnO based hybrids**
14:50	**Jike Lyu**	**Tailoring lattice strain and ferroelectric polarization of epitaxial ferroelectric $BaTiO_3$ films on Si(001)**
15:05	**Vasilis Binas**	**Room Temperature sensing of ozone by p-type Cu_2O nanocubes**
15:20	**Lars Österlund**	**Novel self-cleaning films for the built environment: Functionalized and textured TiO_2 multilayer coatings**

15:40-16:00	**CLOSURE**

Oral talks

Strong Room Temperature and Above *Converse* Magnetoelectric Effect in Nanocomposite Films

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Nanocomposite films with the 3-1 structure, containing ferroelectric and ferro/ferrimagnetic materials have the possibility to achieve magnetoelectric coupling for ultra-high density, non-volatile magnetic recording with low-power electric-writing via voltage driven magnetization switching. $BaTiO_3$-$CoFe_2O_4$ (BTO-CFO) and $BiFeO_3$-$CoFe_2O_4$ (BFO-CFO) nanocomposite films have been intensively studied. However, the relatively low Curie temperature of BTO (*Tc* of 393 K) and large leakage have prevented achievement of electric field control of magnetism at and above room temperature. New materials and precise nanoengineering and growth of these new materials are absolutely crucial factors to achieve the holy grail or magnetoelectric RAM. In this work, we have explored such new materials and have carefully nanoengineered their structures. The leakage problem was overcome and excellent ferroelectric properties and ferrimagnetic properties were achieved. Most importantly, for the first time in a practical system a converse magnetoelectric coupling was achieved, enabling *in-situ* electric field control of magnetism at room temperature and above.

Mottronics in magnetic domain walls

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Domain walls (DWs) in complex oxides have attracted much interest in recent years due to the novel phenomena with which they are associated [1]. The magnetic DWs in mixed-valence manganites with different chemical compositions (and thus variable electron-lattice coupling) have been investigated, as the magnetic DWs in these manganites possess a large electrical resistance due to phase separation at the DW centres [2]. In this work, the creation and destruction of DW arrays in lithographically designed manganite tracks with contact pads at each end has been studied. The DWs have been manipulated magnetically rather than electrically. Photoemission electron microscopy with x-ray magnetic circular dichroism contrast (XMCD-PEEM) is employed to image the resulting magnetic changes while measuring the concomitant changes in track resistance. By combining the magnetoresistance measurements with the magnetic contrast images obtained using XMCD-PEEM, the DW resistance-area product for a range of DW compositions can reliably be quantified, in contrast with studies with no magnetic imaging [3-5]. This study falls into the category of reconfigurable nanopatterning [6], and the formation of insulating regions in a metallic background can be exploited in Mottronic devices for next-generation memory units and transistors with reduced energy consumption.

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Compositional tuning of multiferroic $BiFeO_3$ thin films for next generation PV by low-cost chemical deposition methodologies

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Ferroelectric perovskite oxides, owing a reversible spontaneous electric polarization, have recently emerged as a potential alternative to conventional semiconductor absorbers for the fabrication of efficient solar cells. Unlike traditional silicon based PV cells, they provide unique routes to spontaneously separate charge carriers achieving extremely large beyond band gap photovoltages by a single, homogeneous phase material. Most ferroelectric oxides have bandgaps in the range of 2.7-5 eV which dramatically reduces the solar energy harvesting and shows PV currents orders of magnitude lower than traditional PV cells. Importantly, small changes in film polarization and metal-oxygen bond characteristics (i.e. electronegativity) can impact the built-in electric field and band gap respectively, which will ultimately modify the PV performance of the device.

In this work, we will take advantage of the low-cost chemical thin film growth techniques to perform chemical (co)-substitution in $BiFeO_3$ (BFO), one of the most studied material for its room temperature multiferroicity, and evaluate how these chemical changes influence its structure, morphology, optical properties and photoconductivity. For the first time, we have been able to stabilize by epitaxial growth $BiFe_{1-x}Co_xO_3$ thin films with cobalt contents up to $x\leq 0.7$ identifying a strong decrease in the optical bandgap from 2.7 to 1.4 eV, while preserving the ferroelectric behavior. On the other hand, Bi substitution by rare earth cations has been identified as an effective strategy to further improve film purity, epitaxy and surface morphology. Finally, the preparation of a compositionally graded BFO-based photoabsorber has been experimentally undertaken with the ultimate goal to match the sun spectrum, offering a promising platform to prepare low cost devices.

The intriguing Mott insulating state of Ca_2RuO_4

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In the search for novel quantum material physics the spin-orbit coupling (SOC) plays a key role. A promising scenario is the combination of SOC and strong electron correlations in multi orbital systems. This picture is realized in heavy transition metal oxides composed of 4d and 5d elements.

Of great interest is the complex regime where SOC and crystal field energy scales are comparable. Ca_2RuO_4 is an archetypal example that displays a wealth of physical properties. For example, a high non-superconducting diamagnetic response has been reported, recently. Superconductivity emerges upon application of hydrostatic pressure on crystals or strain to films. The availability of large, high quality single crystals of Ca_2RuO_4 has recently enabled significant progress in the study of the mechanism underlying the Mott insulating state in this system. This talk will present the synthesis of high quality crystals and the low-energy ruthenium band structure as observed by ARPES in the paramagnetic insulating state of Ca_2RuO_4 [1]. These results suggest that Ca_2RuO_4 is a unique example of an orbital differentiated conventional band and Mott insulator. Moreover, a high-resolution oxygen K-edge resonant inelastic X-ray scattering study of the antiferromagnetic Mott insulating state of Ca_2RuO_4 is presented [2,3]. Low-energy (~ 0.3-0.5 eV) weakly dispersive and high-energy (~ 2 eV) non-dispersive excitations are described to show a strong dependence on the incident light polarization. The low-energy excitation has been interpreted as a propagating spin-orbiton, and its nature unveils the intricate interplay of crystal-field splitting and spin-orbit coupling in the band-Mott scenario. In contrast, the high-energy excitation, is closely linked to the Hund's coupling energy scale JH. The excitations reported here on Ca_2RuO_4 are unique features of (1) a band-Mott insulating phase controlled by Hund's coupling and Coulomb interactions, and (2) a composite spin-orbiton resulting from SOC.

Our findings give a unifying picture of the spin and orbital excitations in the band-Mott insulator Ca_2RuO_4.

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[3] L. Das et al., submitted to Phys. Rev. X.

Insights into the spin-orbital entanglement in complex iridium oxides from high-field ESR spectroscopy

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Complex iridium oxides have attracted recently a lot of attention due to an intimate entanglement of spin and orbital degrees of freedom which may give rise to a novel spin-orbital Mott insulating behavior and exotic quantum spin liquid phases. Electron spin resonance (ESR) spectroscopy is known to be an instructive tool for studying the spin-orbital coupling (SOC) effects as it can directly access the relevant parameters sensitive to SOC, such as the g-factor tensor, magnetic anisotropy gaps and spin dynamics. In this talk, our recent results on multi-frequency sub-THz ESR spectroscopy on iridium oxides in strong magnetic fields will be discussed:

(1) Evidence for the inversion of the orbital states in the prototypical spin-orbital Mott insulator Sr_2IrO_4 due to the long-range crystal field effects [1];
(2) Observation of the collective magnetic resonance mode of coupled Cu^{2+} spins $s = 1/2$ and Ir^{4+} pseudo-spins $j_{\mathrm{eff}} = 1/2$ in the aniferromagnetic double perovskite La_2CuIrO_6 [2];
(3) Origin of the unexpected magnetism in the $J = 0$ double perovskite Ba_2YIrO_6 [3].

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On the origin of ferroelectricity in HfO_2-ZrO_2 thin films

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Ferroelectric properties and polar phases have been recently observed in thin films of doped hafnia and solid solution of zirconia with hafnia with composition $Hf_{0.5}Zr_{0.5}O_2$[1]. These materials are of great technological interest owing to their silicon compatibility, the simplicity of their chemistry and low toxicity compared with other commonly used ferroelectric layers.[2] Although robust ferroelectricity has been shown in these materials[3], its origin remains elusive. Furthermore, the factors stabilizing polar phases in ultrathin films, which are otherwise metastable, are poorly understood[4], and understanding these issues are objects of current interest.

To this end, here we report the epitaxial growth of $HfZrO_4$ on (001)-oriented $La_{0.7}Sr_{0.3}Mn0_3$//$SrTiO_3$ substrates. Films below 10 nm relax the bi-axial tensile strain imposed by epitaxy by forming domains, and exhibit ferroelectricity with a large remnant polarization value of 23 $\mu C/cm^2$. Using high resolution electron microscopy, we deduce that these films have a lower symmetry than the commonly reported polar orthorhombic phase ($Pca2_1$). Such a new polar phase in Hafnia-based compounds with a possible symmetry of $P2_1$ or Pc is observed for the first time. $P2_1$ and Pc are sub-groups of polar orthorhombic phase ($Pca2_1$), and can be obtained via in-plane compressive stresses. Through quantitative energy dispersive spectroscopy we estimate that the films are oxygen-deficient ($V_o^{\cdot\cdot}$), and propose a $V_o^{\cdot\cdot}$-strain correlation, in addition to the interface and domain boundaries effects that can create in-plane compressive stresses to stabilize this new phase.

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Oxygen ion conduction and surface exchange reaction tuned by rare earth dopant cations in ceria epitaxial thin films

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Functional properties caused by mobile ions, such as ionic conductivity and surface reaction, are of great importance for a wide range of applications, as for example catalysts, gas sensors, memristors, electrochemical energy storage/conversion systems, and microsolid oxide fuel cells. New possibilities in thin film fabrication allow growth of oxide thin films with a more precise control of the structure and chemical stoichiometry, thus unveiling new perspectives in the study of technologically important properties of oxide materials. While this approach is quite established in the field of nanoelectronics, has been more recently adopted also to study ion conducting materials, raising the question of whether by using epitaxial thin films the functionalities based on mobile oxygen ions can be properly tuned. In this context, doped ceria is widely investigated for the intricate interrelationship between microstructure and chemical substitution defects affecting the transport and catalytic properties. We will discuss the results obtained on the epitaxial doped ceria films by state-of-art techniques, in particular by x-ray photoemission and absorption measurements by synchrotron radiation on in-situ UHV transferred samples. We show how the amount of doping and the different ion radius size of the rare-earth dopants affect the ion conductivity and the activation of the oxygen surface exchange reaction in a non-trivial manner.[1,2]

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Oxide based chemical gas sensing at the nanoscale

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Semiconductor Metal Oxides (SMOX) like SnO_2, ZnO and WO_3 in porous polycrystalline form have been established as the standard sensing substrate for conductometric gas sensors in the market since the 70's. Their success is due to their high surface to volume ratio and to their sensitive band structure dynamics when exposed to both oxidizing and reducing gases. A second generation of SMOX-based sensor started to emerge in the early 2000 as the research community focused on quasi one-dimensional nanostructures like nanowires, nanorods, nano belts etc. To counterbalance the increased stability of the material, contacting may become challenging, especially in the case of individual nanowire devices. Different measurements configuration will be discussed, from the bundle of nanowires to the single nanowire devices, taking into account advantages and drawbacks for obtaining a stable and highly sensitive device [1].
Beside prompted by the fact that worldwide a strong need to develop the third generation of sensitive, stable and reproducible oxides sensors is keeping up and after observing that surface protonation may induce giant conductivity switching of LaAlO3/SrTiO3 heterointerfaces [2], we will present preliminary results obtained on a LaAlO3/SrTiO3 based device.

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Exploring oxide boundaries by Scanning Transmission Electron Microscopy

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Oxide interface engineering can tune charge, lattice type, orbital order and spin, providing new behaviours and functionalities including piezo- and ferro-electricity, colossal magneto-resistance and also unconventional superconductivity, and may lead to wholly new electronic architectures and technologies. Therefore there is growing demand to control the heterostructure interfaces for the development and improvement in device performance. This growing desire to control materials at an atomic level requires the capability to image and analyse material with atomic resolution. In this sense, the development of spherical aberration correctors for electromagnetic established a major improvement in the new generation of electron microscopes. This work focus on the application of state of the art electron microscopy to ferroelectric capacitors.

Using aberration-free scanning transmission electron microscopy (STEM), we analysed in detail the domain structure of Co/$PbTiO_3$/(La,Sr)MnO_3 with ultra-thin active ferroelectric layers. Annular Bright Field (ABF) imaging was used to directly visualise the both heavy and light elements, measuring the relative displacement and dipole distribution unit cell by unit cell. The polarisation maps of different $PbTiO_3$ thin films revealed a clear influence of the depolarization field on the equilibrium domain pattern.

Fano resonances in superconducting gaps near Lifshitz transitions in inhomogeneous transition metal oxides with filamentary hyperbolic interface geometry

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While new functional doped magnetic materials are developed and used in modern nanotechnology the physics of these complex systems is object of active discussions. The multi-scale lattice and electronic complexity from nanoscale to mesoscale in cuprates [1-3] and iron based superconductors [6-6] pushes the fundamental physics of these systems beyond the solid state physics of XX century using simple models based on single band and rigid band approximations.

Here we show that the physics of doped magnetic systems showing high temperature superconductivity is characterized by a dome of Tc controlled by tuning the chemical potential near Lifshitz transitions in strongly correlated multi orbitals systems by pressure, strain, and charge density [6-8]. A major step in the field has been the development of the theory of superconductivity of two components scenarios [7,8] and in particular of a narrow band and a wide band scenarios near Lifshitz transitions [7]. The physics is getting very complex because of frustrated phase separation occurring at the Lifshitz transitions which has been observed by using scanning micro x-ray diffraction [3] and EXAFS method [2] in cuprates, iron based superconductors. Finally we discuss the emerging role of Fano resonances in p-terphenyl [8] and the complex hyperbolic space for the percolation pathways promoting the emergence of quantum coherence at high temperature [3].

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Space-charge effects inducing high-temperature superconductivity in La_2CuO_4 - based heterostructures

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The functional properties of oxide epitaxial heterostructures are the result of a complex interaction between ionic chemistry, local structural parameters and electronic state at the interface level.

In this contribution, we present a comprehensive study in which defect chemistry, striking interface effects (space-charge effects) and the specific cationic distribution resulting from the growth kinetics contribute to the emergence of a fascinating property such as highly confined high-temperature superconductivity.[1]

We employed state-of-the-art atomic-layer-by-layer oxide MBE method in order to synthesize epitaxial thin films of two-dimensionally doped lanthanum cuprate (La_2CuO_4),[2] in which atomic layers of LaO in the crystal structure are substituted by SrO layers with a predefined periodicity. Such SrO layers act as negatively charged surface elements, thus leading to a local redistribution of the mobile defect species. As a result, an electronic phase transformation from insulating into a high-temperature superconducting phase is induced in the material (Tc up to ≈40 K). By employing a number of complementary experimental techniques, including low-temperature DC and magnetic susceptibility measurements, Zinc tomography, HR-TEM imaging and spectroscopy, a number of exciting findings have been highlighted: i) high-temperature superconductivity is confined into a thin region (≈ 3 nm) across the SrO interface, ii) a hole accumulation layer, which is clearly decoupled from the ionic dopant profile (space-charge effects), forms at the side of the interface facing the substrate, iii) as a consequence of the growth kinetics, a certain Sr redistribution occurs from the nominally doped plane, limited to the growth direction,[3] iv) superconductivity can be tuned simply by changing the distance between the active SrO layers.

This works highlights the importance of space-charge effects in the definition of the fundamental properties of oxide interfaces, showing their potential for the local tuning of the functionalities by simply introducing an interface of a-priori known position and charge.

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The Rayleigh Element – Rayleigh Behavior and its Implications for Impedance Spectra of Ferroelectrics

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The Rayleigh law[1] describes the linear dependence of the dielectric permittivity on the amplitude of the applied electric AC field. It is widely accepted as a consequence of the presence of domain walls and their contribution to the effective dielectric response of the measured ferroelectric sample.[2,3]

However, its implications have not been considered when analyzing impedance spectra of ferroelectrics. Here, we report the derivation of a new equivalent circuit element to model these impedance spectra. This allows fits of impedance data based on an actual physical model and a more reliable derivation of relative permittivities than for a single frequency approach. It is emphasized that this is of special importance when characterizing thin films. Only seldom full impedance spectra are shown to justify the selected single measurement frequency. An arbitrary choice of common frequencies such as 10 or 100 kHz can easily be misleading. These points are highlighted using the example of hafnia based ferroelectric thin films.

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Angle-Resolved Photoemission Spectroscopy studies on $EuTiO_3$ thin films and related heterostructures

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The formation of two-dimensional electron gas (2DEG) at titanate surfaces and interfaces have attracted enormous interest in the last decade. Bulk insulating and non-magnetic compounds $SrTiO_3$ and $LaAlO_3$ have been the most employed ones, and the 2DEGs formed at $SrTiO_3$ surface and $SrTiO_3$ / $LaAlO_3$ interface have been widely studied and characterized. Recently, we found that $EuTiO_3$ thin films and $LaAlO_3$ / $EuTiO_3$ / $SrTiO_3$ heterostructures (i.e., traditional $SrTiO_3$ / $LaAlO_3$ interfaces with a ferromagnetic delta-doping $EuTiO_3$ thin layer) are characterized by a 2DEG which shows some similarities to the $SrTiO_3$ and $LaAlO_3$ / $SrTiO_3$ cases [1,2]. This occurrence opens the perspective for the investigation of new functionalities due to the ferromagnetic character of $EuTiO_3$. By carefully acting on the deposition conditions, stoichiometric $EuTiO_3$ films on bare $SrTiO_3$ and on $SrRuO_3$-buffered $SrTiO_3$ substrates, as well as $LaAlO_3$ / $EuTiO_3$ / $SrTiO_3$ heterostructures, were grown for photoemission experiments: we investigated the band structure and the orbital character of such systems by photoemission spectroscopy measurements. We found that $EuTiO_3$ is characterized by a cylindrical Fermi Surface analogous to the one observed in the $SrTiO_3$ and $SrTiO_3$ / $LaAlO_3$ cases. However, the surface and interface states also differ substantially from the "traditional" cases, in particular by the presence of a localized Eu4f band about 2 eV below the Fermi level, and by the presence of only one (and not two as in $SrTiO_3$) ring-shaped Fermi surface components. The data were analyzed and interpreted in order to clarify the interplay between Eu4f states and Ti3d states, and to understand the role of such states in the electronic properties of $EuTiO_3$ films surfaces and interfaces.

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Electronic structure of layered 3d and 5d transition metal oxide architectures

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More than ten years after the initial spark by the discovery of a two-dimensional electron system (2DES) at the $LaAlO_3/SrTiO_3$ interface all-oxide architectures develop rapidly towards device applications. However, sound knowledge about the microscopic physics on which such development efforts could be built is still scarce. Even the origin of the 2DES in LAO/STO is not yet settled. In my talk I will give an overview on what kind of information one can obtain from photoemission spectroscopy on the electronic structure of buried interfaces, surfaces and thin films of such kind of materials.

