Second Short-Term Scientific Mission Workshop on Innovative and Advanced Epitaxy

Organized by European Network for Innovative and Advanced Epitaxy (OPERA), COST Action CA-20116

28 May 2024 (online workshop)

OPERA COST Action CA20116 | STSM

Second Short-Term Scientific Mission Workshop on Innovative and Advanced Epitaxy

The COST Action CA-20116, European Network for Innovative and Advanced Epitaxy (OPERA), is supporting Short-Term Scientific Missions (STSM) to give the opportunity to Researchers or Innovators to carry out specific scientific tasks in a host organization for a well-defined period of time. Since the beginning of the action in September 2021, the Cost Action OPERA has funded near 60 Researchers/Innovators all around Europe.

On May 28, 2024, at 14:00 pm (CEST), the second online STSM workshop will take place. There, 8 STSM grantees will present their experience and results.

Do not hesitate to connect to this STSM workshop!

Link to the meeting by Teams:

https://teams.microsoft.com/l/meetup-join/19%3ameeting_YWQxZjIwYWMtOGZlYy00MjdhLWJmZWUtNmZmMGE2OGZiMTUw%40thread.v2/0?context=%7b%22Tid%22%3a%226afea85d-c323-4270-b69d-a4fb3927c254%22%2c%22Oid%22%3a%225aee3742-8c4b-483d-b9d8-e20290244937%22%7d

The STSM Team and OPERA COST Chair

STSM team members: Sergio Fernández Garrido (STSM Leader), Zoran Jovanović (STSM Vice-Leader), Noelle Cogneau (Action Chair), Tamara Potlog (Action Vice-Chair), Yamina André (Grant Holder Scientific Representative), Laurence Mechin (Grant Awarding Coordinator), Paula Ferreira (Science Communication Coordinator), Gavin Bell (WG1 Leader), Nini Pryds (WG2 Leader), Susana Cardoso (WG3 Leader), Lucian Pintilie, Gertjan Koster, Lucia Sorba, Marta Sawicka and Brian Rodriguez.

Second Short-Term Scientific Mission Workshop on Innovative and Advanced Epitaxy

Program, Tuesday 28 May 2024 (CEST times)

14:00 Opening

14:10 Speaker: Alfredo Blázquez Martínez

Title: Growth of $BiFeO_3$ thin films by pulsed laser deposition

14:25 Speaker: Yu Liu

Title: Superlattice Structural Domain Engineering by Pulsed Laser Deposition

14:40 Speaker: Damian Brzozowski

Title: Structural engineering of LSMO thin films – towards magnetic oxide-topological insulator heterostructures

14:55 Speaker: Matthew P. Wells

Title: Vertically aligned nanocomposite thin film cathodes for reducing critical raw material use in commercial solid oxide fuel cells

15:10 Speaker: Giada Bucci

Title: Zincblende InAsP/InP quantum dots nanowires for Telecom wavelength emission

15:25 Speaker: Mikołaj Chlipała

Title: The influence of metal surfactants on Ge incorporation in AlGaN – the path to UV emitters

15:40 Speaker: Mikołaj Żak

Title: On the path to nanowire-LED hybrid devices emitting single photons

15:55 Speaker: Nayara Carral-Sainz

Title: Second Principles Density Functional Theory Models including first and second order electron-lattice interactions

16:10 Closing remarks

Second Short-Term Scientific Mission Workshop on Innovative and Advanced Epitaxy

Abstracts

Growth of $BiFeO_3$ thin films by pulsed laser deposition

Authors: Alfredo Blázquez Martínez[1], Torsten Granzow[1], Ipek Efe[2], and Morgan Trassin[2]

STSM home institution: [1]Luxembourg Institute of Science and Technology, Luxembourg

STSM host institution: [2]ETH Zürich, Switzerland

Summary: Epitaxial BiFeO3 thin films were grown by pulsed laser deposition on (100) and (111) $SrTiO_3$ single-crystal substrates. A $SrRuO_3$ layer was used as bottom electrode and to promote a stripe-like ferroelectric domain pattern. Additionally, the fabrication of free-standing films was attempted using a $Sr_3Al_2O_6$ sacrificial layer. The films were characterized by X-ray diffraction and piezoresponse force microscopy.

