December 2015

Welcome to the first 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 will regularly keep you up-to-date on the progress made within INREP. You will be given a possibility to discover how the consortium partners cooperate to achieve the project objectives. You will also know how and when we disseminate the INREP results. This is in case you feel like meeting with us!

We take this opportunity to wish you all a great Holiday Season and a Happy New Year!

Word from the Coordination Team

It is with great pride and enthusiasm that we present to you the INREP project and its first Newsletter. We believe that INREP will be successful in identifying possible solutions to replace Indium currently used in electrode materials in the form of ITO for applications such as lighting, photovoltaics and touch screens. INREP adopts a holistic approach in which tailor made solutions are developed for each specific applications, focusing not only on the new material "bare" opto-electronic properties, but also on its interplay with the whole device and all its processing steps.

INREP brings together 13 partners from across Europe, each one contributing with high-level experience and capacities. We are confident that the good team spirit and motivation to deliver the INREP targets will accompany us all along the project!

We also invite you to visit the INREP website (www.inrep.eu) which will be 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

Our webiste is online. The "News & Events" section will be regularly updated with the activities carried out by the INREP partners.

>> Read more

Meet with us at the E-MRS Fall 2016 Meeting on 19-22 September 2016! Several partners plan on representing INREP. Further details will follow soon.

>> Read more

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This project is supported by the European Community's Seventh Framework Programme for research, technological development and demonstration, under grant agreement n°641864.

Word from the Project Officer

Dear Readers,

The era of seemingly plentiful and cheap resources is coming to an end: raw materials, water, air, biodiversity and terrestrial, aquatic and marine ecosystems are all under pressure. The combined impacts of climate change and current production and consumption patterns are undermining our planetary habitat. The European Commission addresses these challenges in its Framework Programme for Research and Innovation, Horizon 2020. Actions are funded in order to address gaps in the knowledge base needed to understand changes in the environment, identify the policies, methods and tools that would most effectively tackle the above mentioned challenges, and support innovators and businesses to bring green solutions to the market.

Research and Innovation Actions under this Framework Programme include the topic of **Innovative and sustainable solutions leading to substitution of raw materials** with specific challenge to find alternative solutions to replace certain Critical Raw Materials (CRM) in concrete applications, or to diversify the supply of raw materials sources. This specific challenge is identified in the Priority Area 'Substitution of raw materials' of the European Innovation Partnership (EIP) on Raw Materials.

INREP (Towards Indium free TCOs), a H2020 funded program under the subtopic **Materials for electronic devices,** works towards the development of innovative and sustainable solutions for the appropriate substitution of Indium in transparent conductive layers (TCO's), targeting appropriately materials and applications that are difficult to recycle and where there are limited prospects to increase primary supply within the EU.

INREP will try to contribute by pushing the EU to the forefront in the area of sustainable raw materials substitution in the long term, while at the same time significant contribution to reduced dependency on CRMs will be targeted in the medium term.

Kind regards,

Dimitrios BILIOURIS
INREP Project Adviser
European Commission
Executive Agency for Small and Medium-sized Enterprises (EASME)

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

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

The activities were launched right after the project start in February 2016. The partners were questioned in detail about the TCO requirements for their applications, with regard to the intrinsic properties, such as absorbance and conductivity, as well as demands stemming from the pre- and post-process of the manufacturing flow of the final product. The results were documented in an internal report “Set of minimum properties of the transparent electrodes for each targeted application, c-Si PV, OLEDs, LEDs and touch screen” to be used as targets for the TCO design and development work in WP2 and WP3. This document will be updated throughout the project.

Since TCOs will be made by different techniques and by different partners in different labs, establishing ways to achieve a ‘fair’ comparison is a major concern. To enable this comparison, techniques and protocols have been chosen to be used by all partners for the determination of the intrinsic opto-electrical properties of the TCOs.