In particular, I will address the roles of oxygen vacancies and the polar discontinuity for the 2DES formation in LAO/STO as well as electron inhomogeneities at bare STO surfaces. Based on similar photoemission measurements on γ-Al_2O_3/STO I will propose a generic mechanism involving a specific type of oxygen vacancies to explain the hugely enhanced mobilities found at this symmetry-breaking spinel-perovskite interface.

With the prediction of topological insulators in 2005 spin-orbit coupling (SOC) driven phenomena have come into focus. While much of the efforts so far have been spent on single-particle aspects, iridates offer a playground to study SOC in the presence of electron correlations. I will report on a metal-insulator transition in ultrathin films of $SrIrO_3$ and reveal based on angle-resolved photoemission in combination with density-functional theory how the film thickness feeds back to the structural, electronic, and spin degrees of freedom to act jointly in driving the transition.

Orbital-selective effects in transition metal compounds: "molecules" in solids against magnetism

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Close to Mott transition several novel states can appear. In particular, "molecular clusters" can be formed in the solid, such as dimers, trimers, etc. In my talk I will illustrate such phenomena, especially dimer formation, on many examples (pyroxenes; La4Ru2O10; Li2RuO3; M1 and M2 phases of VO2; V and Cr hollandites). The concept of orbital-selective Peierls transitions will be proposed and justified. In systems containing structural metal dimers there may exist in the presence of different orbitals a special state with partial formation of singlets by electrons on one orbital, while others are effectively decoupled and may give e.g. long-range magnetic order or stay paramagnetic. Similar situation can be realized in dimers spontaneously formed at structural phase transitions, which can be called orbital-selective Peierls transition. This can occur in case of strongly nonuniform hopping integrals for different orbitals and small intra-atomic Hund's rule coupling J_H. Yet another consequence of this picture is that for odd number of electrons per dimer there exist competition between double exchange mechanism of ferromagnetism, and the formation of singlet dimer by electron on one orbital, with remaining electrons giving a net spin of a dimer. The first case is realized for strong Hund's rule coupling, typical for *3d* compounds, whereas the second is more plausible for *4d-5d* compounds. We discuss some implications of these phenomena, and consider examples of real systems, in which orbital-selective phase seems to be realized.

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Point Defect Characterization in Complex Oxides

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The status of the application of positron annihilation spectroscopy (PAS) to the detection and identification of vacancy defects in perovskite, ABO_3, materials will be briefly reviewed. The application of electron magnetic resonance (EMR) methods for the detection of impurity ion and impurity ion vacancy defect complexes will also be discussed.

Unambiguous vacancy defect identification has been achieved by combining positron annihilation lifetime spectroscopy measurements with coincidence Doppler broadening spectroscopy and with density functional theory calculations. Investigating non-stoichiometry in perovskite thin films showed that vacancy cluster defects are also stable. Combining PAS measurements with high resolution electron microscopy provided valuable insight on the accommodation of non-stoichiometry in $SrTiO_3$ pulsed laser deposited thin films. Evidence for over compensation of Ti-deficiency through the formation extended defects is presented.

The influence of doping will also be discussed. Donor doping at both the perovskite A-site and the B-site positions, and acceptor ion doping at the B-site. Examples will include Fe-doped $SrTiO_3$, Nb-doped and La-doped $SrTiO_3$. The characterization of acceptor and donor ion doped perovskite titanate oxides by EMR methods will also be briefly reviewed. The results of defect characterization of donor (La) doped $PbTiO_3$ will be presented, light-induced electron paramagnetic resonance demonstrates the important role of Ti^{3+}.

Thickness dependent magnetic anisotropy studies of bi-axially strained $La_{0.7}Sr_{0.3}MnO_3$ thin films on LSAT (001) by Magneto-Optical Kerr Magnetometry

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Even though half metallic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) perovskites have been considered prominent materials for spintronics applications, the complexity of competing interactions (electron, orbital, spin, and lattice degrees of freedom) concurring in determining their magnetic and transport properties have slowed down their use in real devices. The magneto-transport properties of LSMO film can be understood through the magnetization reversal thus magnetic anisotropy of LSMO[1]. Hence, it is extremely important to understand the specific thickness dependency of LSMO film magnetic anisotropy (MA) in order to use it in spintronics devices.

Here, we investigate thickness, epitaxial strain, temperature dependent magnetic anisotropy properties of epitaxial LSMO (001) thin films compressively grown on not yet fully explored cubic substrate i.e., $(LaAlO_3)_{0.3}$ $(Sr_2AlTaO_6)_{0.7}$ (LSAT)[2,3] (001) by MOKE. Two different thin film growth techniques are chosen for this study, namely Pulsed Laser Deposition and Molecular Beam Epitaxy that are well-known for achieving high quality epitaxial oxide films. A series of thicknesses are explored to understand the significant changes of the MA. Especially, we discover an intriguing competition between uniaxial and biaxial *in-plane* MA contributions. At low thickness ($t < 12$ nm), the uniaxial (two-fold) is ascribed to either step-surfaces or octahedral rotations of the LSMO, whereas the biaxial (four-fold) contribution comes from the strain induced by cubic substrate. At intermediate (upto 50 nm) and higher thickness ($t > 50$ nm) regime, the uniaxial contribution comes from orthorhombic symmetry of LSMO and biaxial from bulk magneto-crystalline of LSMO. The weight of such contributions depends on the film thickness, strain and growth technique. In addition to this thickness dependency of the *in-plane* MA, we also demonstrate a non-negligible perpendicular magnetic anisotropy that becomes relevant for the large thicknesses ($t > 50$ nm). These findings hint us the importance and complexity of thickness driven magnetic anisotropy transitions in functional oxides.

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Coexistence of high electron mobility, colossal magnetoresistance and magnetism at the γ-Al2O3/SrTiO3 heterointerface

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The plethora of fascinating properties observed in oxide heterostructures has attracted a lot of interest. Most noticeably, the confined electron gas formed at the interface between the two insulators $LaAlO_3$ and $SrTiO_3$ features e.g. gate-tunable superconductivity, ferromagnetism and non-volatile memory effects. Numerous studies have been devoted to understanding the origin of the conductivity along with enhancing its properties, in particular the electron mobility. Recently, we found[1] that substituting $LaAlO_3$ with γ-Al_2O_3 can produce a confined electron gas with a record-high electron mobility exceeding 140,000 cm^2/Vs. Here, we show that the γ-Al_2O_3/$SrTiO_3$ interface conductivity originates from oxygen vacancies and use defect engineering to control various interface properties[2]. In addition, we show that the high mobility coexists with a strain-tunable magnetic order below 40 K and a positive, non-saturating magnetoresistance of up to 80,000% at 15 T. The study evidences that the γ-Al_2O_3/$SrTiO_3$ heterostructure is an exciting alternative to $LaAlO_3$/$SrTiO_3$ and paves the way for combining lattice, spin and electronic degrees of freedom.

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Plume dynamics in pulsed laser deposition with nanosecond and femtosecond pulses

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Pulsed laser deposition (PLD) is a widespread approach for the fabrication of thin film of a variety of materials, starting from the high temperature superconductors 30 years ago to the recent oxide perovskite hetero-structures. The growth of high-quality films is strictly related to a clear understanding of the PLD process, which cannot be complete without a deep knowledge of the properties of the laser ablation plasma plume. Particularly relevant are the effects that the various growth parameters (e.g. laser fluence, background gas pressure, substrate temperature, etc.) have on the growth process that makes PLD an extremely versatile method of material fabrication. In this communication, an overview on the main features of laser plumes generated during PLD with nanosecond laser pulses will be given, addressing the role on many phenomena involved in the propagation dynamics of the ablated species from the target to the substrate. Among the noteworthy examples of PLD physics that will be discussed, the two following are anticipated: i) the striking influence of process parameters (e.g. background gas pressure and substrate temperature) on both the expansion dynamics and the deposition rate in nanosecond PLD of oxides; ii) the influence of the mass ratio between the plume species and the background gas on the stoichiometric transfer of the material blow-off from the target to the substrate. The various experimental findings will be rationalized in the frame of simple theoretical models aiming at establishing a kind of “rule-of-thumb” approach providing a basic understanding of the processes applicable in various experimental situations that is not always achievable with complex modeling elaborated for very specific situations.

As the laser technology has advanced, PLD has kept the pace and nowadays also femtosecond laser ablation and deposition has emerged as an interesting technique for the elaboration of peculiar nanoparticles and nanoparticles-assembled films. The last part of this communication will be devoted to the illustration of the peculiarities of femtosecond laser ablation plumes, involving fast ions and nanoparticles generation, and to fs-PLD as a technique for the elaboration of nanostructured thin films.

Synthesis and characterisation of $SrVO_3$ thin films deposited on varied substrates at low temperature as a new strategic transparent conductive oxide

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The correlated metal $SrVO_3$ is a serious alternative material as a substitute for indium tin oxide (ITO) which suffers from poor mechanical properties and cost fluctuations. This material shows to be an excellent transparent conductor in its crystalline phase. However, the versatility of good $SrVO_3$ layers for their integration into thermally sensitive technologies is currently constrained by its epitaxial growth at high temperature. Therefore, the growth and the electro-optical properties of $SrVO_3$ films deposited at low temperatures were investigated and optimised for a wide variety of substrates. In this work, $SrVO_3$ thin films have been deposited by Pulsed Laser Deposition. A comparative study of the substrate effect on the crystallisation of $SrVO_3$ and its electrical and optical properties is proposed. Furthermore, different strategies have been implemented to improve the transparent-conductive performances of the layers using post-thermal treatments with their pros and cons. These performances have been tracked by electrical and optical characterisations and faced to the structural characterisations and the chemistry of films. The room temperature resistivity, the screened plasma frequency and the transparency in the optical window 400-800 nm were notably used as comparative benchmarks. Optimal films deposited at low temperature show an electrical conductivity of 5.10^{-3} $S.cm^{-1}$ and a transmittance of 80% in the visible range. Both electrical and optical analyses confirm that $SrVO_3$ deposited at low temperature can be a promising material for transparent conductive layers.

Growth and Characterization of Transparent Conducting $SrVO_3$ Thin Films

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Transparent conductors having high electrical conductivity and high optical transparency are of major interest for oxide electronics, particularly for displays and solar panels. So far, tin-doped indium oxide In_2O_3:Sn (ITO) has been most widely used as it reaches a good balance between the two above-mentioned features. However, resources of indium are running out. Also, the improvement of the electronic properties of ITO approaches its limit. This awakens the interest for, so called, transition metal oxides, a class of materials that is abundant in nature and can reach higher conductivities [1,2,3].

Here, we present the growth and characterization of $SrVO_3$ thin films grown by pulsed laser deposition on (001)-oriented $SrTiO_3$ and $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ (LSAT) substrates. It is found that textured, single phase and flat films can be obtained at an oxygen partial pressure P_{O2} of $4x10^{-7}$ mbar and in a range of substrate temperatures going from 700 to 800ºC. Films grown at higher P_{O2} display, in addition to the main $SrVO_3$ phase, the presence of spurious phases (identified as $Sr_3V_2O_8$, etc.) which correlates with an enhanced surface roughness [4] and a higher resistivity. On *in-situ* grown Hall bar devices on LSAT under optimal conditions, we obtain a resistivity of $7.2x10^{-5}$ Ω cm, a carrier density of $2x10^{22}$ cm^{-3} and mobility of 4.4 $cm^2V^{-1}s^{-1}$. This value of resistivity is close to the state-of-art reported value ($2.8x10^{-5}$ Ω cm [1]) and lower than the standard value of ITO (≈ 10^{-4} Ω cm [2,3]).

By spectroscopic ellipsometry measurements we observe a plasma energy of 1.2 eV in two samples deposited on LSAT at optimal conditions. This value confirms the transparency of our films in the visible range as the plasma energy is an indicator of the free carrier reflection edge and hence the onset of light absorption and/or transmission. Moreover, in agreement with earlier results [1], measurements of the transmittance reveal a high transparency over the whole visible spectrum.

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World of high quality complex oxide interfaces:
Oxide Molecular Beam Epitaxy - *tour de force*

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Oxide Molecular Beam Epitaxy (oxide MBE) is a unique technique for the synthesis of high quality oxide thin films and heterostructures devoted to fundamental studies and to the fabrication of nano-sized devices [1]. In recent times, such a growth method has been customized for the realization of different multicomponent oxide materials. In the present article, the most important aspects related to oxide MBE are discussed, including design, control of the growth process, different deposition schemes, advantages and challenges of the method. A focus will be put on the synthesis of oxides heterointerfaces by using atomic layer-by-layer (ALL) oxide MBE, an advanced deposition method which allows for designing materials down to the atomic layer level. Several successful examples of oxide heterostructures and heterointerfaces, which have been fabricated by oxide MBE, are presented, demonstrating the power of the method [2,3,4,5].

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Multiferroic magnetoelectric $BiFeO_3$-$BaTiO_3$ superlattices: Chemical interface features by TOF-SIMS and STEM-EDX

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The understanding of magnetoelectric coupling in multiferroic oxide heterostructures is still a challenge. Very little is known to date concerning the impact of the chemical interface structure and unwanted impurities that may be buried within short-period multiferroic $BiFeO_3$-$BaTiO_3$ superlattices during growth.

Here, we demonstrate how trace impurities and elemental concentration gradients contribute to high magnetoelectric voltage coefficients in thin film superlattices which consist of 15 double layers of $BiFeO_3$-$BaTiO_3$ [1]. Interestingly, the highest ME voltage coefficient of 55 $Vcm^{-1}Oe^{-1}$ at 300 K was measured for a superlattice with a few atomic percent of Ba and Ti that diffused into the nominally 5 nm thin $BiFeO_3$ layers, according to analytical transmission electron microscopy. In addition, clear enhancements of the cation signals were observed in depth profiles by secondary ion mass spectrometry at the interfaces of $BaTiO_3$ and $BiFeO_3$. As these interface features correlate with the magnetoelectric performance of the samples, they point to the importance of charge effects at the interfaces, i.e., to a possible charge mediation of magnetoelectric coupling in oxide superlattices [1].

The challenge is to provide cleaner materials and processes, as well as a well defined control of the chemical interface structure, to push forward the application of oxide superlattices in magnetoelectric devices [1].

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Growth and characterization of SrCuO2/Sr0.9La0.1CuO2/SrCuO2 quantum wells

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The transition-metal oxides (TMO) quantum wells (QWs), in which the carriers can be confined, have raised interest because of the rich and complex physics involved. In these systems it is possible to create new states of matter through manipulation of orbital order, reduced dimensionality and interfacial proximity effects. The quantum confined systems, in fact, often show different properties than their single bulk layer; e.g., SrTiO3 sandwiched in GdTiO3, forming a QW, show metallic and ferromagnetic properties, while bulk SrTiO3 is a band insulator [1]. The possibility of growing *n* and *p*-doped QWs is crucial not only to investigate carrier symmetries in their physical behavior, but to allow the design of ambipolar devices and excitonic systems [2].

We here focus on *n*-type homometallic QWs: SrCuO2/Sr0.9La0.1CuO2/SrCuO2 (SCO/SLCO/SCO), where the SLCO central layer is an *n*-doped infinite layer high Tc superconductor, obtained by doping its parent compound SCO.

The samples have been grown by oxide Reflection High Energy Diffraction (RHEED) calibrated layer-by-layer molecular beam epitaxy (MBE) and they have been characterized by x-ray diffraction and resistivity measurements vs. the temperature also in presence of external magnetic field. These systems have been studied systematically changing the central layer thickness and they present a superconducting transition until the SLCO central layer is 4-5u.c. thick, while for the sample with 3u.c. no metallic behavior and superconductive transition are observed.

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Magnetic order and excitations in metal-oxide heterostructures

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We will show how polarized photon-based methods such as resonant inelastic x-ray scattering (RIXS) and Raman scattering can be used to obtain a comprehensive description of magnetic order and excitations in metal-oxide heterostructures and superlattices, and outline perspectives for control of the phase behavior of correlated electrons in these structures by modifying the occupation of transition metal d-orbitals, the dimensionality of the electron system, and the electron-phonon interaction. We will focus on cuprate and nickelate based superlattices and will also discuss new opportunities afforded by epitaxial integration of 3d and 4f spin systems.

Two-Dimensional Electron Gases at Modulation-doped Oxide Interfaces

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Two-dimensional electron gases (2DEGs) formed at the interface of insulating complex oxides promise the development of all-oxide electronic devices. However, despite of intensive research, it remains a major challenge to increase the mobility of the 2DEG or to order the property on demand. Based on our recent discovery of extreme mobility enhancement at $LaMnO_3$-buffered $LaAlO_3/SrTiO_3$ (LAO/STO) interface [1], we herein explored three different ways to include $LaMnO_3$ into the polar LAO/STO interfaces. Particularly, I will present tunable phase diagram of the LAO/STO interface, which shows a Lifshitz transition at a density of 2.8 × $10^{13}cm^{-2}$, enhanced spin-orbital coupling as well as the consistence of ferromagnetic 2DEG and interface superconductivity [2]. $LaMnO_3$ modulation doping provides much richer phenomena to the LAO/STO system.

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Epitaxial ultra thick LAO/STO films

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Since more than a decade, the $LaAlO_3/SrTiO_3$ (LAO/STO) system has gained the attention of researchers world wide, as an intriguing example of the fascinating properties stemming at the interface between complex oxides compounds. The origin of the two-dimensional electron gas at the interface between such two insulators is still debated, and the occurrence of significant discrepancies between measurements performed on LAO/STO samples grown in different labs enhances the puzzling scenario of the LAO/STO interface. However, despite this aspect, there is a general experimental agreement on 4 u.c. as the minimum critical thickness below which the samples are insulating. On the contrary, the value of the maximum thickness for conducting LAO/STO samples changes noticeably from sample to sample.

The disappearance of the interface conductivity is generally ascribed to defects induced by the gradual relaxation of the tensile strain related to the relatively large lattice mismatch between LAO and STO (~ 3% at room temperature). To our knowledge, the maximum thickness reported in literature for conducting LAO films is around 30 u.c, but there are seldom reports on such topic.

In this work, we present our results on thick LAO films, with thickness varying between 50 and 200 u.c. Interestingly, in the selected windows of PLD parameters, we are able to obtain a stable layer-by-layer growth even for extremely thick films, as confirmed by RHEED intensity oscillations. This layer by layer growth allows us to obtain conducting interfaces well above 30 u.c. The correlation between transport measurements and structural characterizations, obtained by means of AFM and TEM, allowed us to highlight the strain relaxation mechanisms through the occurrence of a film cracking, resulting in flakes. Suck cracked films are insulating but, surprisingly, the structural analysis of each flake section shows the existence of well ordered micrometer-size LAO/STO interface, as the topmost layer of the STO substrate is cut away from the rest of the STO substrate, because of the strong bonding at the interface with the grown thick film. Such epitaxial micrometer LAO/STO interfaces are now under investigation as they might present transport properties similar to the standard LAO/STO samples.

