June 2017

Welcome to the third newsletter from the INREP project!

INREP gathers 13 European partners from 7 countries for a period of three years, until January 2018. Our fundamental goal is to develop and deploy valid and robust alternatives to indium (In) based transparent conductive electrode materials in the following applications: solar cells, LEDs and displays.

Our public newsletters keep you up-to-date on the progress made within INREP. You are given a possibility to discover how the consortium partners cooperate to achieve the project objectives. You can also get to know how and when we disseminate the INREP results. This is in case you feel like meeting with us!

Word from the Coordination Team

The INREP project has started its last implmentation phase. Our INREP adventure has been lasting for 30 months. During this time, the consortium partners have produced many encouraging results.

In the third issue of the newsletter, you will find information on the project-dedicated session that will be held during the TCO2017 meeting in September. You will further get to know how the work progressed within the project work packages. As usual, the interview will let you discover the day-to-day life of people involved in achieveing the INREP goals. Last but not least, the "Get Together" section will inform you about our upcoming dissemination activities.

We also invite you to visit the INREP website (www.inrep.eu) which is regularly updated with pieces of news about the project. Feel free to inform us of any event or activity which should be brought to the attention of the INREP community.

We wish you a good reading!

Duncan Allsopp (University of Bath) and Sylvain Nicolay (CSEM)

NEWS & EVENTS

The special session dedicated to INREP will be held on 22 September 2017 during the TCO2017 – Fundamentals and Applications meeting that will take place in Leipzig, Germany.

Read more

Following the success of the 1st edition of the Raw Meterials Week in 2016, the 2nd edition will take place in Brussels from Monday 6 to Friday 10 November 2017.

Read more

CONTACT US

Mail: contact@inrep.eu

Website: www.inrep.eu

Project Coordination Team:
Duncan Allsopp (University of Bath) and Sylvain Nicolay (CSEM)

Dissemination Manager:
Peggy Favier (L-up)

Follow us:

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INREP SESSION AT TCO2017

The TCO2017 meeting information summary:

Date: 18-22 September 2017

Venue: Universität Leipzig

Felix-Bloch-Institut für Festkörperphysik

Linnéstr. 5, 04103 Leipzig, Germany

Registration fee: 300 Euros

Website: http://research.uni-leipzig.de/hlp/TCO2017/

The TCO2017 meeting will focus on:

- theory of oxide electronic materials
- growth of bulk semiconducting oxides
- epitaxial oxide heterostructures
- metal-like n-type TCOs
- novel oxide semiconductors
- point defects in oxides
- oxide devices and applications

The session dedicated to our project will be held on Friday 22 September and will cover the following topics:

- Optical properties of amorphous Zn-Sn-Ti oxides: A combined molecular dynamics and density functional theory study.
- Atomic layer deposition of MoO_x and Al-doped ZnO for Si heterojunction solar cells.
- Indium-free Transparent Ohmic Contacts to N-polar n-type GaN.
- Towards more sustainable TCO layers: environmental effects of replacement of ITO by alternative materials.

WP1 REQUIREMENTS, SPECIFICATIONS OF IN-FREE TCOS FOR TEST DEVICES

WP1 concerns the specifications and comparison of Indium free TCOs for (O)LED, c-Si PV and touch screen applications.

The partners performed the activities during the first 18 months and produced:

- "Set of minimum properties of the transparent electrodes for each targeted application, c-Si PV, OLEDs, LEDs and touch screen". This report functions as our benchmark for the TCO design and development work in subsequent work packages.
- "Methodology for TCO & test device performance comparisons". This report serves as an inventory of specific methods for use in the TCO development and validation on device level.

WP2 MODELLING AND STRUCTURAL-PROPERTY CORRELATION OF IN-FREE TCOS

The overall goal of the task "Modelling and structural-property correlations in In-free TCOs" of WP2 is materials design and optimisation from first-principles calculations. We use state-of-the-art first-principles electronic structure methods based on density functional theory (DFT). Our results are used in a two-way data-exchange with WP3 to provide a basis for design-led TCO materials, which ultimately supports application-led works in WP5.

