Effect of replacement of tin doped indium oxide (ITO) by ZnO: analysis of environmental impact categories

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Abstract. Abundant use of natural resources is doubtlessly one of the greatest challenges of sustainable development. Process alternatives, which enable sustainable manufacturing of valuable products from more accessible resources, are consequently required. One of examples of limited resources is Indium, currently broadly used for tin doped indium oxide (ITO) for production of transparent conductive films (TCO) in electronics industry. Therefore, candidates for Indium replacement, which would offer as good performance as the industrial state-of-the-art technology based on ITO are widely studied. However, the environmental impact of new layers remains unknown. Hence, this paper studies the environmental effect of ITO replacement by zinc oxide (ZnO) by means life cycle assessment (LCA) methodology. The analysis enables to quantify the environmental impact over the entire period of life cycle of products—during manufacturing, use phase and waste generation. The analysis was based on experimental data for deposition process. Further, analysis of different impact categories was performed in order to determine specific environmental effects related to technology change. What results from the analysis, is that ZnO is a robust alternative material for ITO replacement regarding environmental load and energy efficiency of deposition process which is also crucial for sustainable TCO layer production.

1 Introduction to LCA

Life cycle assessment (LCA) is a technique for evaluating the environmental effects associated with a product or service over the entire period of its life cycle ("from cradle to grave") by:

- Compiling an inventory of relevant energy and material inputs and environmental releases [Fig. 1]
- Evaluating the potential environmental impacts associated with identified inputs and releases
- Interpreting the results to help decision-makers make a more informed decision.

A complete LCA consistent with ISO 14040 series standards is composed of four interrelated phases:

1. Goal Definition and Scoping - define and describe the product, process or activity. Establish the context in which the assessment is to be made and identify the boundaries and environmental effects to be reviewed for the assessment.
2. Inventory Analysis - identify and quantify energy, water and materials usage and environmental releases (e.g., air emissions, solid waste disposal, waste water discharges).
3. Impact Assessment - assess the potential human and ecological effects of energy, water, and material usage and the environmental releases identified in the inventory analysis.
4. Interpretation - evaluate the results of the inventory analysis and impact assessment to select the preferred product, process or service with a clear understanding of the uncertainty and the assumptions used to generate the results [1].

Vast development in LCA methodologies in last 15 years, elaboration of new LCA techniques, and development of huge databases allows obtaining valuable information about environmental load produced by a product within its life cycle.

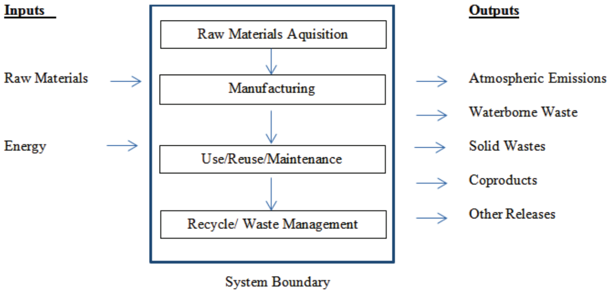

Fig. 1. Life Cycle Stages [2]

1.1 INREP project

INREP "Towards Indium free TCOs" is a Horizon 2020 collaborative research project with the objective to develop and deploy valid and robust alternatives to

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indium (In) based transparent conductive oxides (TCO) materials as electrodes. In-based materials, mainly ITO (Indium Tin Oxide), are technologically entrenched in the commercial manufacture of components like LEDs, solar cells, touch-screens, so replacing them with In-free transparent conducting oxides (TCOs) will require holistic approach. INREP looks for development of new TCOs and their deposition technologies with the optimum opto-electrical properties for the economic and safe manufacture of opto-electronic components. The INREP philosophy aimed at developing solutions for the targeted applications. This action will also bring innovative deposition equipment closer to an industrial level in order to accelerate the deployment of indium free TCOs and achieve cost reduction for large area applications. INREP includes also life cycle assessments of the environmental impact of the developed TCO materials and cost of ownership analyses of their formation technologies over the entire period from application in manufacturing, through component operation into waste management.