First principles calculations of ABO_3 perovskite (001), (011) and (111) surfaces, interfaces and defects therein

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By means of the hybrid exchange-correlation functionals, *ab initio* calculations for main ABO_3 perovskite surfaces, namely $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$, were performed [1-5]. For ABO_3 perovskite (001) surfaces, with a few exceptions, all atoms of the upper surface layer relax inwards, all atoms of the second surface layer relax outwards, and all third layer atoms, again, inwards. The relaxation of (001) surface metal atoms for ABO_3 perovskite upper two surface layers for both AO and BO_2-terminations, in most cases, are considerably larger than that of oxygen atoms, what leads to a considerable rumpling of the outermost plane. The ABO_3 perovskite (001) surface energies always are smaller than the (011) and especially (111) surface energies. The ABO_3 perovskite AO and BO_2-terminated (001) surface band gaps always are reduced with respect to the bulk values. The B-O chemical bond population in ABO_3 perovskite bulk always are smaller than near the (001) and especially (011) surfaces. Electronic and atomic structure of $BaTiO_3/SrTiO_3$ and $SrZrO_3/PbZrO_3$ (001) interfaces are analyzed [6,7]. Systematic trends of *F*-center calculations in ABO_3 perovskite bulk and on their (001) surfaces are analyzed.

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Nano engineering of manganites for miniaturized devices

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In recent years manganites with tailored functional properties have attracted special attention for their use in miniaturized devices such as resistive switching memories, spintronic sensors, micro solar cells and micro solid oxide fuel cells [1]. When prepared in the form of thin films their functional properties can largely vary in comparison to their intrinsic bulk properties. There is thus a large interest in understanding and controlling the influence of different parameters, such as epitaxy, substrate-induced strain and grain boundary effects, for the envisioned use of manganites in applied functional devices.

In this talk I will show several examples of our recent work on functional manganite thin films in views of their application in miniaturized devices. First I will present the fabrication of an artificial mixed ionic electronic conducting oxide by grain boundary engineering thin films of $La_{0.8}Sr_{0.2}MnO_{3+\delta}$ (LSM) [2]. While in bulk form LSM is essentially a pure electronic conductor with a very low concentration of oxygen vacancies, this compound was converted into an excellent mixed ionic electronic conductor by creating a nanostructure with high density of grain boundaries. Next I will show how the mass transport properties at the bulk level can be controlled by modifying the cobalt content in the $La_{0.8}Sr_{0.2}Mn_{1-x}Co_xO_{3\pm\delta}$ perovskite family. Thin film pseudo-binary continuous composition maps were generated by combinatorial pulsed laser deposition. Isotope-exchange depth profiling coupled to secondary ion mass spectroscopy was employed to study the oxygen diffusion at the bulk and grain boundary levels for the whole set of compositions. A very large enhancement of the mass transport properties at the grain boundary level was observed independently of the bulk behaviour. Finally, the memristive properties of both the undoped $LaMnO_{3\pm\delta}$ and the Co-substituted $La_{0.8}Sr_{0.2}Mn_{1-x}Co_xO_{3\pm\delta}$ have been evaluated, showing large differences in resistive switching behaviour. The memristance of these manganites can be tuned by changing the materials composition, by anneal treatments and by varying the nature of the metal electrodes.

Our results lead to fundamental insights into oxygen diffusion along grain boundaries and to the application of these engineered nanomaterials in new advanced solid state ionics devices such as micro-solid oxide fuel cells or resistive switching memories.

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Control of Switching Modes and Conductance Quantization in Oxygen Engineered HfO_x based Memristive Devices

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Hafnium oxide (HfO_x) based memristive devices have tremendous potential as non-volatile resistive random access memory (RRAM) and in neuromorphic electronics. Despite its seemingly simple two-terminal structure, myriad of RRAM devices reported in the rapidly growing literature exhibit rather complex resistive switching behaviors. Using a Pt/HfO_x/TiN based metal-insulator-metal structure as model system, we show that a well-controlled oxygen stoichiometry governs the filament formation and the occurrence of multiple switching modes. The oxygen vacancy concentration is the key factor in manipulating the balance between electric field and Joule heating during formation, rupture (reset), and reformation (set) of the conductive filament in the dielectric. In addition, the engineering of oxygen vacancies stabilizes atomic size filament constrictions exhibiting integer and half-integer conductance quantization at room temperature during set and reset. Identifying the materials conditions of different switching modes and conductance quantization contributes to a unified switching model correlating structural and functional properties of RRAM materials. The possibility to engineer the oxygen stoichiometry in HfO_x will allow creating quantum point contacts with multiple conductance quanta as a first step towards multi-level memristive quantum devices.

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Multi-mode Resistive Switching in Pt/MgO/TaO$_x$/Ta/Ru nanostructures

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The downscaling of conventional non-volatile memories is reaching its fundamental limit and there is thus a tremendous demand for novel scalable approaches. Among the most interesting technologies for novel memories are metal-insulator-metal (MIM) memristive devices[1,2] that exhibit non-volatile resistive switching[2,3] between low (LRS; ON) and high resistive states (HRS; OFF). Resistive switching comprises Set (OFF to ON) and Reset (ON to OFF) processes that can be operated under two modes: unipolar and bipolar. Resistive switching is being studied for a large range of applications such as memory (resistive random access memories; ReRAMs), logic, neuromorphic or sensing.

We obtained unipolar resistive switching in Pt/MgO/Ta/Ru devices, for a 30 nm oxide layer, after a forming step, with a good resistance separation for more than 14h.[4] This behavior was observed with all voltage polarity combinations (50 cycles for each) and the devices can also be arbitrarily switched between modes. We found that the operation is better (lower variability and operating voltages) for positive Set voltages and negative Reset ones (Pt grounded). Therefore the (+,-) mode, with bipolar-like properties, is the one with lower voltage and distribution. The XPS analysis revealed that there is a TaO$_x$ interfacial layer resulting from the migration of oxygen from the MgO, given the high affinity of Ta to oxygen. We also studied the conduction mechanisms involved in the switching and attributed it to the formation and rupture of filaments. The resistive switching behavior can then be explained by the formation and rupture of oxygen vacancies (formed at MgO/Ta) filaments from the Ta to the Pt electrode, with a contribution from joule heating. The shape of the filament (conical or hourglass) was also inferred to be related with the operation mode.

Knowing the influence of the operation mode on the parameters variability, our results open the prospect to improve switching performance in other resistive switching systems.

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Interface-type Resistive Switching in double-perovskite GdBaCo$_2$O$_{5+\delta}$ thin film devices

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GdBaCo$_2$O$_{5+\delta}$ (GBCO) double perovskite is a fascinating material with a rich phase diagram (ferromagnetic, antiferromagnetic and re-entrant paramagnetic phases, metal-insulator transition, colossal magnetoresistance phenomenon, spin state transitions [1]). It is interesting to build a ReRAM device based on different physical properties that can be access by continuous doping of the CoO$_2$ planes with electrons or holes by changing only the O content. Along this line and due to ever increasing device miniaturization (~10 nm CMOS transistors in production) we have studied epitaxial thin films (less than 50 nm thickness) deposited by PLD (pulsed laser deposition) at 700ºC and with P_{O_2}= 60 mTorr. XRD Θ-2Θ diffractograms showed epitaxial growth with only *00l* (*l* = integer, simple pseudocubic perovskite setting) peaks of GBCO. No superstructure *00l/2* peaks were observed characteristic of the layered (ordered) double perovskite [2]. SEM and AFM images showed fully continuous films with low (few nm RMS) surface roughness. The growth mode during the deposition was a 2D islands mode and though a more suitable layer-by-layer mode could be achieved by increasing the deposition temperature, it was kept equal to 700°C to avoid decomposition of the lower electrode LaNiO$_3$ at higher temperatures.

Mechanisms governing resistive switching (RS) for ReRAM memory applications are broadly classified into filamentary and interface types [3]. Interface type RS is usually observed in electrode/complex oxides interfaces (e.g. electrode = metal or semiconductor; complex oxide = simple or double perovskites, Ruddlesden-Popper phases) and is beneficial due to the possibility to have multilevel (multibit) memories rather easily and such interfaces could be integrated in a neuromorphic computing device due to its gradual (analog like) RS. In our memristors GBCO is in contact with metals or semiconductors. Oxygen diffusion and semiconducting transport in GBCO allows the creation of conduction barriers at the electrode-oxide interfaces. The interplay between the created barriers, depletion regions and redox mediated change in oxygen stoichiometry leads to a non-volatile (or volatile) change in the device resistance.

In this work we have examined GBCO heterostructures formed by evaporated top metal (Pt, Au, Ag, Ti) and PLD deposited bottom epitaxial conducting oxide (LaNiO$_3$, SrRuO$_3$) electrodes for its potential application in RS memories. We will show the structural and electrical characterization results (Fig. 1) of GBCO epitaxial thin films and apply a few possible scenarios to elucidate the observed continuous change in the device resistance (possible multilevel) and bipolar RS.

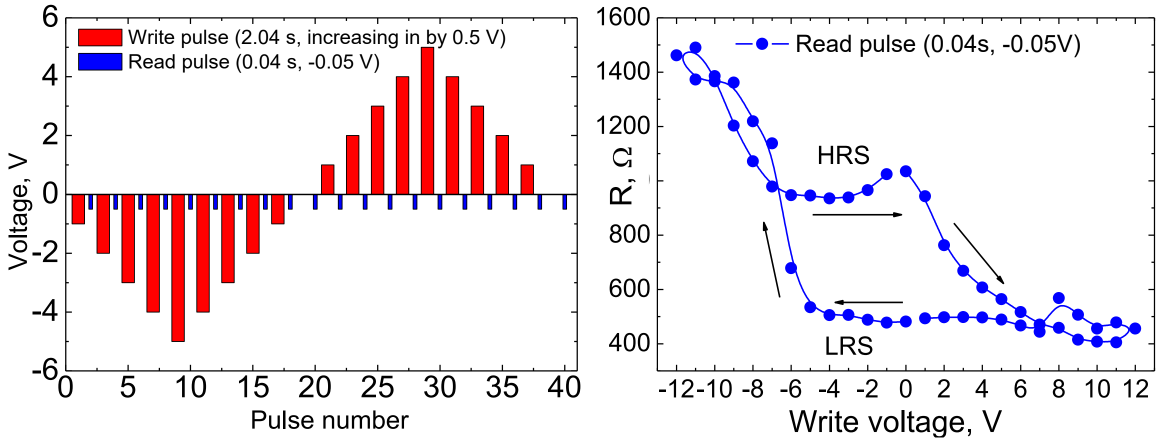

Fig. 1. RS measured in pulse mode on a GdBaCo$_2$O$_{5+\delta}$/ LaNiO$_3$// SrTiO$_3$ heterostructure. a) pulse scheme, b) remnant resistance measured at -0.05V after each write pulse.

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An Overview of the Commercial Prospects for -Ga_2O_3 Based Electronics

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Recently, there has been a surge in interest for the wide bandgap (Eg ~ 4.9 eV) semiconductor gallium oxide (Ga_2O_3). A key driver for this boom is that single crystal wide area bulk β-Ga_2O_3 substrates have become commercially available [1] and a variety of methods have been shown to give high quality epitaxial growth [2,3].

Although Ga_2O_3 has a number of polymorph forms (α-, β-, γ-, δ- and ε) the more stable monoclinic phase (β-Ga_2O_3) has attracted the most attention. Amongst a whole range of potential commercial applications, transparent electrodes, solar blind UVC photodetectors and power electronics have generated the most interest [4, 5]. In this paper we give an overview of the perspectives for these devices with examples from the development work carried out at Nanovation.

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Electrochromic Films for Smart Windows: Coloration and Degradation Mechanisms

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Electrochromic (EC) materials change their optical properties upon the application of a small voltage signal. EC devices are of interest for energy efficient smart windows, as well as for a number of niche applications. The central part of the device comprises EC thin films based on amorphous tungsten oxide (WO_3) and nano-crystalline nickel oxide (NiO_x) joined by a layer of Li^+-containing polymer electrolyte. This arrangement is positioned between transparent and electrically conducting thin films of indium tin oxide (In_2O_3:Sn; ITO) backed by polyester foils. Applying a voltage between the ITO films induces transport of ions between the WO_3 and NiO films, together with charge compensating electron transport through the outer circuit. Insertion of electrons in WO_3 and extraction of them from NiO lead to enhanced optical absorption.

In this paper we report recent results on the mechanisms of coloration as well as degradation under accelerated electrochemical aging of WO_3 and NiO_x thin films. Compositional characterization by Elastic Recoil Detection Analysis (ERDA) gave clear evidence for the species that are active during coloration and bleaching. Coloration in WO_3 is associated with the insertion of Li and degradation occurs because some of the Li cannot be extracted by reversing the voltage signal. In NiO_x the coloration mechanism is more complex and it was found to be due to combined effects of positive Li^+ and negative counter-ions from the electrolyte. These ions are probably adsorbed or chemisorbed at pore surfaces in the film. Degradation occurs because the delicate balance between adsorbed positive and negative ions is altered. Degraded films of WO_3 and NiOx can be rejuvenated i.e. brought back to close to the initial state by electrochemical treatments at high applied potentials. An increased understanding of coloration mechanisms, ageing and rejuvenation will facilitate large-scale practical application of EC materials. It is foreseen to be of major importance for the development of improved EC materials as well as to minimize performance decrease under extended cycling.

Applications of photon-induced phenomena in ZnO based hybrids

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Transition metal oxides are remarkable multifunctional materials with a range of breakthroughs over the past years, which have driven an exponential increase in research activities in the field. RISE Acreo has been active for ZnO based R&D work on optoelectronic applications since 2010 [1-6]. This talk provides an overview on our previous work regarding the synthesis and characterizations of various ZnO nano/micro structures and devices, especially their hybridization processes with p-type Si, GaN, graphene, colloidal CdSe-CdS quantum dots and Poly(3-hexylthiophene) (P3HT) nanofibers for various interdisciplinary applications such as optoelectronic components and bio/chemical sensors listed as follows:

(1) UV photodetectors utilizing ZnO nanorods or nanoflowers on p-type Si substrate
(2) Performance improvement of InGaN/GaN MQW devices by integrated ZnO nanorods
(3) Photovoltaic applications using ZnO composites with colloidal CdSe-CdS quantum dots or P3HT nano fibers
(4) Bio/chemical sensors based on hybrids of ZnO tetrapods and graphene

The structural, optical and electrical properties of the ZnO hybrids verified by AFM, SEM, TEM, FTIR, PL and current-voltage (I-V) characteristics will be presented in the talk, especially the photon-induced interaction between the ZnO structures and their surroundings will be addressed.

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Tailoring lattice strain and ferroelectric polarization of epitaxial ferroelectric $BaTiO_3$ films on Si(001)

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The effects of lattice strain in ferroelectric thin films are known to be generally dramatic. By selection of a proper substrate the elastic strain can be controlled in a certain range, which permits increasing the ferroelectric polarization and the Curie temperature [1]. However the substrate-based strain engineering is limited to relatively small ranges of strain and film thickness due to plastic relaxation. More important, it requires the selection of a specific substrate, whereas for most of the applications the ferroelectric films have to be integrated with silicon. Therefore, alternatives to control lattice strain are required. For this purpose, it is relevant that ferroelectric $BaTiO_3$ thin films deposited by energetic techniques like pulsed laser deposition usually present expansion of the crystalline unit cell [2]. The expansion is likely due to defects, and therefore the relative relevance of thermodynamics and kinetics during deposition of BaTiO3 thin films can influence the amount of defects and consequently of the lattice strain.

We have recently demonstrated that high quality $BaTiO_3$ thin films can be integrated with Si(001) using $LaNiO_3$/CeO_2/YSZ buffer layers [3]. Here we show that epitaxial growth of $BaTiO_3$ can be achieved in broad ranges of deposition parameters, permitting fine tuning of the relevance of kinetics and thermodynamics in the growth, with huge impact on the $BaTiO_3$ tetragonality and ferroelectric polarization. In particular, c-oriented epitaxial $BaTiO_3$ films can be grown in a substrate temperature window wider than 300 ºC, permitting a fine tuning of the c-axis strain from 0 to more than 2%, with remnant polarization scaling with the c-axis up around 11 $\mu C/cm^2$. We present a detailed study of the structural and electrical properties, including ferroelectric loops and leakage curves. The growth strategy presented have permitted an unprecedented level of control and quality in ferroelectric $BaTiO_3$ thin films on Silicon, and can be also used to adjust strain in ferroelectric films on perovskite substrates.

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"Room Temperature sensing of ozone by p-type Cu_2O nanocubes"

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Ozone (O_3) is very useful in everyday life, but also too dangerous for human health as it is toxic. In this work, we present a facile and one pot synthesis at room temperature (RT) of Cu_2O nanocubes. X-ray powder diffraction (XRD), Field – Emission Scanning Electron Microscopy (FESEM), Transmission Electron Microscopy (TEM) techniques were employed to elaborately characterize the structure and the morphology of the sample, revealing Cu_2O nanocubes of high crystallinity Electrical current measurements showed that the nanocubes sensor fabricated in this work was able to detect even 10 ppb O_3 at room temperature and exhibited high sensitivity (28%). At room temperature, the sensor's current increased upon exposure to 10 – 820 ppb O_3, something that can be explained by the gas sensing mechanism of p – type oxide semiconductors. The Cu_2O nanocubes would be promising material in sensor fields.

Novel self-cleaning films for the built environment: Functionalized and textured TiO_2 multilayer coatings

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The possibility to increase human comfort and reduce the global footprint of buildings is a powerful driving force for introduction of new building technology. Introduction of functional coatings in buildings can meet some of these demands. We demonstrate here that photocatalytic and self-cleaning films can be tailored such that they can be up-scaled with available sputtering technologies. Three approaches to achieve these improved functions are presented. First, up to 10-fold enhanced photocatalytic activity is obtained by synthesis of controlled amount of <001> preferential orientation of nanostructured anatase TiO_2 films by reactive dc magnetron sputtering [1]. In a second approach, chemical surface functionalization of TiO_2 by means of photo-fixation of SO_2 and NO_2 are done to bind sulphate and nitrate groups to the surface, and hence acidify the surface [2,3]. By doing so bonding of weak acidic intermediates from VOC photo-degradation and subsequent surface deactivation is avoided. Furthermore, the wetting properties of the TiO_2 films are also modified [4, 5]. In the third approach, TiO_2 is deposited on visible-infrared light absorbing film, whereby heat generated in the underlying light absorbing film heats the TiO_2 film. We show that increasing the temperature of the TiO_2 film results in an increased photocatalytic activity by two mechanisms: thermal activation to increase reaction kinetics, and by shifting the water gas-surface equilibrium coverage to free surface sites for reactant molecules. We generalize the results, and discuss their implications for green building technology and possible scenarios for their implementation.