We have applied a self-consistent hybrid density functional approach to a wide range of oxide semiconductors, including ZnO, SnO_2, TiO_2, MgO, and $BaSnO_3$. These calculations give structural, electronic, and optical properties of these bulk materials that are in very good agreement with comparable experimental data, and that improve on previous theoretical investigations. A subset of these results, concerning ZnO, SnO_2, and MgO, has been published as an open-access article (Self-consistent hybrid functional calculations: Implications for structural, electronic, and optical properties of oxide semiconductors) in the Nanoscale Research Letters [1]. Figure 1 shows the results on the electronic band structures of these materials.

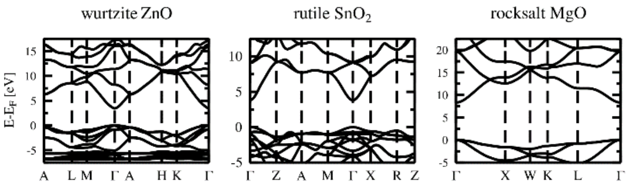

Figure 1 : Electronic band structures of wurtzite ZnO (left panel), rutile SnO_2 (middle panel), and rocksalt MgO (right panel). Energies are in electron volt (eV) and the valence band maximum is set to zero.

Based on the very good description of the bulk oxide semiconductors from this self-consistent hybrid functional approach we want to highlight two further applications. For the first, we have performed detailed calculations to understand the influence of doping on the properties of ZnO. While several trivalent dopants (e.g. Al, B) have been investigated to lower the intrinsic resistivity, additional co-doping (e.g. Mg) has been considered as a route to extend the optical transmission of ZnO into the UV. Preliminary results showing a better performance of B-doped ZnO have already been presented at national and international conferences. The second application refers to the investigation of multi-component amorphous TCOs with ZnO, SnO_2, and TiO_2 as building blocks. An ongoing computational screening of the $(ZnO)x(SnO_2)y(TiO_2)z$ solid-solution aims at

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identifying high-performance compositions (x:y:z) to be fed into WP3 for experimental verification.

Within the task "Microstructural characterisation of the thin films" WP2 we have investigated the microstructure of interfaces between Al-doped ZnO TCO and GaN for inorganic LED applications. TEM images (Figure 2) confirm a sharp high quality interface with no presence of amorphous layer. This information will be used in WP3 and WP5 for optimization of the contact resistance between Al-doped ZnO electrode and GaN in inorganic LEDs.

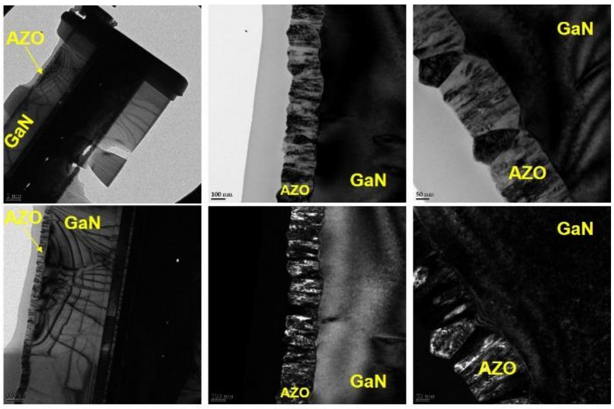

Figure 2: TEM micrographs of Al-doped ZnO / GaN interface.