Superlattice Structural Domain Engineering by Pulsed Laser Deposition

Authors: Yu Liu[1], Gregory Nordahl[2], Susanne Boucher[2], Emma van der Minne[3], Thea Marie Dale[2], Chris Baeume[3], Gertjan Koster[3], Magnus Nord[2], and Ingrid Hallsteinsen[1]

STSM home institution: [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology, Norway

STSM host institution: [3]Department of Inorganic Materials Science, MESA+ Institute for Nanotechnology, Univeristy of Twente, Enschede, The Netherlands

Other institutions involved: [2]Department of Physics, Norwegian University of Science and Technology, Norway

Summary: Transition metal perovskite oxide heterostructures are of great interest for improved device performance from emerging properties due to various effects when coupled. Structural domain can have major implication in functionalities, that can be undesired if not intended. In this work, we present our ongoing work that in part thanks to OPERA-STSM made this possible, on domain engineering in $LaFeO_3$/LSMO/$DyScO_3$(101) superlattices. Where anisotropic strained superlattice forms structural domains without visible structural defects. By inserting a thin buffer layer of $DyScO_3$ per repetition, we were not able to see the domain contrast in 4D-STEM as for the previous sample. The work on growth, AFM and XRD (line scan and RSM) are carried out by the grantee, where growth is done at University of Twente, IMS group. E.v.d Minne are credited for incoming user training.

Second Short-Term Scientific Mission Workshop on Innovative and Advanced Epitaxy

Structural engineering of LSMO thin films – towards magnetic oxide-topological insulator heterostructures

Authors: Damian Brzozowski[1], Felix Trier[2], Daesung Park[2], and Ingrid Hallsteinsen[1]

STSM home institution: [1]Norwegian University of Science and Technology (NTNU), Norway

STSM host institution: [2]Technical University of Denmark (DTU), Denmark

Summary: Pulsed laser deposition system (PLD) was used to grow ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) perovskite oxide films. The films were deposited onto SrTiO3 (STO) substrates with (001) and (111) crystallographic orientations. A series of thin films with varying thicknesses were grown to compare growth dynamics and magneto-structural properties. The in-situ reflection high-energy electron diffraction (RHEED) technique was employed to determine the growth rate and film thickness. Surface morphology was studied using atomic force microscopy (AFM) and x-ray diffraction (XRD). Fully strained epitaxial films were obtained for both crystallographic orientations, preserving clear step-terrace structure of the substrate. X-ray reflectivity (XRR) analysis and fitting confirmed film thicknesses estimated with in-situ RHEED. Temperature-dependent magnetization and low-temperature hysteresis characterization was performed to determine macroscopic magnetic properties, including the magnetic saturation, coercive field, and critical temperature. The films are the initial step for further realization of LSMO-$Bi2Te_3$ heterostructures for investigating magnetic oxide – topological insulator interactions.

Vertically aligned nanocomposite thin film cathodes for reducing critical raw material use in commercial solid oxide fuel cells

Authors: Matthew P. Wells[1], Kosova Kreka[2], Albert Tarancón[2,3], and Judith L. MacManus-Driscoll[1]

STSM home institution: [1]Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom.

STSM host institution: [2]Catalonia Institute for Energy Research (IREC), Department of Advanced Materials for Energy, 1 Jardins de les Dones de Negre, Barcelona 08930, Spain

Other institutions involved: [3]ICREA, Passeig Lluís Companys 23, Barcelona, 08010, Spain

Summary: Low temperature solid oxide cells (SOCs) represent a key technology in next-generation energy devices for portable applications, offering the highly efficient conversion of electrical to chemical energy (e.g. hydrogen), and vice versa. To date, the widespread implementation of SOCs, and therefore the use of hydrogen as a portable energy storage solution, has been prohibited by excessive polarisation resistances at the

device electrodes, together with a heavy dependence on critical raw materials such as La, Co, and Sr. Here, we explore the growth and characterisation of vertically aligned nanocomposite (VAN) films to as thin-film SOC electrodes. State-of-the-art materials are combined in unique nanocomposite structures and the enhancement rendered with respect to equivalent planar films is quantified by electrochemical impedance spectroscopy (EIS). Films are then integrated with commercial SOCs, demonstrating that conventional 'bulk' electrodes can be replaced with VAN thin films, resulting in a 99.5% reduction in critical raw material use. This allows for a detailed study of the VAN growth mechanisms for materials of differing crystal structures, while also giving an improved understanding of the importance of crystalline perfection in thin-film µSOC device performance. Future progress in low-temperature µSOC technology will rely heavily on a detailed understanding of the mechanisms underpinning the performance enhancements achieved in such nanocomposite thin films. Therefore, by building an understanding of the growth mechanisms of state-of-the-art nanostructured materials and quantifying the performance enhancements resulting from a wide variety of VAN structures, this study represents an important step towards the realisation of efficient low-temperature µSOCs for portable applications.