1.1.1 LCA in the INREP project

LCA analysis can be performed with different calculation techniques and a broad variety of approaches was reported so far. However there is no standard methodology, or even no legally accepted guidelines facilitating the choice of LCA method. The only aspect, which can be systematically verified, is accordance with ISO standards ISO 14040 and ISO 14044. Therefore, analysis of each of existing methods should be performed prior to the selection of LCA tool for a given process.

Within the scope of INREP project, LCA is performed as a comparative analysis enabling final ranking of environmentally friendly TCO layers. Hence, the following criteria for subsequent choice of the LCA approach were selected:

- The method must follow ISO standards and have a broad number of applications reported, to ensure that the approach was extensively tested
- The database of materials and utilities related to the method must be very broad to ensure availability of coefficients for all compounds used in the TCO layer deposition process (e.g. Zinc Oxide)
- The method should enable a deep LCA analysis and include all categories of impact on environment and human health
- The result of the calculation should be a single score, enabling easy comparison and interpretation
- LCA calculation tool must enable clear and transparent analysis.

Based on aforementioned criteria, all available methods were screened for availability of coefficients for compounds used in the TCO layer deposition process. As we found, none of the available LCA methods has the coefficients for all of the compounds used in INREP. Consequently, we selected technique based on availability of coefficients for the key compounds (such as Zinc Oxide). Finally, SimaPro methodology was selected for further LCA analysis.

1.1.2 SimaPro for the LCA analysis

SimaPro® methodology, which allows easy modelling and analyzing of complex life cycles in a systematic and transparent way, has been chosen as a basic tool for LCA analysis in INREP

The first steps for setting an inventory analysis are the definition of the functional unit (which is the environmental cost of deposition of 1 cm^2 of TCO) and scope of the analysis. Since the main goal of the INREP project is to develop and bring to the market efficient Indium- free TCOs, the functional unit of analysis is a layer of new TCO.

The next step of LCA analysis consists of collection of detailed data on the process. Based on this data, additional mass and energy balances can be calculated and subsequently all impacts on environment are quantified. Within the scope of INREP project, physical/chemical vapour deposition (PVD) techniques and materials being the promising candidates for ITO replacement e.g. ZnO were analysed.

1.1.3 Life cycle assessment for different layers deposited with PVD technique

For the physical vapour deposition technique (PVD), a solid source of ITO or ZnO for the deposited compound is used, what facilities the exact quantification of materials used for deposition and waste generated by the process [3]. Therefore, only the units of consumption needed to be recalculated. Additionally, the impact of the transport of raw materials was assessed. All recalculated impacts are shown for the ITO layer deposited by the PVD process (Table 1).

Table 1. Data obtained for ITO-based layer, PVD technique.

Inputs/outputs	Unit	Amount
Cooling water	m^3/cm^2	2,80E-05
ITO target	g/cm^2	1,01E-04
Argon gas	m^3/cm^2	1,21E-07
Oxygen gas	m^3/cm^2	9,88E-10
Electricity	kWh/cm^2	7,53E-05
Waste for reuse, recovery, recycling	g/cm^2	6,01E-03
Waste for final disposal	g/cm^2	1,54E-05
Waste water without treatment	m^3/cm^2	1,33E-10

What is crucial in LCA analysis is the availability of impact coefficients in the selected database. In case of PVD processes and related source of ITO or ZnO such data was available, what ensured exact analysis without need for further assumptions. Resulting process tree for the ZnO layer, showing different stages of the deposition process and related impacts is shown in Fig. 2. The values of ecopoints, characterizing the environmental impact, are summarized in Table 2. For the analysed process, the electricity consumption was clearly the dominant contribution to the total environmental impact. Replacement of ITO by ZnO layer proved to a good strategy towards minimization of the environmental impact produced by TCO layer deposition process. The impact of ZnO layer, expressed as a single score accounted for 58% of the ITO layer impact (deposited with the same technique). Consequently, the ZnO material usage is responsible only for a minor part of the environmental impact (ca. 2%).