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Acknowledgements

This work was funded by the European Research Council under the European Community's Seventh Framework Programs (FP7/2007-2013)/ERC Grant Agreement No. 267234 ("GRINDOOR"), Grant Agreement No. NMP4-SL-2013-608950 ("SESBE"), and Swedish Research Agency (VR) contract no. 2015-04757.

Posters

Probing oxide crystal structure using 'digital' electron diffraction

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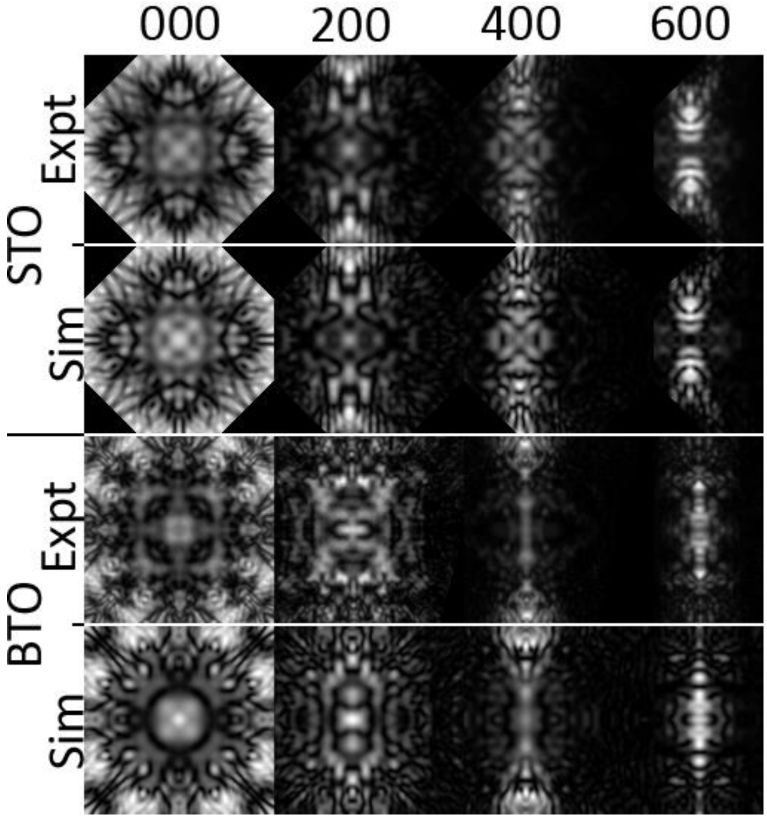
Computer control of electron microscopes now allows thousands of individual convergent beam electron diffraction patterns to be collected, producing data that covers incidence angles of several degrees. These 'digital' large-angle convergent beam electron diffraction (D-LACBED) patterns contain a wealth of information that is sensitive to the fine details of the crystal potential. Here, we investigate their sensitivity to crystal structure using well-known and well-behaved materials such as GaAs and SrTiO3 (STO), and compare these results with similar data from more complex materials such as BaTiO3 (BTO). It is well-known that BTO does not conform to the usual notion of a crystal in at least 3 of the four phases it exhibits (cubic, tetragonal, orthorhombic, rhombohedral) as a function of temperature[1]. Although an average unit cell, symmetry and space group can all be measured and defined for BTO, measurements of interatomic distances are incompatible with the average structure and strong diffuse X-ray scattering is observed for all but the rhombohedral structure. This can only be explained by a 'local' structure, on the length scale of the unit cell, which is different to the larger-scale average structure.

Simulated D-LACBED patterns of GaAs and SRO based on the nominal structure match the experimental data very well and Debye-Waller factors can be separately measured for each atom in the compound. Conversely, simulated patterns for BTO are wildly different from the experimental data, indicating that an average structure is incapable of describing the material.



Processes heat conduction and diffusion in the effects resistive switching memory in thin-film oxide structures

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A resistive switching effect based on the simple binary metal oxides has attracted considerable attention due to the possibility of its application in new electronic memory chips. Experimental data were analyzed by transient electric thermal process of forming unipolar switching memory structure Pt/NiO/Pt. Numerical simulations of the process shows that the channel can be identified with melting of the nickel oxide region, wherein its cross section is determined by the maximum breakdown current, which is a significant contribution to the parasitic capacitance can make. To form a channel parameter estimates are given analytical approximation.

The transition process from the low resistance state into the high resistance state in a Pt/NiO/Pt memory switching structure has been studied by numerical modeling. Detailed analysis shows, that thermally induced diffusion oxidation by nickel vacancies is the key factor for distortion of the channel metallic conductivity. Spatial dynamics of the process of oxidation defines channel narrowing mainly in its central part, and also sets the critical current through the structure sufficient for final rupture of the channel and the transition to high resistance state. The increase in critical current above the limit even by 10% reduces the switching time by an order of magnitude, which is in agreement with experiments. The developed radial diffusion model of conductive channel (or filaments) oxidation may be suitable for the analysis of switching effect a number of other ReRAM oxide structures.

Preparation and study of MoO_3 thin films for realization of MoS_2 2D systems

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Two dimensional (2D) materials have gained great interest in recent years due to their unique electronic, mechanical, and optical properties. Especially transition metal dichalcogenides (TMDs) with the formula MX_2, where M is a transition metal (Mo, W, and so on) and X is a chalcogen (S, Se, or Te), have attracted much attention due to their layer structure and semiconducting properties [1]. Among metal dichalcogenides, molybdenum sulfide (MoS_2) materials have been extensively investigated for its interesting properties including enhanced optical absorption, thermoresponsive photogeneration, efficient hydrogen evolution reaction capability, valley polarization and high on/off ratio with low subthreshold swing, which can lead to ultrathin and highly efficient photovoltaics, photo-thermoelectrics, catalysis for sustainability [3]. Sulfurization of pre-deposited Mo or MoO_3 layers represents a variant of the CVD method for the MoS_2 thin films fabrication. A Mo/MoO_3 layer is annealed in vapors of sulfur at high temperatures converting eventually to MoS_2.

Here we present a preparation of thin MoO_3 films using pulsed laser deposition technique suitable for the fabrication of MoS_2 2D films. As-prepared MoO_3 films were characterized by number of techniques including XRD, AFM, Raman and Auger electron spectroscopy and optical measurements.

MoO_3 films were grown on two substrates – silicon and c-plane sapphire. The first results suggest that only c-plane sapphire will be a suitable substrate for the fabrication of MoO_3 films. From AFM images it is clearly visible that the films prepared on silicon are not continuous and they are growing in the form of flakes. On the other hand, the films on sapphire are continuous. XRD measurements show a polycrystalline character of the MoO_3 film on Si. However, films prepared on c-plane sapphire seems to be at least c-axis oriented. In the symmetric θ-2θ scan only (0 0 l) Bragg-peaks were visible, suggesting a strong texturation in c-axis direction. The in-plane orientation of the MoO_3 phase was studied by ϕ-scans of the (0 2 1) planes and compared with ϕ-scans from the sapphire (1 0 4). Twelve reflections of MoO_3 separated by 30° can be observed in the ϕ-scans. The presence of the reflections will be discussed in detail. The composition and properties of the prepared MoO_3 layers were subsequently studied by Raman and Auger electron spectroscopy and also optical measurements.

After the characterization, the prepared MoO_3 films were used successfully for the fabrication of MoS_2 films.

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Instabilities in functional properties of epitaxial ferroelectric thin films

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Ferroelectric thin films have shown a great potential for application in various electronic devices. To successfully utilize ferroelectric-based devices, the integrated functional layer needs to possess a large stable remnant and switchable polarization between two opposite polarized states. However, as observed in the implementation of these devices, the functional ferroelectric layer often shows instabilities such as a decrease in the remnant polarization after a prolonged period of repeated switching (fatigue) and a change in a possibly present initial preferential polarization state (imprint) upon cycling. The present work aims to identify the causes of the ferroelectric instability as well as to clarify the underlying mechanisms.

$Pb(ZrTi)O_3$ (PZT) was chosen as the model material because of its excellent and unique ferroelectric properties with large remnant polarization, low coercive field and processing temperature. Furthermore PZT is presently the material of choice for most applications. Epitaxial $PbZr_{0.52}Ti_{0.48}O_3$ films were grown with $SrRuO_3$ (or $LaNiO_3$) electrode layers in a heterostructure on $SrTiO_3$ substrates by the pulsed laser deposition method. The films show single (001) out-of-plane growth orientation with excellent crystalline quality and a dense structure without any structural defects.

The pristine SRO/PZT/SRO structure shows a strong imprint as its polarization loop remarkably shifts toward positive direction of the field axis. This indicates that across the PZT film there is an internal electric field which is able to self-polarize the PZT unit cells. A possible origin of this internal electric field is the strain gradient inside the PZT layer due to the misfit dislocations nearby the interface between PZT and SRO bottom electrode. In contrast with the pristine capacitor, the capacitor after being exposed to an external electric field shows a much more symmetric polarization loop with a better switchable polarization, indicating that the film get waked-up during electric application. The effect of the external field strongly depends on its strength, direction, and also the measured temperature. We expect that the internal field and therefore, the self-polarized PZT layer in the treated capacitor is now much reduced.

The fatigue properties of the epitaxial film were also studied. The material of the top electrode plays a crucial role in the bipolar fatigue of the ferroelectric film which was extensively reported in literature. However, we found that the high quality epitaxial films shows an excellent fatigue resistance regardless of electrode material, when unipolar fatigue cycling is applied, irrespective of polarity. This indicates that the well accepted fatigue mechanism model related to the redistribution of charged defects, mostly oxygen vacancies, is not applicable for the epitaxial film.

Novel Carbon Nanotubes Rolled from 6,6,12-Graphyne: Double Dirac Points in 1D Material

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Two kinds of novel carbon nanotubes, namely, (N, 0) and (0, N) 6,6,12-graphyne nanotubes (6,6,12-GNTs), are constructed by rolling up the rectangular 6,6,12-graphyne sheets along two different sides into cylinders [1]. The mechanical and electronic properties of 6,6,12-GNTs with varied N from 3 to 20 are investigated by using density functional theory. Unlike the single-wall carbon nanotubes, the Young's moduli of 6,6,12-GNTs do not remain constant in the case of (N, 0), but the (0, N) tubes possess almost the same around 0.32 TPa. The band structures and density of states also exhibited in our study [1,2]. When the tube sizes N are larger than four, Dirac points appear at Fermi level in the band maps of (N, 0) type 6,6,12-GNTs following an even-odd law, while the (0, N) tubes are narrow-gap semiconductors with tiny band gaps between 5.5 and 247.3 meV.

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First Principles Calculations of $PbTiO_3/SrTiO_3$ (001) Heterostructures

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Using a supercell model and B3PW hybrid exchange-correlation functional in the framework of the density functional theory (DFT), as implemented in the CRYSTAL computer code, we performed *ab initio* calculations for the $PbTiO_3/SrTiO_3$ (001) interfaces [1]. For both PbO and TiO_2-terminations of the $PbTiO_3$ (001) thin film, augmented on the $SrTiO_3$ (001) substrate, the magnitudes of atomic relaxations Δz increases as a function of the number of augmented monolayers. For both terminations of the augmented $PbTiO_3$ (001) nanothin film, all upper, third and fifth monolayers are displaced inwards (Δz is negative), whereas all second, fourth and sixth monolayers are displaced outwards (Δz is positive). The B3PW calculated $PbTiO_3/SrTiO_3$ (001) heterostructure band gaps, independently from the number of augmented layers, are always smaller than the $PbTiO_3$ and $SrTiO_3$ bulk band gaps. For both PbO and TiO_2-terminated $PbTiO_3/SrTiO_3$ (001) heterostructures, their band gaps are reduced due to the increased number of $PbTiO_3$ (001) monolayers. The band gaps of PbO-terminated augmented $PbTiO_3$ (001) films are always larger than those for TiO_2-terminated $PbTiO_3$ (001) thin films. The only exception is the case of 7-layer PbO-terminated and 8-layer TiO_2-terminated augmented $PbTiO_3$ (001) thin films, where their band gaps both are equal to 2.99 eV. For each monolayer of the $SrTiO_3$ (001) substrate, charge magnitudes always are more than several times larger, than for each monolayer in the augmented $PbTiO_3$ (001) thin film. For example, the central $SrTiO_3$ (001) substrate layer Sr and O summary charges varies from +0.45*e* till +0.47*e*. Nevertheless, for the upper $SrTiO_3$ (001) substrate monolayer, the Mulliken charges are quite different, as compared to those in other substrate monolayers. They are found to be changed from -0.28*e* to -0.31*e*, and thereby they approximately correspond to charges averaged between another $SrTiO_3$ (001) substrate monolayers, as well as all monolayer charges in the augmented $PbTiO_3$ (001) film.

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Theoretical prediction of the 5 Volt rechargeable Li ion battery using $Li_2CoMn_3O_8$ as a cathode

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Due to rapid development of computers and forefront research methods, it is nowadays possible to use a quantum-mechanical electronic structure theory of solids and obtain, completely from first-principles, the average voltage of a battery based on intercalation reaction energetics. The results of *ab initio* calculations by means of the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method using the computer code WIEN2k for spin-polarized mixtures of $Li_2Co_xMn_{4-x}O_8$ (x = 0, 1, 2, 3 and 4) treating exchange and correlation effects within the Generalized Gradient Approximation (GGA) are presented [1,2]. The calculated average battery voltage for $Li_2CoMn_3O_8$ cathode material is around 5 Volt. *Ab initio* calculation result of 5 V average battery voltage perfectly describes recently experimentally synthesized $LiCo_{0.5}Mn_{1.5}O_4$ battery cathode material which showed a discharge plateau starting at around 5 V. The calculated average battery voltages for another x values in the mixture $Li_2Co_xMn_{4-x}O_8$ (x = 0, 2, 3 and 4) (3.95 V; 4.47 V; 4.19 V and 3.99 V) are considerably below 5 V.

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Ab initio calculations of $BaTiO_3$ bulk and BaO-terminated (001) surface *F*-centers

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We have performed *ab initio* calculations for the *F*-center in the $BaTiO_3$ bulk and on the BaO-terminated (001) surface using a supercell model and a hybrid B3PW exchange-correlation functional [1]. We find that two Ti atoms nearest to the bulk *F*-center are repulsed, while nearest eight oxygen and four barium atoms relax towards the oxygen vacancy (by 1.06, 0.71 and 0.08% of the lattice constant a_0, respectively). The magnitudes of atomic displacements around the *F*-center located on the BaO-terminated (001) surface in most cases (except for Ti) are larger than those around the bulk *F*-center (0.1, 1.4 and 1.0% of a_0, respectively). Our calculated $BaTiO_3$ bulk Γ-Γ band gap is 3.55 eV. The pristine BaO-terminated (001) surface Γ-Γ band gap (3.49 eV) is reduced with respect to the bulk band gap value. The bulk and BaO-terminated (001) surface *F*-center bands in $BaTiO_3$ matrix are located only 0.23 and 0.07 eV under the conduction band (CB) bottom, indicating that the *F*-center is a shallow donor. The *F*-center in the $BaTiO_3$ bulk contains charge of 1.103*e*, whereas slightly less charge, only 1.052*e*, are localized inside the *F*-center on the BaO-terminated (001) surface. Our calculations demonstrate considerable increase of the chemical bond covalency between the $BaTiO_3$ bulk *F*-center and its two nearest Ti atoms equal to 0.320*e*, and even larger increase for BaO-terminated (001) surface *F*-center and its nearest Ti atom 0.480*e*, in comparison to the relevant Ti-O chemical bond covalency in the perfect $BaTiO_3$ bulk 0.100*e*. The difference between *F*-center formation energy in $BaTiO_3$ bulk (10.3 eV) and on the BaO-terminated (001) surface (10.2 eV) trigger the segregation of the *F*-center from the bulk towards the BaO-terminated (001) surface.

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Bandgap engineering in $KNbO_3$-based ferroelectrics

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Bandgap engineering of ferroelectrics such as $KNbO_3$ allows to explore several photoresponsive phenomena such as photocatalysis and photovoltaic effects. In order to exploit those phenomena in technological applications one should be able to tune the bandgap into the visible range.

The impact of BiMeO3 (with Me=Mn,Fe and Co) doping on the structure, dielectric and optical properties of $KNbO_3$ as been investigated. Both the average and local crystal structures were investigated using XRD combined with Raman Spectroscopy. Reflectivity data collected using a spectrometer with an integrating sphere showed bandgaps to vary from 3.2 eV down to 2.2 eV. In-situ Raman spectroscopy analysis corroborated the polar nature of these materials over a wide temperature range.

The ability to control the bandgap while maintaining the spontaneous polarisation makes $KNbO_3$-$BiMeO_3$ solid solutions interesting for photoinduced processes in a wide temperature range.

Temperature-dependent X-ray absorption spectroscopy study of $CuMoO_4$

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Copper molybdate ($CuMoO_4$) is a thermochromic and piezochromic material, which exhibits structural phase transitions under the influence of pressure and/or temperature. Possible chromic-related applications extend in the range from the user-friendly temperature and pressure indicators to "smart" inorganic pigments. The p-T diagram of pure $CuMoO_4$ has been established in [1]. In this study we focus on α-$CuMoO_4$ and γ-$CuMoO_4$ phases that are stable at high and low temperatures, respectively.

At ambient conditions temperature $CuMoO_4$ has α-phase with triclinic symmetry and a bright green colour [2,3]. Upon decreasing temperature below -73°C the material changes colour to brown due to the first order phase transition from α to γ phase. In addition, a colour change from green to brown but of different origin occurs in α-phase upon heating it up to about 400°C [3].

We used X-ray absorption spectroscopy to study the relationship between structural effects and optical properties of $CuMoO_4$ in the temperature range from -260°C to 700°C. The structural information encoded in the extended X-ray absorption fine structure (EXAFS) spectra was extracted by the simulations-based reverse Monte Carlo method with evolutionary algorithm (RMC/EA) approach [4].

The RMC/EA method allowed us to obtain 3D structure model of the material consistent with experimental data and to analyse the temperature-dependent Cu and Mo K-edge EXAFS spectra of $CuMoO_4$ simultaneously.

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Temperature-dependent EXAFS study of cupric oxide

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Understanding of structure-properties relationship and development of novel functional oxide materials based on design and modelling are key but challenging directions of current research. Successful addressing such needs requires detailed knowledge of materials structure and a proof of reliability for theoretical approaches. Recent experimental and theoretical advances in X-ray absorption spectroscopy (XAS) make it useful and robust tool to tackle such problems [1].