WP3 DEPOSITION OF SELECTED TC(O) LAYERS PREPARATORY TO APPLICATIONS

WP3 is dedicated to the synthesis, either by vacuum based methods (CVD, ALD, PVD) or wet-chemistry approaches, of In-free TCOs/transparent electrodes. Their chemical, opto-electrical and morphological characterization is essential to provide the basis for the selection in terms of TCOs and TCO deposition methods for the application activities addressed in WP5. Furthermore, this WP addresses testing/lab-scale demonstration of the developed TCOs in the target applications of SHJ c-Si solar cells, GaN-based LEDs and touch-sensors. The devices are developed by the partners CSEM, Plessey Semiconductors Ltd, University of Bath and IMEC / Quad Industries NV.

In the last six months, this work package has focused on the following topics:

- Further efforts toward the application of aluminium-doped zinc oxide (ZnO:Al) as contact in crystalline silicon heterojunction solar cells (SHJ). Specifically sputtered ZnO:Al has been further optimized as back contact in SHJ front emitter cells and applied as front and back contact in SHJ rear emitter cells, leading to a conversion efficiency of 22.3% (reference rear emitter cell with both ITO contacts, 21.7%). In parallel, the partners are working on the replacement of the front ITO contact in front emitter cells, where requirements are more stringent, since good in-plane conductivity is needed for carriers to be collected by the screen printed silver fingers, while good transparency is crucial to allow light to be absorbed in the c-Si wafer. Specifically, the focus is on interface engineering solutions where ultra-thin MoOx layers are adopted between hydrogenated amorphous silicon and ZnO:Al.
- Insights into the role of plasma pre-treatment on n-type GaN/ZnO:Al contact resistance have been achieved and initial work on metal interlayers for p-type GaN/ZnO:Al has been carried out. In parallel, a detailed interface analysis of GaN/ZnO:Al has been carried out by means of electroluminescence and electron beam induced current diagnostics.
- Correlations between the ZnO:Al properties and the brightness-to-current density in organic LEDs have been identified.
- Formulation of inks containing Ag nanowires with suitable rheology by screen printing has been developed and transferred to the industrial partners.

WP4 SELECTION, LCA SCREENING OF NEW TCOS ON SELECTED DEVICES

Within WP4, robust alternatives for broadly used ITO-based TCO layers developed in the framework of INREP project are tested in terms of environmental impact. To this end, life cycle assessment (LCA) was performed to assess which components produce smaller environmental impact over the entire period of its life cycle ("from cradle to grave", during manufacturing, operation and waste management). Different materials for TCO layer and different deposition techniques were evaluated: physical/chemical vapour deposition (PVD, CVD), atomic layer deposition (ALD, Fig.3). Results of LCA, expressed as single score (Ecopoints), were benchmarked towards the current industrial standard TCO layer composed from ITO. The LCA calculations, based on data from lab scale devices, showed that ZnO was a proper material for ITO replacement for any of deposition techniques. For the PVD technique, replacement of ITO by ZnO / ZnO:Al reduces environmental load by ca 40.%. ZnO / ZnO:Al layer deposited by PVD seems to be the best option for ITO replacement. Subsequently, effects of process scale-up were studied based on a sensitivity analysis. We found that deposition technique and related energy efficiency were also crucial for sustainable TCO layer production. LCA results support further process improvement and

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help to determine possibilities of environmental impact minimization.