In addition, an inventory was made of specific methods used to compare the effect of the different TCOs effects on actual device. This work was documented in another internal report “Methodology for TCO & test device performance comparisons” for use in the TCO development in WP3 and validation on device level in WP5.

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

The goal of WP2 is to design and optimise novel transparent conducting oxides via numerical modelling. The composition and structural space is immense, so we are combining state-of-the-art materials simulation techniques (University of Bath) with cutting-edge materials deposition and characterisation processess (CSEM).

In the first 6 months, the WP2 activities were focused in two directions:

1. A major goal for first-principles (parameter free) simulation of conductive oxides is the choice of theoretical approach. We have evaluated a new self-consistent approach to electronic structure. Using so-called "non-local hybrid density functionals" we can remove a source of parametrisation that has caused issues in prior investigations. Within this new approach we have established a reliable computational procedure for describing the bulk crystal and electronic structure, and surface properties of ZnO and SnO2. We find good agreement between our calculated parameters and comparable experiments. To illustrate our results, we show the ZnO electronic band structure in Fig. 1. These results also serve as a benchmark for future calculations.

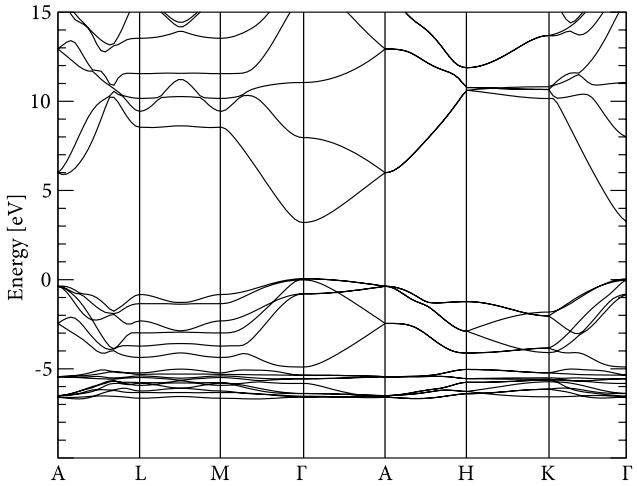

Figure 1: Band structure of wurtzite ZnO calculated by first-principles electronic structure methods employing a new self-consistent approach to non-local hybrid density functionals. The calculated band gap energy of 3.41 eV is in very good agreement with available experimental data (3.44 eV). Zero energy is placed at the top of the valence band.

2. We investigated the properties of reference TCO films that will provide important information for the material simulations as well as for the other workpackages. We used two different deposition techniques to fabricate and study the microstructural properties of intrinsic ZnO and SnO2 films grown on various substrates. We have demonstrated that the choice of the substrate material affects the growth mode and the microstructure of the TCO layers. Figure 2 shows that the ZnO films grown by low pressure chemical vapour deposition (LPCVD) on glass substrates reveal very anisotropic columnar-shaped grains, which exhibit a partial preferential crystallographic orientation, whereas deposition on Si heterojunction structures results in the isotropic growth. Furthermore, the crystallographic orientation of the ZnO films grown on glass were found to depend on the deposition technique (Figure 3).