Being one of direct structural methods, XAS is well suited to perform *ex situ*, *in situ* and *in operando* experiments in a wide range of external conditions as temperatures, pressures and atmospheres. The method provides information on the local atomic and electronic structure around particular element in solids, fluids, metal complexes and gases. Besides, when joined with advanced numerical simulations as molecular dynamics (MD) and reverse Monte Carlo (RMC) methods, the analysis of extended X-ray absorption fine structure (EXAFS) located beyond the element absorption edge can be successfully used to provide information on thermal disorder including correlation effects [2] and to validate theoretical models [3].

Here we will illustrate the use of two advanced methods such as MD-EXAFS and RMC-EXAFS on the example of temperature-dependent study of bulk and nanosized cupric oxide (CuO). Our EXAFS analysis indicates that the first-order Jahn-Teller (JT) effect, which is responsible for the strong axial distortion of CuO_6 octahedra [4], dominates the size effect in nano-CuO. The presence of the JT effect makes challenging theoretical simulations of atomic structure of CuO. We have addressed this problem using molecular dynamics simulations based on the ReaxFF variable charge force field model [5] and will demonstrate the use of the EXAFS data for the force-field model validation. The results of the complementary EXAFS analysis by the reverse Monte Carlo simulations have been used to extract information on the local environment of copper within the first six coordination shells. The temperature dependence of the correlation of atomic motion in CuO lattice has been evidenced along particular directions.

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Raman, FTIR and EPR Spectroscopy of Nano-Sized Zinc Peroxides

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Zinc peroxide (ZnO_2) nanoparticles have pyrite type structure wide band gap (4.6 eV) p-type semiconductor properties and potential applications in multifunctional transparent electronic devices and sensors. In this paper, nanocrystalline ZnO_2 and ZnO_2 doped Mn^{2+} powders were directly produced by hydrothermal process using zinc acetate as precursor and hydrogen peroxide as oxidant agent.

The particles size and morphology of nano-ZnO_2 were characterized using XRD. The XRD spectrum clearly show only the crystalline structure and the various peaks of the cubic structure ZnO_2 (JCPDS card No. 13-0311) with the diameter of nanoparticles about 15 nm.

Optical and vibrational properties were characterized using UV-VIS, low temperature FTIR and Raman spectroscopies. The infrared spectra were measured using the KBr pellet method in the two energy ranges from 200 to 800 cm^{-1} and 500-5000 cm^{-1} employing vacuum Fourier transform infrared spectrometer Bruker VERTEX 80v equipped with the closed circle optical helium cryostat. We found that the low temperature (7 K) infrared spectrum of the samples of as-grown (ZnO_2) have the absorption peaks at about 3431 and 1590 cm^{-1} and are attributed to the stretching vibration of the O-H bond and the bending vibration of H-O-H from water molecules, respectively. The peak positions centered at 1040, 1334, and 1420 cm^{-1} should be relate to the O_2^- ions and may arise from the O-O bands, because the low-temperature heat treated ZnO_2 must contain some O_2^- ions [1]. Other sharp absorption bands of the ZnO_2 samples are observed in far infrared (270, 347 and 434 cm^{-1}) and corresponding to Zn-O vibration bands. Temperature dependence of the Raman spectra of ZnO_2 powder was investigated and thermal decomposition to ZnO was found around ~250 °C.

The EPR spectrum of the manganese doped ZnO_2 is a superposition of two Mn2+ centers – a narrow line sextet (S1) and a much broader signal (S2) similarly as in previous study of ZnO:Mn [2]. Narrow line spectra are characteristic for Mn^{2+} in cubic crystalline fields. [3] The resonance positions of the S1 signal can be simulated with $g = 2.00$ and $A = 89$ G. The broader S2 part of the spectrum is somewhat similar to Mn^{2+} spectra observed in glasses [4], where second order ZFS parameters have to be taken into account in order to fully explain the spectrum.

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Influence of 3d ions on radiation damage of $MgAl_2O_4$

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It has good thermal and mechanical properties, high hardness and low electrical loss. $MgAl_2O_4$ is highly resistant to neutron irradiation and has attracted strong attention for it promising use in a future fusion reactor. $MgAl_2O_4$ is part of the spinel family with general formula AB_2O_4 and Fd3m space group. Oxygen ions create close-packed arrangement with 64 tetrahedral and 32 octahedral interstices per a cell. Divalent A and trivalent B cations are respectively located on the tetrahedral 8a and octahedral 16d.

The present work summarizes the results of absorption and luminescence spectra investigation $MgO.nAl_2O_3$ containing chromium and manganese ions. Preference energy for Cr^{3+} ions in octahedral site is rather big as compared with tetrahedral one. So, chromium ions occupy octahedral sites exclusively, substituting for Al ions. The Mn^{2+} is observed in both tetrahedral and octahedral coordination providing green or orange emission. Absorption bands have been explained in terms of the Mn^{2+} configuration model.

The review will consider the optical, luminescent and EPR properties of manganese and chromium ions and their use for the study of radiation defects in Mg-Al-spinel.

Study the luminescence spectra Cr^{3+} of stoichiometric and non-stoichiometric the irradiated fast neutron Mg-Al- spinel are investigated. The broadening of R- and N-lines takes place after spinel crystals irradiation by fast neutron. The changes in intensities and broadening of the luminescence lines are more pronounced in non-stoichiometric spinels.It should be noted that the fast neutron irradiation causes the increasing of the spinel inversion [1].

In stoichiometric $MgAl_2O_4:Mn^{2+}$ single crystals irradiated with fast neutron, the transition of the manganese impurity ions from tetrahedral to octahedral coordination (more spacious) is detected using luminescence methods.

Using pulse EPR technique, hyperfine sub-level correlation spectroscopy it is shown that an electron from a neutron irradiation induced F^+ centre is located in a hyperfine interaction only with neighbouring octahedral coordinated ^{27}Al nuclei [2].

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WG1-14

Synchrotron X-ray diffraction studies of $NdMn_2O_5$

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After a very brief introduction on ferroelectric and multiferroic materials, we initially discuss the key and unique role of large scale synchrotron X-ray facilities for investigating the structure and dynamics of novel multifunctional materials' in general, and ferroelectrics and multiferroics in particular. We will then focus on $NdMn_2O_5$.which illustrates the use of synchrotron X-ray scattering and the concomitant data analysis and refinement in order to obtain structural insights on its multiferroic behavior. We will address the role of the form (single crystal, powder) on the crystal structure and properties of $NdMn_2O_5$, a member of the family of materials RMn_2O_5 (R is a rare-earth), where the multiferroelectricity is present or absent depending on the nature and thus the size of the R cation. The structural differences between the various forms of this material as obtained from synchrotron and conventional X-ray diffraction will be presented and the structure-property relationship will be discussed.

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Tunable electron gas at the non-isostructural oxide interface of γ-Al2O3/SrTiO3 by electric-double-layer gating

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Using electric fields to control the interface properties is the backbone of modern electronics. 2D electron gases (2DEGs) formed at $SrTiO_3$-based interfaces provide a rich platform for fundamental researches and device applications[1,2]. In conventional configuration of field-effect devices, the $SrTiO_3$ substrate was often used as the dielectric insulator, and high voltages of tens to hundreds of volts were required[3,4]. In contrast, field effect in electronic double layer transistor (EDLT) configuration with ionic liquids as the dielectric layer provides a more powerful means of tuning the carrier density and exploring the resultant modulation of novel properties with only a few volts[5]. Herein, we demonstrate, for the first time, an ionic-liquid-gated γ-Al_2O_3/$SrTiO_3$ interface. Remarkably, we observed strong enhancement of Rashba spin-orbit coupling (SOC) of the 2DEG: When a gate is swept from negative to positive voltage to tune the band filling, the SOC increases strongly as evidenced by the intensive weak-antilocalization effect. The quantum oscillations with significantly enhanced mobility and the transition from one- to two- carrier transport by gate voltages were observed and will also be discussed[6].

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PVDF polymer composites with enhanced electrical properties

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The present work is based on idea that the dielectric properties of polymer membranes may be enhanced by using carbon nanotubes (CNTs) and it was study the effects of multiwalled carbon nanotubes (MWCNTs) inclusions on crystalline structure of polyvinylidene fluoride (PVDF), and on the dielectric properties of PVDF/CNT nanocomposites. The extraordinary mechanical, electrical and thermal properties of CNTs make the polymer composites proper to be utilized in microelectronics and flexible electronics which why is considered as high potential material filler for polymer matrices. Polyvinylidene fluoride (PVDF) is known as ferroelectric in its beta phase. Their specific electrical properties allow its utilization for sensors, actuators and transducers, biomedical and optical applications [1].

The PVDF/CNT composites were prepared by dispersing multiwalled carbon nanotubes in PVDF resulting mixed-matrix membranes via solution-sonication method in different volume percent, in concentrations within the range 0.1vol% - 5vol% above threshold of percolation. Flexible and transparent films with high mechanical strength were obtained for composites with small amounts of MWCNTs crystallized at 165°C, but the transparency is decreasing as MWCNTs loading increases. The composite materials were characterized by various spectroscopic, microscopic and dielectric spectroscopy techniques such as XRD and SEM analyses. The XRD analysis of prepared polymer composites show a mixture of α and β crystalline phases and SEM microstructures of the surface fractures allow to characterize the morphology.

Dielectric investigations were performed at low field using Impedance Spectroscopy in the temperature range of (25-150)°C and frequency range of 20Hz–2MHz. The dielectric constant was found sensitive to the MWCNTs loading at room temperature, while in the temperature dependence are highlighted only the polymer relaxations. MWCNTs inclusions in PVDF matrix enhances the electrical conductivity and their mechanical properties, without affecting the membranes flexibility.

Acknowledgements: The collaboration within TO-BE COST Action MP1308 is highly acknowledged.

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THERMAL DECOMPOSITION OF TRONA OF CARBONISED GLASS FIBER FABRICS

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There are continued the research [1,2] of behavior of glass fiber fabrics containing shell of trona ($Na_2CO_3 \cdot NaHCO_3 \cdot 2H_2O$) crystals on its glass elementary filaments [2] at elevated temperatures and different atmospheric condition, that has practical interests. Another motivation is the small sizes (below one um in two directions) of trona crystals in a shell that increase attitude of surface to volume and facilitate investigation of surface phenomena itself.

The aim of this research was to elucidate decomposition of trona at different temperatures (up to 155^0C by step about of 5^0C during a hour) by change its adsorption possibilities after preheating in the terms , defined earlier by relation (1) in [2], that characterize the kinetic of CO_2 and H_2O mass adsorption from atmosphere during first 0.25 hr.

Analysis of obtained relations showed the steep adsorption increase of CO_2 and H_2O after known decomposition beginning of trona at 57^0C and untill approache to its maximum values at about 70 and 80^0C accordingly. Fom trona decomposition beginning (57^0C) up to 155^0C there are revealed at least three maximums of water adsorption and only one sharp adsorbtion maximum of CO_2. The adsorption (physical) increases could be associated with derive the new absorption sites from degradation of crystals surface and increase its area.The adsorption sites are not saturated with adsorbements. The adsorption values are determined by equelibrium with CO_2 and H_2O concentration in surraunding atmosphere and can be changed.

The degradation stages along preheating temperature increase of trona are dicussed.

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We are grateful to State programm of Latvia IMIS2 for financial support

TSL and Cathodoluminescent studies of ScF_3 single crystals at 80 – 300K

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ScF_3 has a simple cubic ReO_3 type structure down to at least 10 K and exhibits a rare property of isotropic negative thermal expansion (NTE) over a large temperature range.

In order to reveal the manifestations of the NTE effect in optical spectra, we have performed the following investigations:

(a) cathodoluminescence analysis of ScF_3 single crystals,

(b) VUV-luminescence excitation using synchrotron radiation at MAX-Laboratory in Lund,

(b) Thermally stimulated luminescence (TSL) study between 80 and 350 K, excited by an electron-beam (10 keV) or VUV radiation.

From the TSL data analysis and the comparison with other metal fluorites, we can conclude that in ScF_3 there is the effective self-trapping of holes in the form of V_k centres and their thermal destruction occurs at about 100 K. From the creation (excitation) spectra of several TSL peaks as well as the VUV-luminescence excitation spectra, we can conclude that the value of band gap energy in ScF_3 exceeds 11 eV.

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Role of Defects in Functional Properties of Irradiated Simple and Complex Oxides Containing Transition Metal Ions

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Natural and synthetic materials are not always pure, they can contain optically active dopant ions. The most common activators found in natural minerals and synthetic materials are transition metal ions (Cr, Mn, and Fe). The type, site distribution and oxidation state of dopant ions strongly influence properties of materials. The current understanding of the role of transition metal impurities in optical absorption and photoluminescence in single and complex oxides is not yet completely established, particularly in relation to the effect of neutron irradiation in this material. It is very important to study color enhancing by neutrons in order to understand the coloration processes and the structure of the color centers. The photoluminescence (PL), its excitation (PLE) and optical absorption of magnesium oxide (MgO) and magnesium aluminium spinel ($MgO.nAl_2O_3$), crystals containing transition metal ions and defects produced by fast neutron and electron irradiation are investigated.

In the most of the investigated MgO samples there can be distinguished three ranges of luminescence: 380-460 nm, 650-850 nm and 900-1300 nm. The intensity of emission in each of these regions is strongly dependent on concentration of transition metal ions, temperature of annealing and irradiation conditions. These luminescence bands are attributed to presence of Fe^{3+}. The broad emission band, which spreads from 650 to 800 nm in topaz and beryl crystals belong to presence of Fe^{3+}, too.

The Cr^{3+} impurity ions prefer to localise in the octahedral sites in order to maintain the local charge neutrality of crystal. The broad band emission of Cr^{3+} ascribed to the ${}^4T_{2g} \rightarrow {}^4A_{2g}$ transition and narrow bands due to ${}^2E_g \rightarrow {}^4A_{2g}$ transition are observed is all investigated crystals. The broadening of R- and N-lines takes place after crystals irradiation with fast neutrons.

Electron and hole centers usually produce coloration in minerals and they are produced in general by irradiation. Exchange interaction between radiation defects and impurity ions during neutron or electron irradiation leads to appearance of additional absorption lines and luminescence band broadening in magnesium oxide (MgO) and magnesium aluminium spinel ($MgO.nAl_2O_3$) crystals.

Channels modification using low energy electron irradiation for potential coherent vortex motion applications in YBaCuO thin films superconductors.

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Dissipation associated with vortex motion in type II superconductors opens new possibilities for superconducting electronic devices. A system of coherently moving superconducting vortices leads to appearance of quasi-Josephson effects. In order to enforce coherent vortex motion it is necessary to confine vortices to channels of easy vortex motion. The most common technique of increasing pinning in high T_C superconductors consist in controlled introduction of defects by ion or electron irradiation.

We demonstrate the feasibility of low energy electron writing for creating artificial channels for easy vortex motion. Multiple transversal channels were prepared in the $YBa_2Cu_3O_{7-x}$ (YBCO) bridges using low energy 30 keV electron irradiation. The irradiated area was arranged into the 0.5 – 4.0 µm narrow channels periodically repeated with distances of 7.5 - 15 µm between the channels, oriented transversal across the bridges with the aim to repress superconductivity in the channels.

The YBCO films were prepared on MgO and $(LaAlO_3)(Sr_2AlTaO_6)_7$ substrates using a pulsed laser deposition technique. The films were patterned into bridges and used for investigation of electrical properties before and after electron irradiation. Depending on the channel width at the point of fluency 10^{20} electrons/cm^2 the measurements of irradiated bridges can show no changes, or enhancement or restriction of the electrical properties.

As the first results show it is not possible to observe any changes in electrical properties of the 0.5 µm - 1.5 µm wide channel. In this case the channel width is too narrow and oxygen diffusion from the non-irradiated parts of the YBCO film to the channels occurs. This lateral diffusion could suppress the difference in oxygen concentration between the channels and non-irradiated area of the film. If the irradiation area width is increased to 2 µm we observe a repression of superconducting properties. On the other hand, for 4 µm wide channels we detect enhancement of superconducting properties. The changes in electrical properties could be connected with electron scattering on the substrates as we illustrated by computer simulations. A possible interpretation of difference between the substrates will be discussed.

Polarised Luminescence of $LiGaO_2$ Crystal

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Lithium metagallate $LiGaO_2$ is a wide band gap ($E_g \approx 6$ eV) ternary mixed-metal oxide compound (I-III-VI) potentially attractive for various practical applications, including use as a substrate for semiconductor heteroepitaxy. Recently a large β-$LiGaO_2$ single crystal was grown by the Taiwan group with an aim to provide a high quality lattice-matched substrate for ZnO heteroepitaxy [1]. Though the basic characterisation of the sample, including cathodoluminescence, was done by the crystal producers, still more detailed study of $LiGaO_2$ properties, especially those connected with luminescence seems to be necessary.

The comprehensive spectral study of lithium metagallate $LiGaO_2$ crystal was done by methods of optical absorption, photoluminescence, luminescence kinetics, thermoluminescence and polarised luminescence in broad temperature range.

Excitation with UV light and X rays causes the main emission bands at 280, 330, 520 and 700 nm (Fig.1). Excitation spectrum of the 280 nm emission band is located entirely in the spectral range of fundamental absorption, structure of the excitation spectrum most probably corresponds to superposition of exciton and band-to-band transitions of $LiGaO_2$ crystal.

The main attention of the present work is focused on the 280 nm band. Dependence of the photoluminescence properties on excitation intensity and other experimental results allow conclusion that the 280 nm band is due to tunnel recombination of donor-acceptor pairs with random distribution of separation distance. The 280 nm band's intensity shows the unusual behaviour with temperature rise – it increases up to the turning point, which depends on the excitation intensity, and then decreases. Studies of the polarised luminescence provide additional information about luminescence processes in $LiGaO_2$ crystal. Measurements of polarised luminescence demonstrate that both 280 nm luminescence emission and excitation bands consist of several subbands with different luminescence polarisation. The emission and excitation subbands with mutually orthogonal polarisation are characterised with different thermal evolution of intensity and spectral position of maximum. The study of polarised luminescence of LiGaO2 is still in progress.

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WG1-23

Towards novel functional properties by interface reaction in $BaTiO_3$-ferrite composites

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In this study, the dielectric and magnetic properties of $BaTiO_3$–ferrite multiphase magnetoelectric composites are reported. The composite ceramics were prepared starting from di-phase mixtures of appropriate amounts of α-Fe_2O_3 and $BaTiO_3$ powders (10, 20, 30 and 40 vol% α-Fe_2O_3), that were uniaxially pressed into pellets at 150 MPa and sintered at 1200°C for 1 h.

M(H) loops at room temperature show a "wasp-waisted" feature (Fig. 1), determined as result of the formation of magnetic phases with contrasting coercivities (hard $BaFe_{12}O_{19}$ and soft $Ba_{12}Ti_{28}Fe_{15}O_{84}$) in different ratios, according to the X-ray diffraction patterns. These extrinsic contributions play an important role, modifying the electrical properties of ceramics with large amount of magnetic phases, causing space charge effect and Maxwell-Wagner relaxations[1,2]. Thus, measurements in the MHz – GHz range (Fig. 1) were carried out for determining intrinsic contributions to electrical response of this kind of composites. The present approach demonstrates that by an appropriated choosing of the system, the chemical reactions at interfaces in ferroelectric–magnetic oxide composites can be controlled and new functional properties can be tailored.

