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

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

3 April 2025 (online workshop)

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

The COST Action CA-20116, European Network for Innovative and Advanced Epitaxy (OPERA), supports Short-Term Scientific Missions (STSMs), providing Researchers and Innovators with the opportunity to carry out specific scientific tasks at a host organization for a well-defined period.

Since the launch of the action in September 2021, COST Action OPERA has funded more than 80 Researchers and Innovators across Europe.

On April 3, 2025, at 14:45 (CEST), the third online STSM workshop will take place, where 11 STSM grantees will present their experiences and results.

Don't miss the opportunity to join us for this STSM workshop!

Link to the meeting by Teams:

https://teams.microsoft.com/l/meetup-join/19%3ameeting_MTM3NzZjMzAtMjYzYS00YmY0LTk1MDMtMzE0ZTA0MDZlNDc5%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.

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

Program, Thursday 3 April 2022 (CEST times)

14:45 Opening

14:55 Speaker: Aysha Riaz

Title: Investigating and engineering surface band bending of MBE-grown semiconducting oxide layers as a tool to tailor electronic contact properties

15:10 Speaker: Nataša Tomić

Title: Nanostructured functional oxide thin films TiO_2 and V_2O_5 for photocatalytic and energy applications

15:25 Speaker: Safya Elsharkawy

Title: Designing Multilayer Perovskite Oxides through Advanced Epitaxy for Enhanced Oxygen Evolution Electrocatalysts

15:40 Speaker: Iris C. G. van den Bosch

Title: Model system electrocatalysts for operando characterization at oxygen evolution reaction potentials

15:55 Speaker: Marlene Anzengruber

Title: Pushing the limits of µSOFCs – from freestanding thin films to single repeating units

16:10 Speaker: Lamiya Balayeva

Title: Manufacturing and Investigation of Epitaxial Layer based on Boron-Doped GaSe Thin Film

16:25 BREAK

16:45 Speaker: Calisa Carolina De Oliveira

Title: Epitaxial Growth and Characterization of Graphene over SiC

17:00 Speaker: Karl Graser

Title: The growth of dislocation filter layers for the epitaxy of III-Sb on Si for in-situ microscopy investigations

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17:15 Speaker: Oliver Rehm

Title: Towards in-operando HAXPES of ferroelectric AlScN-based capacitors

17:30 Speaker: Elçin Akar

Title: Top-down fabrication of nanowires containing a GaN-based p-n junction for advanced microscopy studies

17:45 Speaker: Žarko Gačević

Title: Selective area growth of GaN nanowires on GaN-on-sapphire pseudosubstrates

18:00 Closing remarks

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Abstracts

Investigating and engineering surface band bending of MBE-grown semiconducting oxide layers as a tool to tailor electronic contact properties

Authors: Aysha Riaz[1], Andrea Ardenghi[2], Georg Hoffman[2], Anna Regoutz[1] and Oliver Bierwagen[2]

STSM home institution: [1]University College London (UK)

STSM host institution: [2]Paul Drude Institute for Solid State Electronics (Germany)

Summary: The objective of this work was to explore the impact of wet oxygen annealing on the surface band bending of semiconducting layers grown by molecular beam epitaxy (MBE) and its correlation to contact properties. Surface treatment of both (-201) and (100) epitaxially grown β-Ga_2O_3 was conducted by dry oxygen annealing (60 min, 900°C) and wet oxygen annealing (30 min, 600°C) in a tube furnace under O_2 flow. Contact properties of the samples were investigated using a four-point probe and measuring the current-voltage (I-V). To correlate contact properties with surface band bending, X-ray photoelectron spectroscopy (XPS) was measured to observe core level shifts relative to the EF.