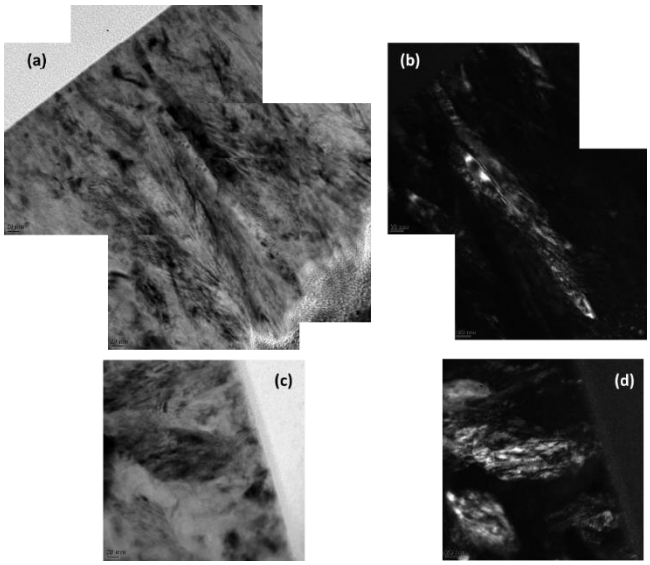

Figure 2: (a, b) Bright and dark field transmission electron microscopy (TEM) images of the undoped ZnO sample grown by LPCVD on glass, respectively. (c, d) Bright and dark field TEM images of the undoped ZnO sample grown by LPCVD on the Si HTJ, respectively.

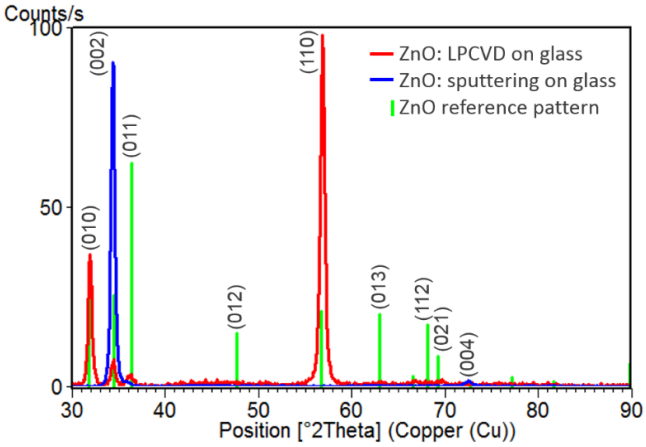

Figure 3: Comparison of the normalized X-ray diffraction patterns of ZnO films deposited by LPCVD and sputtering on glass substrates. Both samples reveal pure ZnO phase. However, the preferred crystallographic orientations are very different between the samples. Vertical green strokes on the graph represent the theoretical positions and relative intensities of the crystallographic reflections for the hexagonal ZnO (PDF card No. 98-000-9341).

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Having demonstrated the applicability of a new first-principles simulation method, we are now investigating the role of defects and surfaces based on the experimental results on the microstructural properties of real TCO systems. We are also using the electronic structure calculations to screen novel TCO materials, e.g. by including a co-doping approach to finely control carrier concentrations and conductivity.

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.

The synthesis of In-free TCOs/transparent electrodes is carried out from the INREP partners CSEM, TNO, Plasma Quest Ltd, TUe and IMEC. The deposition methods range from low pressure (plasma-enhanced) chemical vapor deposition to temporal and spatial atomic layer deposition, sputtering and screen printing.

The layer characterization includes electrical conductivity, carrier concentration, carrier mobility and optical properties. Furthermore, in specific cases the characterization extends to the whole device, as in the case of the assessment of the electrical integrity of contacts in structured LED and the acquisition of EBIC maps and I-V curves of individual nanorods (partners Slovak University of Technology and University of Bath).