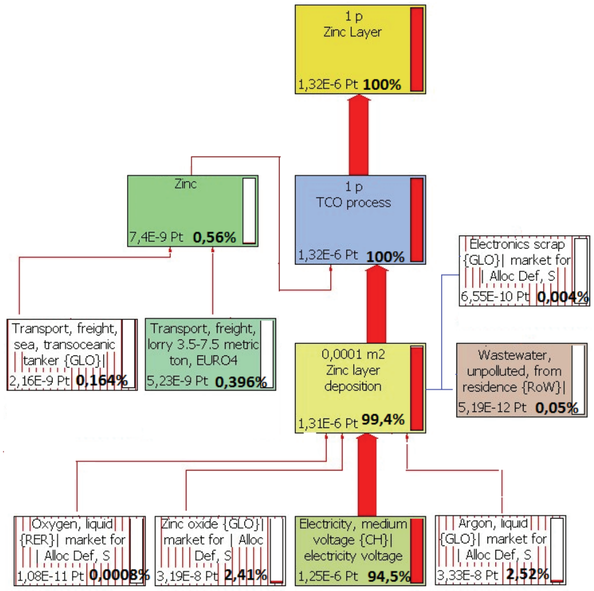

Fig. 2. Exemplary process tree for ZnO, PVD technique, SimaPro®.

Table 2. LCA results for TCO layers deposited with the PVD technique.

No.	Compound	Deposition Technique	Single Score [Pt]	Main impact [%]
1	ITO (reference case)	PVD	2,29E-6	Indium tin oxide 93,3
2	ZnO	PVD	1,32E-6	Electricity 94,5

2 Impact categories

The impact categories are defined and selected in order to describe the impacts caused by the emissions and the consumption of natural resources during the production, use and disposal of the product or processes. In most of Life Cycle Impact Assessment (LCIA) methodologies, the emissions and consumption of resources are attained to three main areas: ecosystem quality, human health and natural resources depletion (Fig. 3).

ReCiPe Endpoint H/A method was applied in INREP project to end up life cycle analysis with single score, SimaPro®.

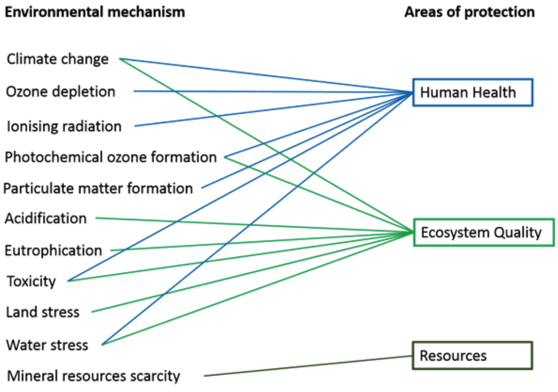

Fig. 3. An example of overall scheme of the environmental life cycle impact assessment framework linking life cycle impact results to midpoint categories to damage categories (areas of protection) [4].

A single score methodology requires subjective opinions in order to weight the relative importance of different environmental impact categories [5].

The subjective views are represented by (quantitative) weighting factors, which represent the relative importance of different environmental impacts and are used to calculate one single, aggregated value (single score). Results of LCA in a form of a single score makes decision making process clear and easier, especially when it is difficult to have an overall conclusion merely based on midpoint results [6-8].

Results of the LCA analysis indicate that for damage categories, the highest environmental impact is connected with human health, than resources depletion and finally ecosystem quality for both ZnO and ITO (Fig. 4 and 6). However specific values of ecopoints for ZnO are lower than for ITO. For human health category, ZnO has 6E-7 Pt while ITO: 1,1E-6 Pt, in case of resources: ZnO has 4.51e-7, ITO – 9,4E-7 Pt, for ecosystem both values are similar – 2,5E-7 Pt.

Total single score for ZnO is 1,32E-6 Pt whereas for ITO is 2,29E-6 Pt.

In terms of impact categories (Fig. 5 and 7) fossil depletion is mostly effected for production of ZnO layer, and also climate changes due to the gas emissions and transportation (Fig. 5). For the production of Indium layer, the biggest environmental effect is for human toxicity and metal depletion.