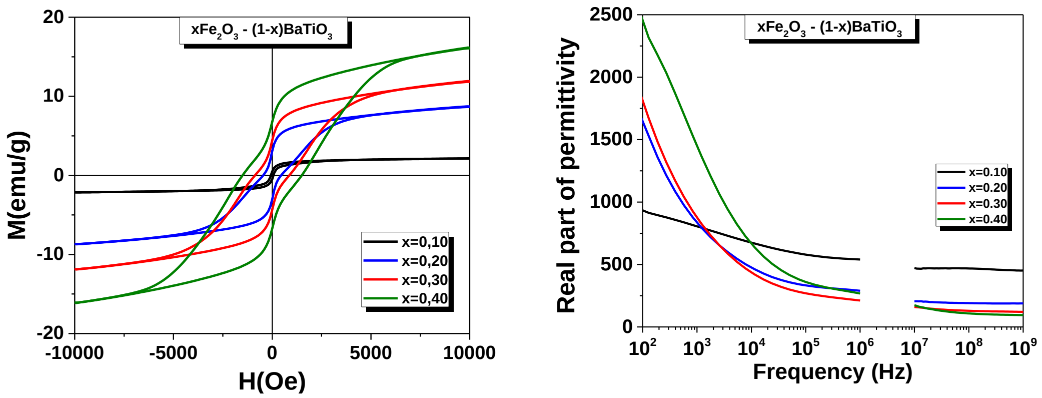

Figure 1. M(H) loops of Fe_2O_3-$BaTiO_3$ at room temperature – left; Real part of permittivity frequency dependencies of Fe_2O_3-$BaTiO_3$ at room temperature – right.

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Spin dynamics in the frustrated system $CoAl_2O_4$

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We present here the results of the combined experimental study of magnetic properties of the frustrated diamond lattice antiferromagnet CoAl2O4 with Co2+ electron spin resonance, 27Al nuclear magnetic resonance, and muon spin rotation/relaxation techniques. In this compound, the frustration of spin interactions and the Co/Al site disorder strongly affect the spin dynamics. The short-range electron spin correlations occure far above a characteristic temperature $T* = 8$ K at which the spin system turns into in a quasistatic state. The results of three spectroscopy techniques highlight a nontrivial role of structural disorder for the magnetism of a frustrated diamond spin lattice at the proximity to the critical point.

Unraveling the magnetoelectric enhancement of $TbMnO_3$ by Fe^{3+} doping

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$TbMnO_3$ is a well-known multiferroic material. Its phase sequence is reported in the literature, and can be summarized as follows. At T_N = 41 K, $TbMnO_3$ undergoes a magnetic phase transition into a incommensurate antiferromagnetic phase, with a longitudinal spin density wave propagating along the *b*-axis, in a P*bnm* symmetry setting. Below T_{lock} = 27 K, a commensurate cycloidal magnetic order in the *ac*-plane becomes stable, which allows the emergence of spontaneous electric polarization along the *c*-axis, according to the Dzyaloshinskii-Moriya mechanism.[1]

Recently it has been shown that the inclusion of a magnetic non-active Jahn-Teller cation (Co^{3+}, Cr^{3+}, Fe^{3+}) in the octahedral site of $TbMnO_3$, even in small concentrations, is a very effective route to reach a substantial change of its physical properties.[2,3] These studies however have been mainly focused on the effect onto the magnetic structure,[2] and only few on the consequent ferroelectricity through the magnetoelectric coupling.[3]

Our work aims at unraveling the effect of Fe^{3+} substitution, up to x = 0.05, in the magnetic, ferroelectric and magnetoelectric properties of the $TbMn_{1-x}Fe_xO_3$ system, both as a function of temperature and applied magnetic field, up to 9 T.[3] A strong decrease of the polarization with increasing Fe^{3+} substitution is observed. However, a significant increase of the magnetic sensitivity of the polarization is obtained, resulting in a high magnetoelectric effect.[3] With single-crystal neutron diffraction we explain this result by the evolution of the magnetic structure responsible for the emergence of the ferroelectricity. The crucial effect of Fe^{3+} substitution is also discussed in the scope of available theoretical framework, understood as a consequence of the competition between ferromagnetic and antiferromagnetic interactions, very sensitive to both local fields and distortions.[3]

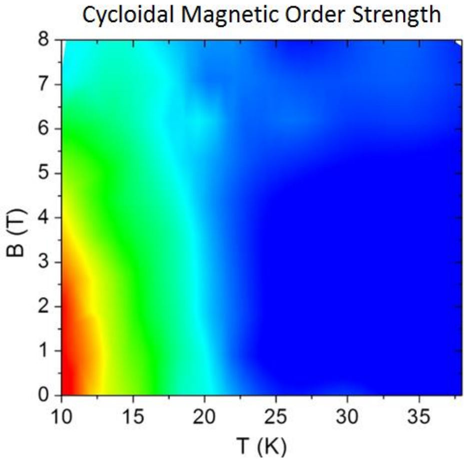

Figure: Cycloidal magnetic order strength obtained from single-crystal neutron diffraction.

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Nanoscale devices and low temperature transport properties at the γ-Al_2O_3/$SrTiO_3$ interface

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Within the last decade, the interface between $LaAlO_3$ and $SrTiO_3$ has been found to host a huge variety of physical phenomena, such as magnetism, and superconductivity. Recently, we have discovered a new two-dimensional electron system at γ-Al_2O_3/$SrTiO_3$ (GAO/STO) interface with exceptional high electron mobility [1]. Here we report on progress with the room temperature fabrication, and low temperature transport properties in the GAO/STO system. Using conducting AFM (cAFM) it is possible to write high precision nanoscale patterns, and surpass the limits of traditional patterning techniques [2]. We show that with a gentle oxygen annealing it is possible to tune thick (above the critical thickness) GAO films into a regime that allows for cAFM writing of devices, without sacrificing its properties [3]. Finally, we will discuss the implications of fabricating more advanced devices such as superconducting nanowires and rings.

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Tuning the ground state of polar $LaAlO_3/SrTiO_3$ interface by an electron sink

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Most of the intriguing properties of two-dimensional electron gases (2DEGs) at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface are sensitive to the electrons located in 3d-orbit of Ti. However, tuning the electronic structure of the system remains challenging due to the intrinsic high carrier density. Herein, instead of using $LaMnO_3$ (LMO) as buffer layers [1], we show that Mn doping in $LaAlO_3$ (LAMO) creates an electron sink that alters the ground state of 2DEG by suppressing the carrier density at the interface, without changing the polarity of the system. By precise control of the Mn-doping level, we found that 2DEGs in our system experience a change from two-band to one-band transport with decreasing carrier density, which is accompanied by a Lifshitz transition at a critical carrier density of 2.76×10^{13} cm^{-2} at 2K. Significantly, the peak value (255.7mK) of superconducting transition temperature is observed at Lifshitz point. In addition, our experiments realize the coexistence of ferromagnetism (FM) and superconductivity (SC) by Mn doping.

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Tuning the Two-Dimensional Electron Gas at the TiO_2-based Surfaces/Interfaces by Ti-O-Ti Configurations

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Chemical redox reactions in $SrTiO_3$ (STO)-based heterostructures can lead to an oxygen-vacancy-induced interfacial two-dimensional electron gas (2DEG) between TiO_2-terminated STO substrate and another oxide insulator, such as the metallic interface between the amorphous $LaAlO_3$ (aLAO) and the TiO_2-terminated STO [1, 2]. The interfacial redox reaction is generally controlled by the formation heat of metal oxide and the work function of the capping layers [3, 4], i.e. the affinity to oxygen and the band-alignment across the interface. Herein, we show that the formation of interfacial 2DEG can also be tuned by the Ti-O-Ti configurations of the TiO_2-based surface/interfaces. This was determined by using two kinds of TiO_2 polymorphous (rutile and anatase) to substitute the STO substrate for the metallic interface of aLAO/STO. Interestingly, these three heterointefaces are all conductive at room temperature, but have dramatically different behaviors upon cooling: the aLAO/STO keeps metallic; the aLAO/TiO_2(A) shows Kondo effect when the temperature is lower than 125 K and the aLAO/TiO_2(R) exhibits metal-insulator transition at 45 K. The above differences mainly come from the abilities with regards to the diffusion of oxygen vacancies at the surface of the three substrates which is determined by the atom species and the atom distributions (Ti-O-Ti configurations) of the three substrates.

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WG1-29

Morphology and Properties of 1D Transition Metal Oxide Nanostructures: First Principles Simulations

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A number of transition metal oxides were proposed and intensively studied as candidates for technologically important applications. Binary oxides TiO_2 and ZnO were found to be rather the cheap, non-toxic and stable among them. On the other hand, regular syntheses of the corresponding one-dimensional nanostructures, first of all nanotubes (NTs) and nanowires (NWs), occurred at the end of 90s and resulted in finding of additional properties important for technological applications and stimulated their intensive theoretical studies.

In most theoretical simulations on periodic 1D nanomaterials, the model of 3D→2D→1D structural transformations has been applied as appropriate [1]. 3D bulk phase is transformed either to a lamellar 2D product, later bent and rolled to 1D NT [2], or to 1D NW after bulk sectioning by 2D planes symmetrically arranged around the chosen crystallographic axis [3]. Initially, symmetric models of defectless nanotubes and nanowires are applied for further first principles calculations using the hybrid DFT-HF Hamiltonian [4]. At last, we consider different types of point defects implemented in pristine NTs and NWs [5], which change structural and electronic properties of 1D nanostructures attached to support of electrode immersed in aqueous media, e.g., improve their photocatalytic suitability for dissociation of water molecules.

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Formation of oxide nanoparticles in ODS steel manufacturing process.

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Oxide dispersion strengthened (ODS) steels are promising materials for fusion reactors and other challenging applications, where uniformly distributed oxide nanoparticles increase radiation resistance, strength and working temperature of the steel matrix.

In this work, we have studied ODS steel materials produced by a recently developed method of manufacturing: Surface Treatment of gas Atomized powder followed by Reactive Synthesis (STARS). We have used X-ray absorption spectroscopy of the Y K-edge and Ti K-edge to reveal local structure changes around Y and Ti atoms. Analysis of X-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS) revealed valuable information about changes in the local structure and valence of Y and Ti after different processing conditions (hot isostatic pressing and following heat treatment temperature). This allowed us to detect formation and character of the nanoparticles in the steel matrix.

Microstructural, optical and glucose sensing characteristics of pulsed laser deposited silver nanoparticles

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Plasmonic nanostructures have been widely investigated due to their potential applications in photovoltaic devices and sensors [1-4]. In general, the efficiency of the photovoltaic devices made from silicon (Si) decreases seriously due to its high reflectivity to the visible and near infrared light. In order to overcome the intrinsic disadvantage of silicon, a new method has currently emerged by the use of light scattering from noble metal nanoparticles (NPs), excited at their surface plasmon resonance (SPR).

This work reports the substrate temperature influenced change in the structural, morphological, optical and glucose sensing properties of silver (Ag) nanoparticles (NPs) deposited on p-type Si (100) wafers. AgNP films grown at temperatures ranging from RT to 600 ºC clearly shows a dependence of orientation texture and surface morphology on substrate temperature (Ts). Moreover, the AgNP shape also changes from ellipsoid to sphere as Ts increases from RT to 600 ºC. Surface plasmon enhancement in photoluminescence intensity is observed with increase in Ts. It is also found that the AgNP film deposited at 300 ºC has considerable reflectance reduction relatively to the silicon substrate, in wavelength range of 300-800 nm and a progressive red shift of localized surface plasmon resonances caused by the adding of increasing quantities of glucose.

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Recent advances in large area Pulsed Laser Deposition; epitaxial growth of complex oxides on silicon

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Pulsed Laser Deposition (PLD) has been established in recent years as a versatile thin film deposition technique for the near stoichiometric synthesis of materials including complex transition metal oxide thin films that offer a variety of exploitable properties. Despite this rich potential for use in electronics, actual industrial applications are relatively few as they rely on growth of films on substrate materials with sizes suitable for industrial applications, were silicon wafers define the standard of CMOS technology. This demands upscaling of the PLD process to grow high quality films on silicon wafers.

Twente Solid State Technology B.V. has developed a PLD system with which oxide heterostructure growth on 4” silicon wafers is investigated and optimized. For thin film growth on silicon wafers using PLD, two important challenges have been the focus of research in recent years. First, epitaxial growth of oxides on as-received silicon wafers is intrinsically prohibited by a native silicon dioxide layer. Growth of YsZ buffer layers has proven to be an effective method to reduce and remove the native silicon dioxide layer to form an epitaxial basis for oxide growth. Second, in PLD the dimension of the plasma plume is smaller than commonly used industrial wafer sizes, which is solved by scanning the plasma plume over the full wafer area.

We present the results on growth of $SrRuO_3$ and $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) on optimized high quality YsZ//CeO_2 buffer layers on 4" silicon wafers. Film morphology and structural characteristics are investigated with Atomic Force Microscopy and X-Ray Diffraction. We show that over the full wafer, films are nearly single phase epitaxially oriented and highly crystalline with atomically sharp interfaces. Subsequently, investigation of the magnetic properties of LSMO shows behaviour comparable to small scale experiments.
Futhermore, we present the results of the effect of an additional $SrRuO_3$ buffer layer on the growth temperature dependent structural and magnetic properties of LSMO films, where LSMO films show ferromagnetic behaviour for growth temperatures as low as 250°C. We speculate that the occurance of this LSMO high quality crystal growth at these remarkable low growth temperatures could be understood by an improved surface diffusion induced by the SRO buffer layer.

Electrical, optical and structural properties of ITO thin films deposited by reactive plasma assisted thermal evaporation

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Transparent and conductive layers are widely used for many microelectronics applications, such as transparent in the visible and near infrared regions electrical contacts electrodes in displays, heat able glass and thin films solar cells. Tin doped indium oxide (indium tin oxide, ITO) is a wide band gap n-type semiconductor (Eg=3.5–4.3 eV) with high transparency in the visible light wavelength range. ITO is one of the most investigated and used transparent conductive oxides due to the small electrical sheet resistance (5-1000 Ω/sq). The electro-optical and structural characteristics of the ITO films are strongly dependent on deposition method and parameters.

In this study ITO thin films were deposited on soda lime glass substrates by reactive plasma assisted thermal evaporation in O_2 gas environment (oxygen pressure of 4 Pa). Metallic In and Sn pieces (Kurt J. Lesker Company (of 99.999% purity)) were thermally melted in the molybdenum evaporation boat and used as the evaporated material. The formation of the films was done at 350 °C temperature substrates. The surface morphology of the samples was analyzed using scanning electron microscopy. The elemental compositions of the deposited ITO structures were measured by energy dispersive spectrometry. The crystallographic structure of thin films was investigated by X-ray diffraction. Sheet resistance and resistivity dependence on temperature of the films were measured by a four point probe technique. This dependence was used for calculation of band gap of ITO films. The transmittance and reflectance spectra of the films were measured at a normal incidence with UV–VIS–NIR spectrophotometer. The absorption edge of the transmittance spectra was analyzed using Tauc method and optical band gap (Eg) was determined.

It was obtained that the ITO films with the porous and uniform surface morphology and columnar structure were formed. The films have a low resistivity of 16.9·10-3 Ω cm (sheet resistance 211 Ω/sq) and a transparency above 80 % was obtained. The band gap values determined by Tauc method and by resistivity dependence on temperature were 3.4 eV and 3.5 eV, respectively. The XRD profile showed the polycrystalline structure of the films.

Magnetic properties of Zn-doped cobalt ferrite nanoparticles: influence of magnetic structure

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In the last two decades spinel ferrites nanoparticles have been one of the most versatile systems due to their potential applications in a wide variety of fields such as catalysis, environment, and especially biomedicine. Among them, cobalt ferrite ($CoFe_2O_4$, CFO) is material with the large magnetocrystalline anisotropy and high magnetization; also it shows good chemical and thermal stability and good mechanical properties.

In the present work, cobalt ferrite nanoparticles with different zinc content ($Co_{(1-x)}Zn_xFe_2O_4$; x=0, 0.05, 0.1, 0.3 and 0.5) were prepared by solvothermal synthesis method. The XRD patterns of samples show single crystalline phase, with all the reflections corresponding to the cubic spinel structure. TEM analysis revealed the presence of sphere-like particles with equal diameter and distribution of diameter for all the samples ($<D_{TEM}>\sim 5$nm). The FT-IR analysis confirms the presence of oleic acid on the surface of the nanoparticles. Field dependence of magnetization recorded at 300 K show the superparamagnetic behavior of all synthesized samples, while M vs H recorded at 5 K show a hysteretic behavior with decrease of coercive field with increase of zinc content. Temperature dependence of magnetization, recorded by Zero Field Cooled and Field Cooled protocols, indicates that all the samples are superparamagnetic at room temperature. M_{ZFC} show a maximum for all the samples, with T_{max} decreasing with the increasing of Zn content. In order to study the influence of Zn content on the magnetic structure Mössbauer spectra has been recorded at low temperature (10 K) under an intense magnetic field (8T). These measurements evidenced the modification of inversion degree, with the content of iron in A site decreasing with the increase of Zn content. This induce also a change in magnetic disorder, with a non-monotonic behavior of the mean canting angle.

Transition Metal Oxide Heterostructures with Photo-Catalytic Activity

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We are living in the age when feasible methods and materials are searched for active pollution degradation. One of proposed solutions to the problem is photocatalytically active materials and pollution degradation due to availability of the Sun light. Stable and active materials are necessary to manage feasible photoanodes for effective energy conversion to split chemical bonds of pollutants.

It is well known that titanium dioxide (TiO_2) is a prominent material [1] as a photoanode with advantages of pronounced stability [2,3], accessibility, environmentally friendly with high photocatalytic activity [4,5], reduction and oxidation potentials. Nevertheless large band gap energy is responsible for low amount of catch solar light photons (mostly from near UV region) and pressed photo-activity accordingly [6]. Another prominent photoanode material widely researched recently [7] is iron oxide (hematite Fe_2O_3), with long lifetime of light-induced electron and hole pair, natural prevalence and, most importantly - lower band gap energy. Obvious choice next step is to create Fe_2O_3/TiO_2 structure to ensure activity under visible light, create higher charge separation with that higher photocatalytic activity. But to create a device feasible for use synthesis methods must be relatively simple and cost effective.