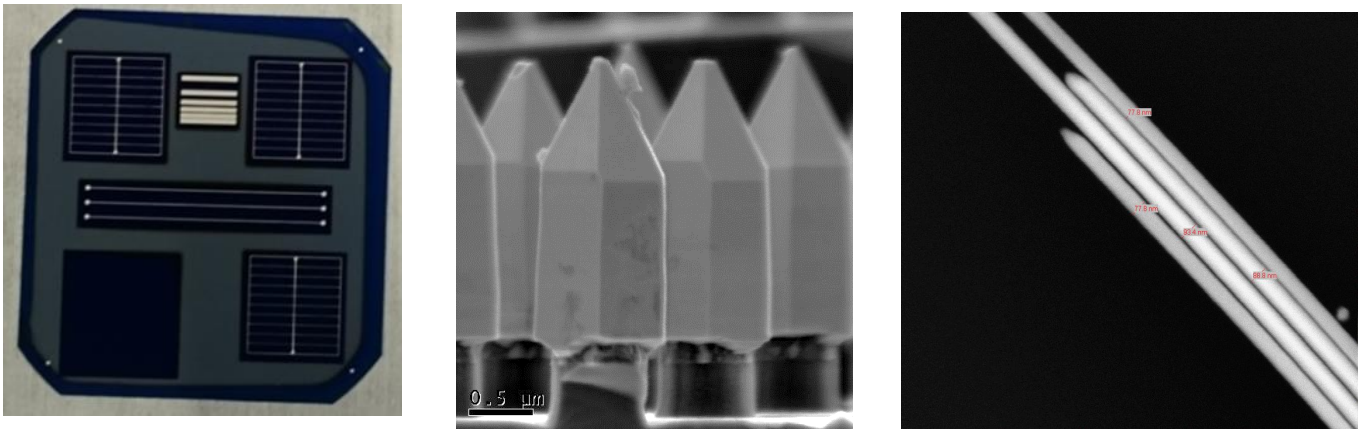

Figure 4: (left)-standard test sample consisting of four c-silicon heterojunction solar cells; (middle)-GaN on sapphire core-shell nanorods LEDs; (right)-Ag nanowires (diameter in the range of 70-90 nm) ink.

WP4 SELECTION, LCA SCREENING OF NEW TCOS ON SELECTED DEVICES

In the framework of WP4, Life Cycle Assessment analysis (LCA) will be carried out to assess the environmental impact of different TCO materials composition over the entire period of its life cycle (manufacturing, operation and waste management). A complete LCA analysis performed in this workpackage will consist of goal definition and scope, inventory analysis, impact assessment with four sub-phases: classification, characterisation, normalisation, weighting and improvement assessment which is consistent with ISO standards. Therefore, this analysis will enable a profound and objective assessment of sustainability of TCO materials. The LCA results will be included in further workpackages of the INREP project-e.g. in the final product design phase. As a result, the environmental impact of TCO will be considered in the design of the final product, allowing to achieve the highest environmental quality of the TCO being developed to a manufacturing standard. As there is no standard LCA methodology, in order to perform the LCA calculations for the project, in the first step, the most suitable environmental assessment method must be chosen for TCO application in devices as PV, LCD, OLED, ILED. The method once chosen and applied for TCO LCA calculations may be used as a standard against which new TCO can be tested. Optimization of a final composition of in-free TCOs for different materials and different doping will allow us to minimize environmental impact and production costs.

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WP5 APPLICATION AND TESTING OF NEW TCOS ON SELECTED DEVICES

This work package will take the new TCO layers developed within INREP, mainly from WP2 and WP3, and evaluate their performance in a range of device technologies at a pre-production scale. These devices include: High Efficiency Solar Cells, Inorganic LEDs, Organic LEDs and Touch Screens. This close collaboration with end users will allow process steps to be developed that ensure the TCO can be incorporated into demonstrator devices which fully exploit the improved material properties. Although this work will start later in the project, the partners developing these devices are already working closely with the research partners to define and guide the TCO development for the specific applications. This will ensure that the layers developed closely match the requirements of real world devices.

Another aspect of this work package is the development of production capable deposition techniques with high throughput, high uniformity and low cost of ownership. This will ensure that the TCOs developed are compatible with industrial scale deposition processes and are suitable for commercial device production allowing the outcomes of the project to be exploited as soon as possible. The systems being developed cover a range of deposition technologies including Large Area (30mmx30mm) Spatial Atomic Layer Deposition (S-ALD) and plasma based systems. Development of the production scale systems has already begun and is already demonstrating high quality TCO layers.

Figure 5 : Extended Planar Plasma Source (EPPS) being developed at Plasma Quest Ltd for the large area deposition of a range of Transparent Conducting Oxides.

GET-TOGETHER

The full list of scientific and technological events related to the INREP research areas can be found on our website. Don't hesitate to inform us of any event likely to interest the members of the INREP community.