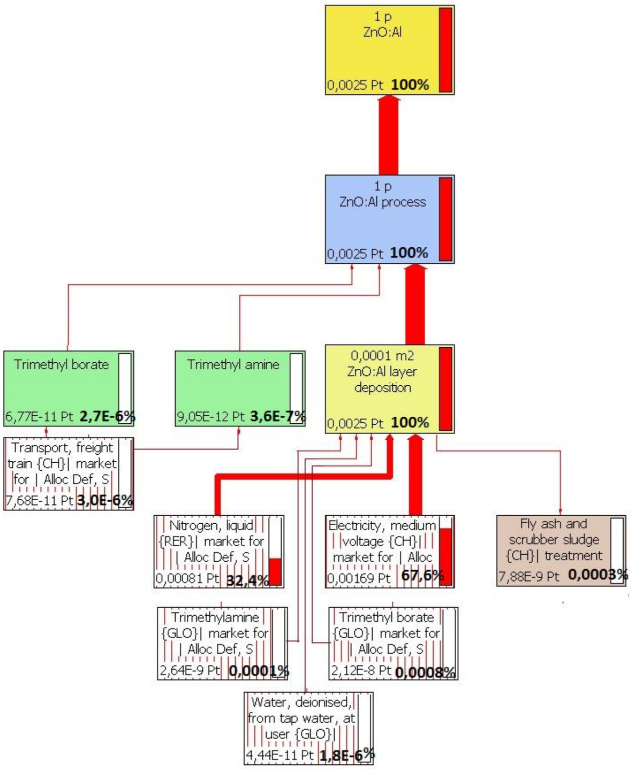

Figure 3 Process tree for ZnO:Al layer deposited by ALD technique.

WP5 APPLICATION AND TESTING OF NEW TCOS ON SELECTED DEVICES

WP5 will introduce new Transparent Conductive Oxide (TCO) materials developed within the programme onto real world applications while developing manufacturing tools to ensure scaled production. Four target applications identified at the programme outset (Solar Cells, Inorganic LED's, touch-screens and Organic LED's) naturally define stringent properties for the new TCO materials and provide a natural feedback loop between fundamental material research and their end application.

Scaled production of TCO materials currently focus on the replacement of the back contact to solar cells since the transparency and conductivity requirements are less strict. Both ALD and PVD approaches have been extended to full scale 156x156mm^2 solar cells. Further work is required to resolve the more stringent front side (p-type) Indium Tin Oxide (ITO) replacement.

Figure 4 highlights the work for TCO scaled manufacturing as carried out by Netherlands Organisation for Applied Scientific Research with their sheet to sheet ALD deposition.

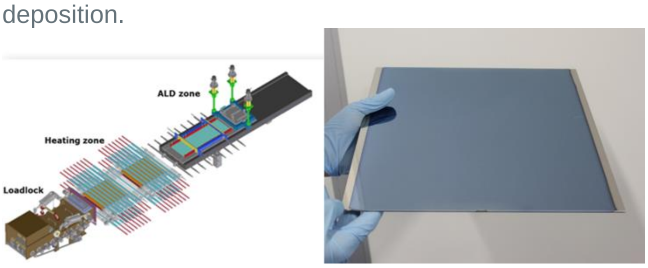

Figure 4 : Schematic (LHS) for plasma spatial ALD sheet to sheet deposition manufacturing tool being developed by Netherlands Organisation for Applied Scientific Research with example of deposited TCO (99.4% thickness uniformity) RHS.

Meyer Burger have successfully transferred PVD AZO onto their industrial scale tool targeting 2400 solar cells/hour while Plasma Quest have successfully demonstrated PVD AZO deposition using their large area application tool.

The true test for the new TCO materials will be their ability to match, and ideally, outperform ITO in real world end user applications. These commercial applications require the new material to pass product reliability tests usually through the use of accelerated life time testing.

In addition, the TCO properties are also being tested by our commercial partners through Quad industries Touch sensors and Plessey GaN LED's. The TCO material performances within the applications will be continually feedback to enable further understanding and development from a base scientific level to allow the advancement of these new and exciting materials.

Figure 5: Working touch screen demonstrator by Quad industries utilising TCO.

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Figure 6: Optical picture of emitting MOCVD GaN LED with blanket TCO electrical contact.

INTERVIEW

INREP newsletters offer you the possibility of getting to know some of the project partners a little better… Thus, the Interviews section will let you discover the day-to-day life of the people involved in achieving the INREP goals.

In this edition of the INREP Newsletter # 3, we propose you three tags which will lead the interview: **stakes** – **challenges** – **achievements** – **results – trends in industry – gender aspects.**

MARIADRIANA CREATORE
ASSOCIATE PROFESSOR
EINDHOVEN UNIVERSITY OF TECHNOLOGY

Q1: You are the leader of work package 3 (WP3) "Deposition of selected TC(O) layers preparatory to applications" within INREP. Can you please remind us the objectives and stakes of this work package?