Nanostructured functional oxide thin films TiO2 and V2O5 for photocatalytic and energy applications

Authors: Nataša Tomić[1], Zorica Konstantinović[1], Borivoje Vasić[1], Milica Vujković[3], Lluis Balcells[2] and Benjamin Martinez[2]

STSM home institution: [1]Institute of Physics Belgrade (Serbia)

STSM host institution: [2]Institute of Materials Science of Barcelona ICMAB-CSIC (Spain)

Other institutions involved: [3]Faculty of Physical Chemistry (Serbia)

Summary: Topics dealing with Energy and Environmental issues will be always of great importance. Research is highly oriented towards designing TiO_2 and V_2O_5 thin films with improved photocatalytic and electrochemical properties. Vacuum deposition methods (RF sputtering and/or laser deposition-PLD) were used under different growth atmosphere (argon, oxygen) in order to examine their influence on structural properties

and crystallinity of obtained nanomaterials. ITO glass was used as a substrate, while pure metal foil of Ti and V were used as target materials. Besides the morphology analysis, the final goal of this research was to analyse how these growth conditions affect the photocatalytic activity of TiO_2 thin film in degradation process of organic dye Reactive Orange (RO16) and to test V_2O_5 thin film as an electrode material in Li-ion battery for Energy storage.

Designing Multilayer Perovskite Oxides through Advanced Epitaxy for Enhanced Oxygen Evolution Electrocatalysts

Authors: Safya Elsharkawy[1], Ellen M. Kiens[2] and Christoph Baeumer[2]

STSM home institution: [1]Faculty of Non-Ferrous-Metals, AGH University of Krakow, al. Mickiewicza 30, 30-059 Krakow (Poland)

STSM host institution: [2]MESA+ Institute for Nanotechnology, Faculty of Science and Technology, University of Twente, Enschede (Netherlands)

Summary: Epitaxial thin films of perovskite oxides, including $LaCoO_3$ and $LaNiO_3$, were synthesized on $SrTiO_3$ substrates using pulsed laser deposition (PLD). Multilayer structures incorporating $LaAlO_3$ as an insulating layer were also fabricated with precise unit-cell control. X-ray diffraction (XRD) and atomic force microscopy (AFM) confirmed high crystallinity and smooth morphology. The oxygen evolution reaction (OER) performance was evaluated in purified, iron-free KOH electrolyte using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). Among the tested structures, the three-layer configuration ($LaAlO_3$/$LaCoO_3$/$LaNiO_3$) exhibited the best OER activity, correlating with its lowest charge transfer resistance. Additionally, the electrochemical performance was studied at different pH values (12, 13, and 14), revealing a positive pH dependence, where increasing alkalinity enhanced catalytic activity. These findings highlight the influence of multilayer design and pH conditions on perovskite oxide electrocatalysts, emphasizing the need for fresh electrolyte use to ensure reliable measurements.

Model system electrocatalysts for operando characterization at oxygen evolution reaction potentials

Authors: Iris C. G. van den Bosch[1], Edwin Dollekamp[2], Nini Pryds[2] and Chris Baeumer[1]

STSM home institution: [1]University of Twente (The Netherlands)

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

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

Summary: The electrochemical water-splitting, needed to reach sustainability goals, is limited by the sluggish kinetics of the oxygen evolution reaction. Using electrocatalysts this hurdle can be reduced. Traditionally, catalysts are optimized using so-called descriptors that relate electronic structure to activity. However, this approach is limited, because their composition and electronic structure are different during the reaction compared to the pre/post-catalyst. Therefore, we will utilize operando x-ray absorption spectroscopy to investigate the catalyst at operating conditions. Here we will demonstrate a measurement geometry and catalyst design that allows for illumination through the back of a thin, x-ray-transparent catalyst membrane. Preventing measurements through the electrolyte, which is a large x-ray absorber. This catalyst will be an epitaxial thin film model system, grown on a single-crystalline substrate with a sacrificial layer. By dissolving the sacrificial layer the catalyst thin film can be transferred onto x-ray transparent substrates. This enables operando x-ray studies of epitaxial model electrocatalysts.