Zincblende InAsP/InP quantum dots nanowires for Telecom wavelength emission

Authors: Giada Bucci[1] ,Valentina Zannier[2], [3]Francesca Rossi, [4]Anna Musiał, [4]Jakub Boniecki, Grzegorz Sęk, and [2]Lucia Sorba

STSM home institution: [1]Scuola Normale Superiore di Pisa, 56127 Pisa, Italy

STSM host institution: [4]Department of Experimental Physics, Wrocław University of Science and Technology, 50-370 Wrocław , Poland

Other institutions involved: [2]NEST, Istituto Nanoscienze-CNR, 56127 Pisa, Italy, [3]IMEM-CNR, Parco Area delle Scienze, 43124 Parma, Italy

Summary: InAsP quantum dots (QDs) embedded in InP nanowires (NWs) have been investigated as a platform for emission at the telecom wavelength, with potential applications in quantum information technology. Typically, InAsP QDs have been grown along the <111>B direction InP NWs characterized by a wurtzite crystal structure. However, NWs grown along the <111> direction suffer for the easy formation of stacking faults, which strongly affect the optical properties of the QD. Conversely, InP NWs grown along the <100> direction show a pure zincblende (ZB) crystal phase for a wide range of growth conditions and diameters. In my contribution, I will present and discuss the epitaxial growth of defect-free ZB InAsP QDs in InP NWs employing Au-assisted vapor-liquid-solid growth in a Chemical Beam Epitaxy system. Employing micro-

photoluminescence measurements, the tunability of the emission as a function of the QD composition and dimension is demonstrated, remarkably observing an emission at the telecom O-band.

The influence of metal surfactants on Ge incorporation in AlGaN – the path to UV emitters

Authors: Mikołaj Chlipała[1], Henryk Turski[1], Eva Monroy[2], and Jesus Cañas[2]

STSM home institution: [1]Institute of High Pressure Physics Polish Academy of Sciences ul. Sokolowska 29/37 01-142, Warsaw, Poland

STSM host institution: [2]Quantum Photonics, Electronics and Engineering Laboratory (PHELIQS), CEA-IRIG, 17 av. des Martyrs, 38054, Grenoble cedex 9, France

Summary: The recent COVID outbreak has caused a greater interest in UV LEDs as a reliable and efficient disinfection solution. Doping is one of the most significant issues that high Al-content AlGaN-based emitters face. The goal of this work is to explore the influence of metal surfactants on Ge incorporation in AlGaN, grown by plasma-assisted molecular beam epitaxy (PAMBE). This will be the first step to realizing the idea of UV LED and tunnel junctions. Four samples were grown, two GaN and two AlGaN with 30% of Al content doped with Ge. We varied the growing conditions by changing the metal surfactant on the surface, two utilized In as a surfactant, while the other two employed Ga. Preliminary findings obtained from Hall measurements and secondary ion mass spectrometry indicate that the utilization of In as a surfactant yields a more uniform incorporation of Ge.

On the path to nanowire-LED hybrid devices emitting single photons

Authors: Mikołaj Żak[1], Marcin Siekacz[1], Czesław Skierbiszewski[1],
Amalia Fernando-Saavedra[2], Miguel A. Sanchez-Garcia[2], and Enrique Calleja[2]

STSM home institution: [1]Institute of High Pressure Physics Polish Academy of Sciences, Poland

STSM host institution: [2]ETSI Telecomunicación, Universidad Politécnica de Madrid, Spain

Summary: Single photon sources (SPSs) are key components of almost all new quantum technologies, such as linear optical quantum computing, quantum key distribution and quantum memories. Developing SPS requires a nanoscale control of the device making process e.g. with molecular beam epitaxy. As shown by a group from the Polytechnic University of Madrid, it is possible to achieve single photon emission (SPE) at temperatures below 80K from optically pumped quantum dots (QDs) located in InGaN/GaN core-shell nanowires. On the other hand, at the Institute of High Pressure

Physics we are able to produce very efficient LEDs that operate at cryogenic temperatures. The STSM in Miguel A. Sanchez-Garcia's groups has allowed work to begin on the fabrication of a hybrid device in which QDs will be optically pumped by an LED placed below the NW. During this talk, I will present the concept of this hybrid devices and show the preliminary results.

Second Principles Density Functional Theory Models including first and second order electron-lattice interactions

Authors: Nayara Carral-Sainz[1], Javier Junquera[1], Pablo García-Fernández[1], and Philippe Ghosez[2]

STSM home institution: [1]Universidad de Cantabria, Spain

STSM host institution: [2]Université de Liège, Belgium

Summary: From first principles, as DFT, simulations at operating conditions as finite temperatures or electric fields remain practically limited by computational resources to very small length and time scales. To overcome these limitations, a first-principles-based method called Second-Principles has been developed. Second-Principles are based on a parametric tight-bindding Hamiltonian model where geometry distortions in systems are caught by first and second order electron-lattice parameters computed through finite differences in real-space. The finite differences formulas are fed with data from first-principles calculations characterized by specific atomic displacements with respect to a reference atomic geometry. According to stress distortions, one might think these can be captured by the previous electron-lattice parameters. However, as atoms are located farther away from the origin, atomic displacements relative to the reference atomic structure increase significantly, leaving the perturbative regime. At this juncture, the aim is to determine the term in our Hamiltonian model capable of accurately capturing the effects of strain.