Mariadriana Creatore (MC): This work package is scientifically and technologically exciting because it hosts all INREP core research activities: synthesis of new transparent conductor layers, their direct integration in demonstrator devices (solar cells, organic and inorganic LEDs and touch sensors), and fundamental studies on key interfaces in devices. WP3 brings together a wide range of scientists, from academia to research institutes and industry and this has brought us to achieve key-results already at the very early stages of the project.

Q2: What is innovative about these research activities? What are the challenges?

MC: The INREP team looks into valid, reliable, cost-effective material solutions alternative to the usage of ITO. INREP goes beyond the merely development of alternative materials, and integrate them directly into state-of-the art devices (at early stages in WP3 and on large-area prototypes in WP5). Because integration starts right from the early phases of the project, the research team critically looks into the challenges related to integration by proposing and developing interface solutions toward efficient, cost-effective devices. The word "interface" has now appeared several times in this interview and it is no coincidence. The opto-electronics devices addressed by INREP are all relying on efficient, selective (electron, hole) charge carrier processes and educated engineering of interfaces is key to achieve them.

Q3: What do you think have been / will be the most significant achievements of the activities performed in WP3?

MC: The WP3 team has been extremely busy in exploring aluminum-doped zinc oxide (ZnO:Al) as valid alternative to ITO in crystalline silicon heterojunction solar cells (SHJ). Our studies show that ZnO:Al is an excellent back contact in front emitter SHJ cells and parallel work on rear emitter SHJ cells shows that it is feasible to have both front and back contacts made of ZnO:Al. It would be great if we could replace ITO with ZnO:Al also in front emitter SHJ cells but for this to happen we need again to focus in the coming months on the interface. Specifically, we need to develop transparent, hole selective transport layers exhibiting good interface properties with ZnO:Al and hydrogenated amorphous silicon, which is fundamental to passivate the surface defects of crystalline silicon.

Of course, WP3 is not only about solar cells! The team's work has led to major achievements also in the field of inorganic, GaN-based LEDs: we have generated insights into the role of plasma treatment on the quality of the contact resistance at the interface between GaN and ZnO:Al, especially thanks to academic groups expert in developing interface-sensitive key-diagnostics. And we have developed silver nanowire solutions with optimized opto-electrical properties, compatible with touch sensors requirements.

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And finally, we should not forget that all material science and development carried out within INREP finds its roots in reliable, state-of-the art, innovative deposition methods and tools which are explored by the team at the several partners' locations.

Q4: What is the key-strength of WP3 in the INREP consortium? How will the results be beneficial to the INREP partners?

MC: The synergy among the partners in terms of brainstorming and collaborative, joint-experiments is definitely playing a key-role in defining a robust knowledge and expertise background to explore alternative materials to ITO. Scientific output is definitely a reliable way to measure the impact of the joint-work for the academic and R&D partners and presently there is a plethora of initiatives in the directions of joint-scientific contributions to peer-review journals and conferences/workshops. Industrial partners acknowledge the benefits of joining this consortium because they can measure the impact and strength of the materials alternative to ITO directly in devices.

Q5: In broader terms, how does the work align with contemporary **trends in industry**? How does the consortium plan to bridge the gap from the lab to the market?

MC: We plan to bridge the gap from the lab to the market by exploiting the contacts with customers which the INREP industrial partners have, by presenting the current work which we are carrying out in WP5, fully dedicated to implementation of transparent conductors in large area devices. Furthermore, INREP has an industrial board, which keep all INREP partners sharp on the latest (and future) market developments.

Q6: Research and development are generally perceived as a mainly male domain. As a female researcher participating in INREP, can you tell us how gender aspects are considered in European research & innovation collaborative projects? What would be your recommendations to make science and technology more women-friendly and to increase women's visibility in this field?