Pushing the limits of µSOFCs – from freestanding thin films to single repeating units

Authors: Marlene Anzengruber[1], Benedikt Winter[2], Kosova Kreka[1], Isabell Schloder[2], Raimund Förg[2] and Albert Taracon[1]

STSM home institution: [1]Institut de Recerca en Energía de Catalunya – IREC (Spain)

STSM host institution: [2]Technische Hochschule Deggendorf - THD (Germany)

Summary: The performance of solid oxide fuel cells (SOFC) is governed by the efficiency and dependability of the oxygen transport pathways within the material. The reduction of the vertical dimension in freestanding thin films results in an increased surface-to-volume ratio thus presenting an attractive optimization approach which is being exploited for the fabrication of low to intermediate temperature SOFCs. Existing challenges in traditional bulk oxide materials, like restricted kinetics at moderate temperatures and limited mechanical flexibility, are being addressed by the introduction of freestanding thin films based on the release from the original substrate via sacrificial layers. Hereby, microstructure and chemical composition can be tailored explicitly during Pulsed Laser Deposition. During the STSM the growth and release of high-quality thin films with vertical dimensions of well below 1 µm could be achieved. Subsequently, the fully functional freestanding SOFC membranes were encapsulated in a single repeating unit.

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Manufacturing and Investigation of Epitaxial Layer based on Boron-Doped GaSe Thin Film

Authors: Lamiya Balayeva[1] and Elias Stathatos[2]

STSM home institution: [1]Baku State University (Azerbaijan)

STSM host institution: [2]Electrical and Computer Engineering Department, University of the Peloponnese (Greece)

Summary: The Short-Term Scientific Mission (STSM) focused on synthesizing and studying boron-doped GaSe crystals and their epitaxial layers. GaSe and $Ga_{1-x}B_xSe$ (x = 1, 3, 5%) crystals were prepared using vapor-phase epitaxy (VPE) to form homoepitaxial layers. Structural and optical properties were analyzed using X-ray diffraction (XRD), scanning electron microscopy (SEM), and optical measurements. XRD revealed new peaks (2θ = 47.55° and 54.102°), confirming successful boron incorporation into the GaSe lattice. SEM images showed reduced layer thickness and modified surface morphology due to boron doping, indicating structural and electronic property changes. Optical measurements highlighted improved absorption in boron-doped layers, suggesting enhanced optical properties. Although photoluminescence spectra could not be obtained due to instrument limitations, other goals were achieved, providing valuable insights. Discussions on future collaborations and joint publications were initiated, with plans to further explore boron-doped GaSe for high-performance photodetectors. The findings hold promise for advancing photodetector technology.

Epitaxial Growth and Characterization of Graphene over SiC

Authors: Calisa Carolina De Oliveira[1], Vlado Lazarov[2], Andrew Pratt[3] and Amilcar Bedoya-Pinto[4]

STSM home institution: [1]University of Valencia (Spain)

STSM host institution: [2,3]University of York (England)

Summary: The work to be presented focuses on the growth of graphene through thermal treatment in an Ultra High Vacuum (UHV) system, made possible by the short-term scientific mission (STSM) at the host institution, the University of York. The research includes in-situ structural characterization using Low-Energy Electron Diffraction (LEED). Additionally, post-treatment evaluations are conducted ex-situ using techniques such as Raman spectroscopy and Atomic Force Microscopy (AFM) for structural and morphology characterization. This study contributes to a broader understanding of graphene production under controlled vacuum conditions, providing a foundation for the future reproduction and optimization of the methodology at our home institution (University of Valencia) using the Molecular Beam Epitaxy (MBE) method to achieve a high-quality

monolayer of graphene. Furthermore, this presentation aims to outline the next steps in our research, focusing on establishing a framework for nanoscale device production and exploring superfluidity and spin transport within graphene-based systems.

The growth of dislocation filter layers for the epitaxy of III-Sb on Si for in-situ microscopy investigations

Authors: Karl Graser[1], Audrey Gilbert[2], Jean-Baptiste Rodriguez[2], Eric Tournié[2] and Achim Trampert[1]

STSM home institution: [1] Paul-Drude-Institut für Festkörperelektronik, Leibnitz Institut im Forschungsverbund Berlin e.V. (Germany)

STSM host institution: [2] Institut d'Electronique et des Systèmes, Université de Montpellier (France)

Summary: The heteroepitaxy of III-V semiconductors on Si(001) paves the way for various photonic devices integrated into Si circuits. However, III-Sb-based structures face significant challenges due to their large lattice mismatch with Si, which leads to a high density of threading dislocations that degrade device performance. In collaboration with our French partners, we are investigating the use of AlSb dislocation filter layers embedded in GaSb on Si to reduce threading dislocations. During the STSM, specific filter layer samples were synthesized, and ECCI measurements were conducted on the grown samples. Back at the home institution, these ECCI results were correlated with STEM investigations to analyze the interaction between threading dislocations and misfit dislocations formed at the AlSb filter layer interfaces. Additionally, in-situ heating STEM experiments were performed to observe the effect of temperature on these dislocation structures, providing deeper insights into their behavior and reduction mechanisms.