In this work Fe_2O_3/TiO_2 system was created using time and equipment efficient electrochemical methods. TiO_2 nanotubular substrate was synthesized using electrochemical anodization on titanium foil, whereas Fe_2O_3 deposited on TiO_2 galvanic deposition from electrolyte. Samples were heat treated to ensure crystallinity and the presence of necessary structures (anatase and hematite for TiO_2 and Fe_2O_3 accordingly). Morphological, optical, structural and electrochemical properties were studied. Conclusions on Fe_2O_3/TiO_2 electrochemically synthesized system synthesis properties, material electrochemical activity and composition as well as upscaling of synthesis were made.

Acknowledgment: Authors express their deep gratitude to Latvian National Research Program project LATENERGI for the financial support.

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Influence of temperature on structure and properties of lead titanate and bismuth titanate films

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Thin films of lead titanate and bismuth titanate have a great interesting and perspectives in application in electronics devices, such as: pyroelectric infrared detectors, capacitors, ultrasonic transducers, thermistors, optoelectronics, microsensors and actuators [1-2]. The most perspective applications of lead titanate and bismuth titanate are used in ultra-fast, very dense and non-volatile memory application (FRAM) [3-4].

Bismuth titanate and lead titanate thin films were deposited on heated platinized silicon substrates (400-550^{o}C) using in situ layer-by-layer reactive DC magnetron sputtering. The thickness was determined using Linnic micro-interferometer and tested with profilometer and SEM cross-section. The surface morphology of the films was analyzed using scanning electron microscope. The crystallographic structure of thin films was investigated by X-ray diffraction. Sawyer and Tower method for polarization–electric field (P-E) loop measurements were used for hysteresis loops measurements.

The results indicated that the surface morphology, structure and ferroelectric properties strongly depend on the formation temperature. Variation of the temperature allows controlling the structure of the films and obtaining the films with the highest ferroelectric properties. Hysteresis measurements showed that the highest coercive field of 150 kV/cm and the remnant polarization of 60 $\mu C/cm^2$ were reached for the lead titanate film produced at the 550 ˚C substrate temperature. The highest coercive field of 130 kV/cm and remnant polarization of 73 $\mu C/cm^2$ was obtained for the bismuth titanate film deposited at 450 ^{o}C.

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A comparative study of heterostructured CuO/CuWO$_4$ nanowires and thin films

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In this work we present the results of a comparative study of heterostructured CuO/CuWO4 core/shell nanowires and double-layer thin films, which were synthesised by a simple approach based on a two-step process. Amorphous WO3 thin layer was deposited first on top of CuO nanowires or thin film by reactive DC magnetron sputtering of tungsten, and high temperature annealing was used next to induce a solid-state reaction between CuO and WO3 resulting in a formation of CuWO4 phase. The morphology evolution of heterostructured core/shell nanowires and thin films upon heating was studied by scanning and transmission electron microscopies. A formation of crystalline CuWO4 phase around nanowires or at the thin film surface was observed upon annealing of CuO/WO3 system at 650ºC in air and is due to thermally stimulated diffusion of copper ions into WO3 layer, revealed in SEM-EDX analysis. The emergence of CuWO4 phase was confirmed by X-ray diffraction and confocal micro-Raman spectroscopy.

Resistive switching in $0.5Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.5(Ba_{0.7}Ca_{0.3})$/ZnO heterostructures

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Resistive random access memories (RRAMs) have been considered as one of the most potential candidates for next-generation non-volatile memories because of their remarkable characteristics such as low power consumption, high operation speed, high integration density and nondestructive readout. The intrinsic physical phenomenon behind RRAMs is resistive switching (RS). A wide variety of materials such as perovskite-type oxides, ferroelectric oxides and binary transition metal oxides (TMOs) has been extensively investigated [1]. However, RS effects in most of these materials are based on a certain type of defect (ionic or electronic) mediated phenomenon [2]. On the other hand, RRAMs based on ferroelectric-semiconductor heterostructures have been attracting considerable attention as an emerging non-volatile memory with ultrahigh density and operational speed [3]. In these heterostructures, low and high resistance states can be tuned via intrinsic switching of ferroelectric polarization without invoking the charged defect migration.

In this work, in-situ reflection high-energy electron diffraction (RHEED) was used to determine the growth mechanisms of $0.5Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.5(Ba_{0.7}Ca_{0.3})$ thin films deposited by pulsed lased deposition (PLD) on Nb:STO substrates. The RHEED pattern changes from streaks to spots, indicating that after 8.0 nm deposition the surface tends to become rougher. Moreover, the streaky pattern until the thickness exceeds 8.0 nm suggests the 2D growth mode, while after 8.0 nm deposition the growth mode changes from layer by layer to Stranski-Krastanow growth. The presence of the perovskite and wurzite phases of $0.5Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.5(Ba_{0.7}Ca_{0.3})$ and ZnO, respectively, was confirmed by X-ray diffraction measurements. The butterfly features of the capacitance–voltage characteristics and P-E hysteresis loops confirm the presence of ferroelectric nature in present heterostructures. An electroforming free RS was obtained in $0.5Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.5(Ba_{0.7}Ca_{0.3})$/ZnO heterostructures and its governing mechanisms are highlighted.

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TwinBeam PLD - new possibilities for advanced functional films

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At present the growth of thin films by using the PLD technique is limited to the availability of dense ceramic targets of the stoichiometric compounds. Some phases do not withstand the sintering conditions and therefore poorly sintered or composite targets are used instead. This may bring some problems of particle ejection and composition deviations in the growing film. Another typical problem in PLD arises when some element in the compound has a higher volatility (Pb, Bi, etc), which induces serious deviations in the film composition. This is normally compensated by preparing targets enriched in the volatile element, which needs to be adjusted for each deposition conditions. These limitations can be overcome by the use of simultaneous ablation of two targets to composit the final film material.

The new SURFACE Twin Beam PLD technology makes use of a dual laser beam of the same laser, separated by a laser beam splitter and a new target manipulator that combines three standard single targets (2"diameter) ablation with a Twin Beam target pair (2 x 1"diameter) position for the simultaneous ablation. The angle of the twin targets can be adjusted from a confocal to a cross beam configuration.

This new technology does not need a new PLD system, it is an available upgrade for all SURFACE PLD-Workstation systems. The new TwinBeam option includes only an upgrade of the standard target manipulator to the TwinBeam version. The necessary additional beam line is an extension to the existing one and the tuning of the fluence will be done with two manual or motorized laser beam attenuators. A software upgrade incorporates this new feature in the highly flexible PLUMEmaster user interface.

New process features are integrated and fully software controlled:

- software controlled in-situ fluence variation between the two targets
- fluence modulation of one beam synchron to the RHEED oscillation of the film growth
- synchronic variation of the plume angle at TwinBeam targets from a cross-beam1) to confocal plume to parallel plume orientation
- enhanced combinatorial features:
    - + in-situ composition spread deposition (ICSD) of two materials
    - + better material mix with no limitation of film thickness and no post-annealing step
    - + large fluence differences and modulation possible to combine metals with oxides

The TwinBeam option extends the flexibility of the SURFACE PLD workstation and is a powerful support of the SURFACE wedge heater which allows other combinatorial operations like wedge shaped films or deposition through shadow masks.

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MiniTonpilz : Device Application of Crystallographically Textured Piezoceramics

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Single crystals exhibit superior properties compared to the polycrystalline piezoelectrics with randomly oriented grains, but growth of single crystals is usually a difficult and expensive process. Thus, usually polycrystalline ceramics are used in many applications owing to their easier and cheaper processing methods. However, studies on textured polycrystalline ceramics with preferred grain orientation have increased in recent years. An anisotropy is developed as a result and properties that are comparable to the single crystal values are attainable in certain directions. Although there are numerous novel examples on textured piezoceramics in the literature, there are hardly any application examples of them. The main reason for this lack of application is the fact that the processing methods are limited in terms of possible shapes and dimensions. Thus, niche applications, where only thin ceramics are required, can provide the driving force for the practical implementation of textured piezoceramics.

In this study, textured $Pb(Mg_{1/3}Nb_{2/3})O_3$-$Pb(Zr,Ti)O_3$ (PMN-PZT) based piezoceramics were produced in thin, ring form by templated grain growth method using $BaTiO_3$ (BT) template particles with plate-like morphology. The BT template particles were synthesized in 3 steps using topochemical microcrystal conversion (TMC) method. The template particles were aligned in the fine grained PMN-PZT matrix by tape casting method. PMN-PZT ceramics with randomly oriented equiaxial grains have also been produced for comparison. Green tapes have been cut and laminated in ring form and sintered for densification and texture development.

A piezoelectric transducer in minitonpilz form with square aluminium head mass and cylindrical steel back mass was designed using finite element analysis and fabricated using two PMN-PZT piezoceramic rings. The rings were of either random or textured ceramics, for comparison. The bandwidth of the mintonpilz with textured ceramics was more than twice that of the random one, demonstrating the positive effect of texture on the physical properties and performance of the device.

WG3-2

Towards full-ceramic microdevices for oxygen sensing applications integrated in silicon

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The demand for solid state oxygen sensors is expected to undergo a huge increment in the next years in view of the more stringent legislation in terms of safety and emissions control, which requires their application in a number of new fields spanning from domestic systems to portable devices. However, state-of-the art sensors, which are based on the electrochemical response of bulky Yttria Stabilized Zirconia (YSZ) (lambda sensors), suffer from a series of intrinsic limitations related to their size (about 2 cm), to the operating temperature (above 400 ºC) and to the start-up response (≈10 s), which make them insufficient to respond to such future demands.

In this contribution, we present a novel concept for lambda sensors consisting of a cross-plane micrometeric device based on a self-sustained YSZ membrane. The device processing consists of the deposition of nanometric thin films (≈200 nm thick) of YSZ and ceramic electrodes on Si by means of large area PLD, combined with cleanroom microfabrication steps.

The proposed system addresses the main limitations regarding the "classical" lambda sensors, allowing for a drastic reduction of the material cost, of the thermal mass and of the operating temperature. Most importantly, a great flexibility in the selection of the ceramic electrode material and in the design (e.g. the possibility of introducing contact and heating paths) tackles some important issues related to the system mechanical and chemical stability and to the heat distribution.

Preliminary results related to film stress engineering, to the fabrication of differently shaped membranes, to their thermal response and to electrode materials are shown, demonstrating the potential of such nano-membrane architecture not only as a base for micro sensing device, but also opening up interesting opportunities for fundamental studies on oxide engineering and on their practical application in devices.

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WG3-3

Reduced Graphene Oxide - $LiFePO_4$ Composite Electrodes for Li-Ion Batteries

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Lithium ion battery market is estimated to currently be over US$30 bn. Although the portable electronics are currently driving the most growth of the market, electric vehicles and hybrid electric vehicles are also expected to become an increasingly significant branch of application. However, improvement of specific power and energy is still needed along with an increased material stability.

One of the most popular cathode materials for lithium ion batteries is $LiFePO_4$. It is also increasingly studied as a model material in order to uncover the fundamental characteristics and relations governing the behavior of lithium insertion materials in general. In this work we investigate the electrochemical properties of $LiFePO_4$/reduced graphene oxide (rGO) composite as a function of the composite preparation and morphology.

We find that the synthesis stage at which graphene oxide and $LiFePO_4$ are mixed has a significant influence on the electrochemical properties of the obtained cathode. More evenly distributed rGO sheets with more $LiFePO_4$ grains anchored on rGO lead to an increased rate capability. Such structures can be best obtained when mixing graphene oxide and $LiFePO_4$ at the initial synthesis steps.

Acknowledgment: Authors acknowledge Cooperation Project from Latvian Science Council No 2014/666 for the financial support.

Band offsets at the amorphous Al_2O_3 – $SrTiO_3$ interface

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The recent discovery of oxide 2D electron gases (2DEGs) at amorphous-crystalline oxide interfaces has attracted considerable interest. 2DEGs formed at such interfaces provide important input on the fundamental aspects of oxide 2DEGs, and they further provide a low-cost route towards applications in devices.

We used amorphous atomic layer deposition (ALD) Al_2O_3 on single crystalline $SrTiO_3$ as a simple model system, and investigated its electronic structure and underlying mechanisms. X-ray photoelectron spectroscopy has been employed for studying the chemical states and the electronic structure at the amorphous-crystalline oxide interface. Based on the spectroscopic data, the band gap was determined and significant barriers for electrons and holes (>1 eV) were observed. Our results highlight the advantages of ALD-Al_2O_3 as a robust insulator for oxide electronic devices.

Laser processing and its effect on thermoelectric materials based on CaMnO3

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Today a particular interest is given to the oxide-based thermoelectric materials, due to enhanced thermal and redox stability, attractive properties at high temperature, the absence of toxicity, and natural abundance of the constituent compounds [1,2]. The objective of this work is to assess the possibilities for processing oxide thermoelectrics through laser floating zone (LFZ) method, including identification of the appropriate treatment conditions and main structural and microstructural factors affecting the thermoelectric performance [3]. Known Nb- and La-substituted calcium manganite-based materials, possessing promising thermoelectric properties, were selected as a model system. Detailed structural (XRD) and microstructural (SEM/EDS) studies were performed for the samples, grown at various pulling rates. The results on electrical conductivity, Seebeck coefficient and thermal conductivity indicate that high thermoelectric performance can be triggered by laser processing. Long-term stability tests revealed gradual improvement of the electrical properties at high temperatures, including both increases in electrical conductivity and Seebeck coefficient. The effects provided by the pulling rate are discussed, and observed variations in electrical properties are attributed to the significant difference in redox conditions during processing and, possibly, the presence of frozen-in redox states. The obtained results clearly indicate a need the optimization of laser treatment conditions, when seeking high thermoelectric performance by LFZ processing of oxide thermoelectrics.

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Sb^{3+} ion as Effective Sensitizer of Blue, Green and Red Emission of $LaInO_3$-based Oxide Phosphors doped with Pr^{3+}, Ho^{3+} ions

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Single-phased $La_{1-x}Pr_xInO_3$ (x = 0.001, 0.002, 0.003), $La_{1-x}Ho_xInO_3$ (x = 0.03, 0.05, 0.07, 0.15) perovskite samples as well as samples of nominal composition of $La_{0.997}Pr_{0.003}In_{0.98}Sb_{0.02}O_3$, $La_{0.95}Ho_{0.05}In_{0.98}Sb_{0.02}O_3$ that contain a small amount of the impurity phase probably referred to $LaSbO_3$ were obtained by the solid-state reactions method from oxides. Their excitation and photoluminescence (PL) spectra were measured at room temperature using automatic spectrofluorimeter SDL-2. A DKsSh-120 xenon lamp was used as the excitation source. SEM-images of samples were obtained with scanning electronic microscope JEOL JSM – 5610LV. In the excitation spectra of all the samples obtained there were excitation bands located in the ultraviolet and visible spectrum regions. In the photoluminescence spectra of $La_{1-x}Ho_xInO_3$ (x = 0.03, 0.05, 0.07, 0.15) at λ_{ex} = 275 and 333 nm the maximum intensity of the green emission band of Ho^{3+} ions with λ_{max} = 543 nm was observed for the sample with x = 0.03. In the PL spectra obtained at λ_{ex} = 362 and 455 nm the maximum band intensity with λ_{max} = 543 nm has a $La_{1-x}Ho_xInO_3$ sample with x = 0.05. As for the $La_{1-x}Pr_xInO_3$ (x = 0.001, 0.002, 0.003) samples the maximum intensity of all photoluminescence bands in the PL spectra at λ_{ex} = 255 and 440 nm was observed for a sample with x = 0.003. It was established that the intensity of photoluminescence bands of $La_{0.997}Pr_{0.003}In_{0.98}Sb_{0.02}O_3$ at λ_{ex} = 445 nm, $La_{0.95}Ho_{0.05}In_{0.98}Sb_{0.02}O_3$ at λ_{ex} = 275, 333 and 455 nm is much higher than the intensity of the PL bands of $La_{0.997}Pr_{0.003}InO_3$, $La_{0.95}Ho_{0.05}InO_3$ samples respectively in which Sb^{3+} ions are absent. This can be caused by sensitization effect of Sb^{3+} ions on the of Pr^{3+} and Ho^{3+} ions PL. In the SEM-images of $La_{0.997}Pr_{0.003}In_{0.98}Sb_{0.02}O_3$ and $La_{0.95}Ho_{0.05}In_{0.98}Sb_{0.02}O_3$ samples no signs of impurity phase could be seen. All the samples were composed of spherical and ellipsoid particles with sizes around 0.5–2.5 μm. The samples obtained can be used as phosphors for white light emitting diodes, FED displays and other optoelectronic devices. In addition the samples investigated are magnetically dilute solid solutions in which the paramagnetic contribution of Pr^{3+}, Ho^{3+} rare-earth ions to the magnetization and magnetic susceptibility differ insignificantly from the diamagnetic contribution of the $LaInO_3$ matrix. Hence they can be used as new microelectronic and spintronic oxide materials.

Thermoelectric Properties of Layered Cobaltates and Perovskite Plumbates

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Layered cobaltates (Na_xCoO_2, $Ca_3Co_4O_{9+\delta}$, $Bi_2Ca_2Co_{1.7}O_y$ etc.) and perovskite plumbates ($BaPbO_3$, $SrPbO_3$) are the prospective materials for the high-temperature thermoelectric devices because of their high values of electrical conductivity and Seebeck's coefficient, low thermal conductivity and stability in air at high temperatures. Thermal, electrical, and functional properties of these phases can be essentially improved by substitution of different cations in their crystal structure. So study derivatives of these complex oxides is in scientific and practical interest.

We have prepared a number of solid solutions and composite materials based on layered cobaltates and perovskite plumbates – $Na_x(Co,M)O_2$, $(Ca,A)_3(Co,M)_4O_{9+\delta}$, $(Bi,Pb)_2Ba_2(Co,M)_2O_y$, $(Bi,Pb)_2Sr_2(Co,M)_{1.8}O_y$, $(Bi,Pb)_2Ca_2(Co,M)_{1.7}O_y$, $(Ba,Sr)Pb_{1+y}O_{3+2y}$ (M = transition and heavy metals, A = Bi, rare-earth metals) – and studied their phase composition, microstructure, thermal (thermal expansion, thermal diffusivity, thermal conductivity), electrical (electrical conductivity, thermo-EMF) and functional properties (power factor, figure-of-merit).

It was found that layered cobaltates are *p*-type conductors but perovskite plumbates are *n*-type conductors, and their conductivity character (metallic or semiconducting) depends on their composition and (for some samples) on temperature. The values of linear thermal expansion coefficients and apparent activation energy of conductivity of the samples were calculated as well as the electronic and lattice parts of thermal conductivity of the compounds were determined. The effect of preparation method, cationic composition, microstructure and temperature on the physic-chemical and functional characteristics of the samples investigated was analyzed. It was also found that creation of phase inhomogeneity in the layered calcium cobaltate $Ca_3Co_4O_{9+\delta}$ and $(Ba,Sr)Pb_{1+y}O_{3+2y}$ plumbates solid solutions improves their thermoelectric (functional) properties. It was shown that several of samples prepared due to their good thermoelectric properties are the promising candidates for p- and n-branches of high-temperature thermoelectroconverters. So, for instance, layered sodium cobaltate $Na_{0.89}CoO_2$ possesses high values of figure-of-merit at elevated temperatures ($ZT > 1$ at $T > 900$ K) and composite $Ba_{0.2}Sr_{0.8}Pb_{1.1}O_{3.2}$ ($Ba_{0.2}Sr_{0.8}PbO_3$ + PbO) has very large values of power factor at high temperatures ($P > 1$ mW/(m·K) at $T > 900$ K).