MC: INREP has an exceptionally high female researchers participation: 4 principal investigators at the locations of University of Bath, CSEM, University of Lodz and Eindhoven University of Technology, supported by the excellent team of L-up with two female employers. Definitely, an example to be followed in future EU collaborative projects! My recommendation is making science and technology more visible and tangible already in primary education. At the same time, female talent in higher academic (as well as R&D and industrial) position should be better stimulated and promoted by introducing personal development plans and coaching tools.

GET-TOGETHER

The full list of scientific and technological events related to the INREP research areas can be found on our website. Feel free to inform us of any event likely to interest the members of the INREP community.

By the end of the year, INREP will be represented during the following events:

ICNS-12, 24-28 JULY 2017, STRASBOURG FRANCE

The ICNS-12 conference will present high impact scientific and technological advances in materials and devices based on group-III nitride semiconductors.

Source: ICNS-12

NANOENERGY, 26-28 JULY 2017, AALTO UNIVERISYT FINLAND

The 4th NANOENERGY conference will address the theory, design, research, discovery and development of new materials and nanotechnologies in relation to the field of energy applications (e.g. in energy harvesting, production, storage, transfer and use, etc.). NANOENERGY aims to bring together academia, industries and policy makers interested in the application of nanotechnology in the energy sector. The conference will discuss the state-of-the-art and latest development of nanotechnology, nanomaterialsand thin filmsfor energy applications but also investigate possible avenues ahead.

Source: NANOENERGY

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MICROSCOPY CONFERCENCE 2017, 21-25 AUGUST 2017, LAUSANNE SWITZERLAND

The scientific program features three main topical areas addressing advances in instrumentation and methods, life sciences and materials science. Each main topic is split in seven thematic sessions covering invited and contributed talks as well as poster sessions.

Source Microscopy Conference

EEMS 2017, 13-15 SEPTEMBER, POLANICA ZDROJ POLAND

The International Conference Energy, Environment and Material Systems 2017 will cover topics such as sustainable energy, environmental and material development to bring together scholars, leading researchers and experts from diverse backgrounds and applications areas.

Source: International Conference Energy, Environment And Material Systems

ICOSSE '17, 2-4 OCTOBER 2017, BARCELONA SPAIN

6th International Congress on Sustainability Science & Engineering will discuss the trends towards greater sustainability that are driving innovation and present the latest achievemnts in new sustainable process technologies.

Source: ICOSSE '17

SURFINT-SREN V, 20-23 NOVEMBER 2017, FLORENCE ITALY

The main goal of the conference Progress in Applied Surface, Interface and Thin Film Science 2017 is to contribute to new knowledge in surface, interface, ultra-thin films and very-thin films science of inorganic and organic materials by the most rapid interactive manner - by direct communication among scientists of corresponding research fields.

Source: SURFINT-SREN V

RAW MATERIALS WEEK, 6-10 NOVEMBER 2017, BRUSSELS, BELGIUM

Following the success of the 1st edition of the Raw Meterials Week in 2016, the 2nd edition will take place in Brussels from Monday 6 to Friday 10 November 2017.

It will be a great opportunity for the raw materials community to discuss and exchange on all relevant issues such as policy, technology, international cooperation and framework conditions.

The Raw Materials Week is centred around a series of events organised by the European Commission addressing the latest news regarding raw materials in the EU:

- 6 November: Copernicus for raw materials
- 7 November: EU advanced mining country raw materials diplomacy dialogue and EU critical raw materials event
- 8 November: 5th annual high level conference of the European Innovation Partnership (EIP) on raw materials
- 9 November: Horizon 2020: societal challenge 5 infoday & brokerage event and Reconciling biodiversity protection and extractive activities within Natura 2000 Network

Further details about these events will be published shortly.

Source: Directorate-General (DG) for Internal Market, Industry, Entrepreneurship and SMEs of the European Commission (Growth).

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