SILICONPV 2016 — 07-09 MARCH 2016

The 6th International Conference on Silicon Photovoltaics will be held in Chambéry, France. It will focus on advanced technologies, materials and concepts for crystalline silicon solar cells and modules.
Source: https://www.siliconpv.com/home.html

ICCG 11 — 12-16 JUNE 2016

The International Conference on Coatings on Glass and Plastics will be organised in Braunschweig, Germany. The ICCG 11 will address the advanced coatings on glass and plastics for large-area or high-volume products.
Source: https://11.iccg.eu/en/home

E-MRS FALL MEETING — 19-22 SEPTEMBER 2016

The 2016 E-MRS Fall Meeting and Exhibit will be held in Warsaw University of Technology. The topics addressed will range from electronic nanomaterials to biomaterials for applications in Electronics, Energy saving and production and Health sectors. Source: http://www.european-mrs.com/meetings/2016-fall

TCM 2016 — 09-13 OCTOBER 2016

The 6th International Symposium Transparent Conductive Materials will take place in Crete, Greece. The topics will cover among others TCMs in TTFTs, OLEDs, LCDs and paper electronics, oxydes for PVs, sensor coatings…
Source: http://www.european-mrs.com/endorsed-meeting/tcm-2016-conference

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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 # 1, we propose you three tags which will lead the interview: **Application - Literature review – Silver nanowires – Rheology analysis**

DR LAURENCE LUTSEN & DR KEN ELEN

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Q1: Could you explain to the readers your involvement in INREP? What application do your research activities address?

A1: Many devices rely on printed electronic technologies for function, form and flexibility. IMEC-imomec is involved within the INREP project for the development of novel transparent printable conductive inks for screen printing. Printed electronics allows for high volume, high-throughput and cost-effective manufacturing of many products. IMEC-imomec is working in close collaboration with the INREP consortium and more especially with the company Quad Industries, a leading manufacturer and developer of user interfaces and control panels in Belgium.

Q2: One of the activities that IMEC has carried out since the start of the project is the literature review. Could you tell us what information you were looking for?

A2: A literature and patent search is the process by which prior knowledge, know-how, inventions or ideas are examined, with the goal being to find information on a given (or eventually very similar) topic. IMEC-imomec has started its activity in the INREP project with such activity to draw the state-of-the-art on transparent printable conductive inks for screen printing.

Q3: Why are silver nanowires of interest for INREP? What kind of synthesis of nanowires have you performed within the project?

A3: Since bulk silver (Ag) has the highest electrical and thermal conductivity among all metals, it has received considerable attention as the conductive material in conductive inks for printed electronics. One-dimensional nanostructures “nanowires” of silver can be used to deposit conducting networks on a surface. In these networks, the nanowires will conduct electricity, while the open areas allow the transmission of light.
There are several methods to synthesize silver nanowires including chemical synthesis, electrochemical technique, hydrothermal method, ultraviolet irradiation photodetection technique, DNA template, porous materials template, and polyol process. Among these, the polyol process is simple and inexpensive, and provides a relatively high yield. The polyol process proceeds by chemical reduction of silver ion in the presence of a polymeric surfactant. In this method, ethylene glycol (EG) is used as both solvent and reducing agent, poly(vinylpyrrolidone) (PVP) is used as stabilizing agent, and silver nitrate ($AgNO_3$) is used as silver source.

Q4: **What were the results of the rheology analysis and how do they influence your further work within INREP?**

A4: For each novel ink formulation, a rheology study is first carried out as the printed pattern characteristics depend strongly on the rheological properties of the ink. Inks for screen printing should exhibit thixotropic rheological behavior with both time dependence and shear thinning. The suitable inks should have high viscosity at low shear rates when the ink is charged to the printer, low viscosity during printing at high shear rate, and finally viscosity recovery of high viscosity after printing. After this first screening, the most promising ink are screen printed at laboratory scale and finally tested within the context of production processing schedules.

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