The work had been carried out at financial support of State Program of Scientific Investigations "Physical Materials Science, New Materials and Technologies", subprogram "Materials Science and Materials Technology", task 1.26, Ministry Education of Belarus Republic and Belarusian Republican Foundation for Fundamental Research.

Properties of Layered Bismuth Titanate with Aurivillius Phase Structure Doped by La or Pr

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Aurivillius phases ($Bi_2A_{n-1}B_nO_{3n+3}$) are a family of layered bismuth oxides which structure consists of perovskite-like blocks $[A_{n-1}B_nO_{3n+1}]^{2-}$ sandwiched between the bismuth oxide layers $[Bi_2O_2]^{2+}$ along *c* axis, where 12-fold-coodinated A-site is occupied by large mono, di, or trivalent cations, and oxygen octahedral coordinated B-site is occupied by small tetra, penta, or hexavalent cations, and *n* indicates the number of corner-sharing BO_6 octahedra forming the perovskite-like slabs. $Bi_4Ti_3O_{12}$ is three-layered Aurivillius phase which high Curie temperature ($T_C \approx 948$ K) and good ferroelectric properties in a wide temperature range allows us to consider it as a promising material for radio-, acusto-, and optoelectronics, suitable for manufacturing optical displays, piezoelectric transducers, radio capacitors as well as nonvolatile random access memories. It is known that functional properties of $Bi_4Ti_3O_{12}$ can be improved at partial substitution in its structure of bismuth by rare-earth element (REE) so study of structure and properties of $(Bi,R)_4Ti_3O_{12}$ (R = REE) solid solutions is very important problem.

In this work the $Bi_{4-x}R_xTi_3O_{12}$ (R = La, Pr; x = 0.05, 0.10, 0.15) solutions using solid state reactions method had been prepared, their crystal structure using X-ray diffraction and IR absorption spectroscopy had been studied, and their thermal expansion, electrical conductivity, thermo-EMF, dielectric constant and dielectric losses had been investigated in a wide temperature range.

According to the results of investigation of electrical properties of the $Bi_{4-x}R_xTi_3O_{12}$ solid solutions they are *p*-type semiconductors. It had been found that partial substitution of bismuth by lanthanum in $Bi_{4-x}La_xTi_3O_{12}$ solid solutions results in slight increasing of their lattice constants, decreasing of their Curie temperature, dielectric constant and dielectric losses, activation energy of electrical transport in them and slightly affects the values of their electrical conductivity, Seebeck' and linear thermal expansion coefficients. Substitution of bismuth by praseodymium in $Bi_{4-x}Pr_xTi_3O_{12}$ leads to the decreasing their Curie temperature, values of electrical conductivity and Seebeck' coefficient, dielectric losses and increasing of their dielectric constant. It had been found that $Bi_{3.95}R_{0.05}Ti_3O_{12}$ solid solutions was characterized anomalously low values of electrical conductivity, dielectric properties and linear thermal expansion coefficient among the samples studied.

The work had been carried out at financial support of State Program of Scientific Investigations "Physical Materials Science, New Materials and Technologies", subprogram "Materials Science and Materials Technology", task 1.17.

Nanostructured Fe_2O_3 , TiO_2 and reduced graphene oxide with excellent electrochemical performance as anode material for lithium ion batteries

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Two metal oxides, α-Fe_2O_3 and rutile phase TiO_2 with a particle diameter 50 nm and 21 nm respectively, were mixed with graphene oxide. Electrophoretic thin film deposition procedure from water suspension under potentiostatic mode was performed and the following composite thin films on a stainless steel substrate were obtained: α-Fe_2O_3/rGO, TiO_2/rGO, α-Fe_2O_3/TiO_2/rGO. Subsequently reduction of graphene oxide were performed. Thickness of acquired thin films were in the range of 2-6 μm. Electrochemical properties of all samples were studied by chronopotentiometry, cyclic voltammetry and electrochemical impedance spectroscopy. Gravimetric capacity was calculated for each synthesized material. Values of gravimetric capacity as well as rate capability after charge/discgarge cycles were figured out. Structure and morphology investigations for each sample were performed by SEM, AFM, XRD and Raman spectroscopy.

Our synthesized composite material α-Fe_2O_3/TiO_2/rGO showed excellent electrochemical properties for application as lithium ion battery anode material compared with a α-Fe_2O_3/rGO and TiO_2/rGO and as well as previously synthesized material containing α-Fe_2O_3 with a main particle diameter of about 150 nm. The results showed that the obtained composite material is a promising anode material for high energy and high power lithium ion batteries.

Acknowledgements

Authors acknowledge the Latvian Council of Science Cooperation Project No. 666/2014 for financial support.

WG3-11

Historical Summary about Researches of TMO in Electrochromic and Photoelectrochromic devices at ISSP UL

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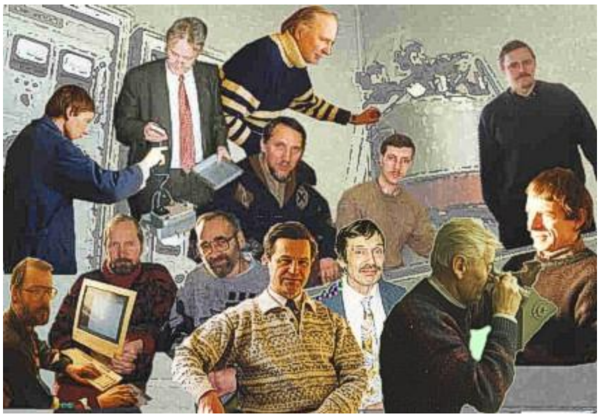
This report is devoted to the memory of Andrejs Lusis (1939-2017), Founder and Head of Semiconductor materials Department at Institute of Solid State Physics (1968-2017); also Founder of solid-state-ionics research school in Latvia. Andrejs Lusis together with Professor E.A. Ukshe (1928–1993) from Institute of Problems of Chemical Physics of the RAS (Chernogolovka, Moscow district) organized series of international scientific conferences "Fundamental problems of Solid State Ionics" in Latvia. The research direction, related with electrochromism in transition metal oxides (TMO) started at ISSP UL on 1972 on guidance of Andrejs Lusis and already first electrochromic devices were obtained in 1974 by J.Klavins, T.Zamozdiks, O.Rode. On the end of 1970th the Semiconductor Material Department of ISSP UL was largest and powerful scientific organization in previous Soviet Union, connected with electrochromic materials and devices. The prosperity period of Department was 1981-1990, when were defended 12 doctoral dissertations, 23 university diploma works in physics and chemistry, received 14 patent applications and published more than 200 scientific papers.

The main research subjects were amorphous tungsten oxide films (a-WO_3 films) themselves and in cells or in multi-layer thin film systems of type: indium–tin oxide ITO/WO_3/SiO_x/Au; ITO/CdS/WO_3/SiO_x/Au and ITO/WO_3/SE/MO_x/ITO, where SE is an proton conducting solid electrolyte based on solid antimony acid hydrate or hydrogen uranyl phosphate, and M – iridium or nickel. Morphologic, structural, optical, electric and magnetic properties of tungsten trioxide are investigated and mechanisms of electrochromic and photo-electrochromic phenomena explained. Thin film devices were cycled from colored to bleached states more than 10^6 times without remarkable degradation; electrochemical and optical properties studied using self-made equipment. Original apparatus with multichannel facilities was constructed and built at ISSP UL to study cycling and aging of electrochromic thin film systems.

Apparatus to cycle electrochromic systems with pulses of different length.



Main researchers at Semiconductor Materials Department of ISSP UL in 1990s

The radiation response of the high dielectric-constant hafnium silicate

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In this study, the electrical characteristics of the capacitors were determined by after series resistance correction C–V and G/ω–V measurements for several frequencies from 30 kHz to 2 MHz. Before the MOS capacitor was irradiated, the initial interface trap density (N_{it}) was evaluated from 2MHz frequency (HF) and 30 kHz frequency (LF) capacitance method and the N_{it} was calculated as $10.78x10^{11}$ cm^{-2}. This results show that $HfSiO_4$/p-Si interface quality is convenient for microelectronics applications. The Co-60 gamma irradiation responses of $HfSiO_4$ (MOS) capacitors were examined in various radiation doses. The 2 MHz C-V measurements of the samples were taken at each irradiation step and the radiation sensitivities of the devices were examined using flat band and midgap voltage shifts. Simple equivalent circuit model have been proposed for the MOS capacitor to determination interface and oxide the trapped charge. The radiation sensitivity of the $HfSiO_4$ MOS capacitors was found to be 4.41 mV/Gy for 300 nm-thick $HfSiO_4$ gate dielectric. Hafnium silicate is not sensitive as much as to radiation compared to SiO_2. Hence it may have important usage in high radiation field areas.

Keywords: $HfSiO_4$ MOS capacitors; Irradiation Hard Materials, Interface states, Oxide trapped

This work is supported Ministry of Development of Turkey under the contract number 2016K121110

Calcium manganite coatings for energy conversion

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Calcium manganite, $CaMnO_3$, is a ceramic material of perovskite structure with the attractive property of transformation of thermal into electric energy. But perovskite materials also have excellent properties as the absorption layer in photovoltaic cells. Most commonly researched are lead halides, which have poor stability when exposed to higher temperatures or humidity, and the synthesis of which involves harmful and toxic compounds. Calcium manganite is both chemically and thermally stable, as well as easily synthesised from widely accessible raw materials (i.e. calcium carbonate, $CaCO_3$ and manganese dioxide, MnO_2). Electron structure of $CaMnO_3$ makes it suitable for the absorption layer in photovoltaic cells, and its optical properties largely match those of a commonly used lead halide, which makes it an interesting alternative to those compounds. The goal of our research is to synthesise $CaMnO_3$ in a form suitable for thin film deposition (e.g. by doctor blade or spin-coating).
We have prepared crystalline $CaMnO_3$ powder by auto-combustion method (CMc) and by powder homogenisation (CMh). The first method consists in preparation of aqueous solution of nitrate salts of Ca^{2+} and Mn^{2+} with citric acid as a complexing agent and “fuel”. Upon boiling, the solution self-ignites due to decomposition of nitrates and rapid oxidation of the citric acid. The resulting ashes were found to contain $CaCO_3$ and probably poorly crystallized MnO_2. The second method consists in repeated homogenisation of mixture of pure $CaCO_3$ and MnO_2 powders in an agate mortar. Both the ashes and the homogenised mixture were calcined at 900 °C for 2 h in order to obtain fully crystallized perovskite structure. Resulting crystalline powders were $CaMnO_3$ with traces of $CaMn_2O_4$, with following mean particle diameter and specific surface area: 38 μm and 4.1 m^2/g for CMc and 226 μm and 4,3 m^2/g for CMh. Scanning electron microscopy (SEM) has shown that diameters correspond to sintered branched agglomerates of particles whose primary size is under 1 μm. Both powders were suspended in ethanol using ultrasonic agitation in order to obtain a stable suspension, and suspension of CMh has proven more stable. Suspension of CMh was deposited by drop-casting and the resulting coatings examined under SEM: quality was poor, and it will be necessary to obtain finer powders for this manner of $CaMnO_3$ deposition. Calcined CMh powder was compacted into a tablet and sintered at 1200 °C to obtain a target for pulsed laser deposition (PLD). There was no change in phase composition during sintering. PLD was carried out in a vacuum chamber using Nd:YAG laser with 1064 nm, 10 J/cm^2 and 5 Hz repetition rate. Thin film was deposited on a silicon substrate with 2000 laser pulses while distance between target and substrate was 3 cm. The film was characterised by grazing incidence X-ray diffraction. The results show that $CaMnO_3$ during the deposition process dissociates into CaO and most likely Mn_2O_3 with a bixbyite structure (space group Ia3). To avoid dissociation of deposited films we plan to further optimize PLD parameters such as laser wavelength, fluence and deposition atmosphere (addition of inert or reactive gas, deposition within plasma medium and deposition in with colliding laser plasmas).

This work has been supported in part by Croatian Science Foundation under the project (IP-2014-09-9419).

Anisotropic magnetoresistance in $La_{0.7}Sr_{0.3}MnO_3$ thin films

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The bypass of a damaged section of the spinal cord can be accomplished by detecting the neuronal signals before their reinjection into undamaged neurons. Among the various possible detections, magnetic detection has the advantage of being non-invasive unlike electrodes that measure the action potential of nerve impulses. In order to carry out the detection of the magnetic field of the neurons, which should be of the order of few nT or even below, the sensor must have excellent sensitivity at ambient temperature as well as being insensitive to external disturbances.

One major problem with low-field magnetic sensors is their low frequency noise, also named 1/f noise [1]. Thanks to the low 1/f noise the rare earth manganese oxides, such as $La_{0.7}Sr_{0.3}MnO_3$ (LSMO), may then find important applications in magnetoresistive sensors [2, 3]. In addition, LSMO exhibits a Curie temperature of about 350 K, which allows room temperature applications. In this paper, we will present our advances towards the optimization of LSMO-based low-noise magneto-resistive sensors. We measured the anisotropic magnetoresistance (AMR) and the low frequency noise in patterned LSMO thin films deposited on different substrates. Around zero field promising values of AMR could be measured. The corresponding magnetic detectivity at room temperature is equal to 25 $nT \cdot Hz^{-1/2}$ at 1kHz. These preliminary results open the route towards optimization of the AMR in LSMO thin films by optimizing thickness, anisotropy fields, bias current and geometries in order to lower the measured magnetic detectivity at values of $nT \cdot Hz^{-1/2}$, or below.

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FABRICATION AND CHARACTERIZATION OF CRYSTALLOGRAPHICALLY TEXTURED TERNARY PIN-PMN-PT PIEZOELECTRIC CERAMICS FOR NOVEL PIEZOELECTRIC APPLICATIONS

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Single crystal (1-x)Pb($Mg_{1/3}Nb_{2/3}$)TiO_3-xPbTiO_3 (PMN-PT) and xPb($In_{1/2}Nb_{1/2}$)O_3-(1-x-y) Pb($Mg_{1/3}Nb_{2/3}$)O_3-yPbTiO_3 (PIN-PMN-PT) ternary systems have been drawn attention in field of electronic device applications because of their giant piezoelectric coefficient and outstanding coupling factors of <001> direction. The Curie temperature (T_c) of PMN-PT is reported in literature between 130-170°C, which is restricted to application areas. PIN-PMN-PT ceramics have a thermal stability and Tc chances from 160°C up to 320°C with regard to composition in morphotropic phase boundary (MFB) [1,2]. However, single crystal growth techniques are required high cost equipment and show stoichiometric deviations. The crystallographic textured ceramics exhibits higher electrical properties than conventional ceramics which is comparable with single crystal [3].

In this study, textured pure 0.26Pb($In_{1/2}Nb_{1/2}$)O_3-0.40Pb($Mg_{1/3}Nb_{2/3}$)O_3-0.34PbTiO_3 (PIN-5BT) and 1.5 mol. % doped (PIN-5BT-1.5Mn) ceramics were synthesized by templated grain growth method (TGG) by using 5 vol % plate-like $BaTiO_3$ (BT) templates. Random and textured PIN-PMN-PT ceramics were sintered at 1150oC for 6 h. Lotgering factors of the both textured, PIN-5BT and PIN-5BT-1.5Mn ceramics were obtained as 94%, respectively. The maximum field induced bipolar strain of PIN-R, PIN-T5, PIN-1.5Mn and PIN-T5-1.5Mn was measured as 0.16%, 0.25%, 0.12% and 0.24%at 40kV/cm, respectively.

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The metal oxide resistivity sensors are the most common sensors for reducing and oxidizing gases, due to their low cost, easiness of preparation and signal processing. The sensing properties of a metal oxide film depend on the surface roughness, porosity, crystallinity and some other factors, which differentiate for each preparation method. Moreover, the addition of noble nanoparticles on the surface of the films, improves the sensing properties of the films. In this work two different techniques were used to prepare thin films of metal oxides doped with noble metals and their sensing properties for different reducing gases were investigated. Namely we used the PLD technique and the Sol-gel technique to prepare metal oxide thin films (ZnO CuO etc) doped with noble metals. All the films are characterized and tested as gas sensors. A significant response to several concentrations of the analytes was demonstrated at temperatures lower than 200°C.

Investigation of Gamma Irradiation Response on Interface State and Series Resistance of Y_2O_3 MOS Capacitors for Future Radiation Sensors

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Investigation of gamma irradiation responses on interface state and series resistance of Y_2O_3 MOS Capacitors for future radiation sensor applications was studied and initial valuation of the Y_2O_3 dielectrics used in gamma radiation sensors was discussed. Charge trapping and relevant irradiation responses of the devices are significant for requirement of high-k dielectrics for a long-term dependability of high-k dielectric materials. Therefore, irradiation effects on the series resistance (R_s) and interface state (D_{it}) characteristics of the Y_2O_3 MOS capacitors were investigated and analyzed. The electrical improvements of the thin films were analyzed using capacitance-voltage (C-V) and conductance-voltage (G/ω-V) measurements. On the other hand, the composed oxide traps densities increase with irradiation while interface state density trend changes by irradiation. The results show that both series resistance (R_s) and interface state (D_{it}) characteristics critically varied with gamma irradiation. Positive Y^{+2} and Y^{+3} atoms ionized by irradiation, may be the reason of the composed trap densities in the device.

Design of transparent ZnO:Ga,Al,Bi thin film electrodes with thermoelectric properties

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One of the biggest challenges to face in the near future will be to meet the energy demand (+35% by 2030) in an economically, efficient, and environmentally responsible way [1]. Beyond the materials for photovoltaic systems, there is another class of materials under intense investigation, the thermoelectric [2]. These can convert thermal differences into electrical energy, or reciprocally, cool down. Recent research has demonstrated the effectiveness of ZnO-based coatings for thermoelectric applications [4-5]. In this work, ZnO:Ga,Al,Bi thin film electrodes were developed with the objective to enhance the efficiency of photovoltaic systems [3]. For this purpose, besides having good electric and thermoelectric properties, these thin films are need to be optically transparent. To do so, it is necessary to study and understand the inherent physical properties, such as, the electrical conductivity, transport properties (carrier concentration and mobility), and optical transmittance in the visible region, and establish the relation between these properties and the chemical composition, crystal structure and microstructure. Besides the theoretical considerations of the problem, it is described the production method and charge transport properties of several doped ZnO thin films deposited by magnetron sputtering. Furthermore, these results are correlated in view of XPS and ToF-SIMS characterization.

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