Towards in-operando HAXPES of ferroelectric AlScN-based capacitors

Authors: Oliver Rehm[1], Mehrdad Farahani[2], Ignasi Fina[2], Florencio Sánchez[1] and Martina Müller[1]

STSM home institution: [1]Universität Konstanz (Germany)

STSM host institution: [2]The Institute of Materials Science of Barcelona ICMAB-SCIC (Spain)

Summary: During my Short-Term Scientific Mission (STSM) at the Institute of Materials Science of Barcelona (ICMAB-CSIC), I acquired hands-on experience with ferroelectric switching measurements utilizing the Aixacct TF3000 system and probe station.

My research concentrated on exploring the frequency and voltage dependence of ferroelectric switching in HfO_2 and AlScN-based capacitors, which is a crucial preparatory step for conducting in-operando hard X-ray photoelectron spectroscopy (HAXPES) experiments at a synchrotron facility. I discovered a significant correlation between the switching response, frequency, and applied voltage, which provided vital insights for optimizing experimental conditions. After my STSM, I conducted the first in-operando HAXPES measurements on ferroelectric AlScN, revealing a strong voltage-induced oxidation. Analysis of pre-cycled devices further uncovered local chemical changes and global energy shifts, providing insights into ferroelectric breakdown mechanisms.

Top-down fabrication of nanowires containing a GaN-based p-n junction for advanced microscopy studies

Authors: Elçin Akar, Amine Arsalane, Matteo Knebel, Marcin Siekacz, Anna Feduniewicz-Żmuda, Grzegorz Muzioł, Czeslaw Skierbiszewski, Martien Ilse Den Hertog, and Eva Monroy

STSM home institution: Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) (France)

STSM host institution: Institute of High Pressure Physics (IHPP) of the Polish Academy of Sciences (Poland)

Summary: This mission aimed to study the electrical behavior of top-down p-n junction GaN nanowire using correlated microscopy techniques. With this purpose, I contributed to growing planar GaN LED structures (p-n junction) via plasma-assisted molecular beam epitaxy at the Host Institution. The sample structures were designed to improve the contact properties by inserting a tunnel junction at the end of p region. These layers were then etched using reactive ion etching and crystallographic-selective chemical etching at the Home Institution to form nanowires over 3 µm long and ~200 nm in diameter. The nanowires were detached, dispersed on an electron-transparent membrane, and electrically contacted via electron beam lithography. This setup enables electrical field assessment at the junction using STEM-EBIC and 4D-STEM. These contacted nanowires were characterized for their photodetector performance.

Selective area growth of GaN nanowires on GaN-on-sapphire pseudosubstrates

Authors: Mikołaj Żak,[2] Marcin Siekacz,[2] Žarko Gačević[1] and Czesław Skierbiszewski[2]

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STSM home institution: [1]Institute for Optoelectronic systems and Microtechnology, Universidad Politécnica de Madrid (Spain)

STSM host institution: [2]Unipress (Poland)

Summary: The STSM is focused on achieving selective area growth of GaN via molecular beam epitaxy to control the formation of pencil-like GaN nanowires for monolithic single-photon sources. The study used GaN pseudo-substrates, covered by Ti masks, of two types: (I) micrometric parallel stripes and (II) nanohole matrices with varying diameters and pitch. Initial growth trials on type I substrates explored selective growth conditions by maintaining fixed Ga and N fluxes while varying temperature. The samples were assessed based on (i) Ti mask quality, (ii) GaN nucleation kinetics, and (iii) GaN faceting into thermodynamically stable crystal structures. Once optimal conditions were identified, they were applied to type II substrates to grow nanowire matrices with different diameters and pitch. These results are now under detailed analysis.