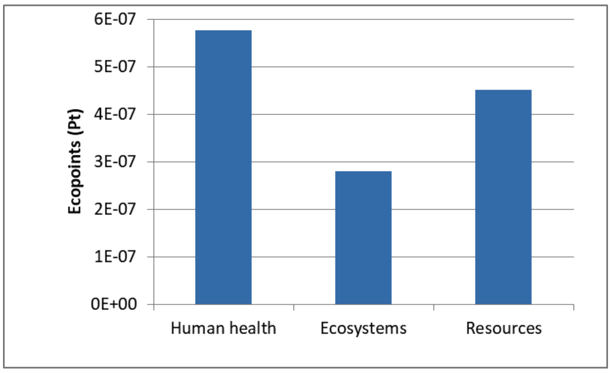

Fig. 4. Single score results per damage categories for TCO production process: ZnO, PVD technique.

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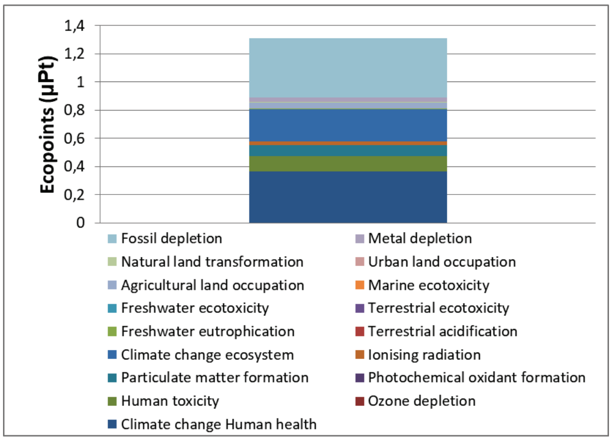

Fig. 5. Single score results per impact category for TCO process: ZnO, PVD technique.

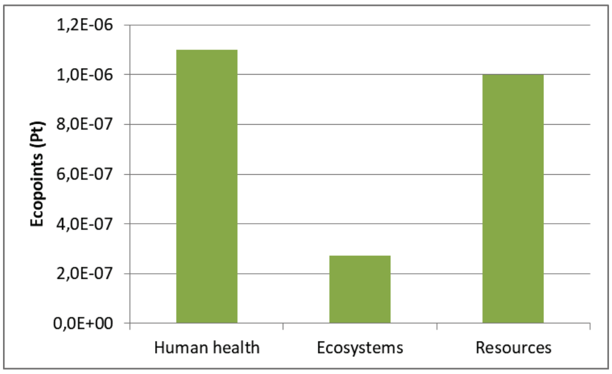

Fig. 6. Single score results per damage categories for TCO production process: ITO, PVD technique.

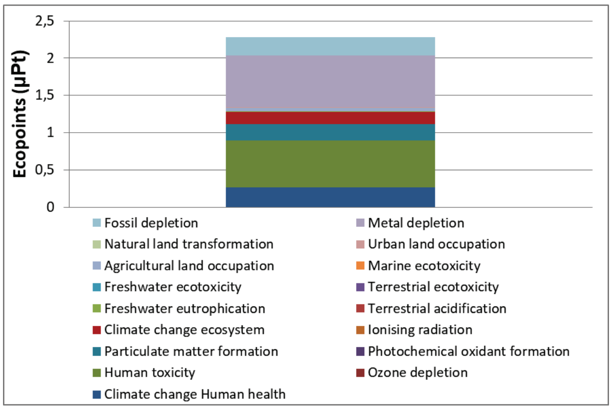

Fig. 7. Single score results per impact category for TCO process: ITO, PVD technique.

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.

3 Conclusions

Within the INREP project, robust alternatives for broadly used ITO-based TCO layers are tested in terms of environmental impact. To this end, life cycle assessment (LCA) was carried out to assess environmental impact over the entire period of its life cycle ("from cradle to grave", during manufacturing, operation and waste management) for each component of the layer. 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 the PVD technique, replacement of ITO by ZnO reduces environmental load by factor of 58%.

Results obtained from LCA support further process improvement and help to determine possibilities of environmental impact minimization.

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References

1. International Organization for Standardization 14040. Environmental Management — Life Cycle Assessment — Principles and Framework (2006)
2. J.C. Bare, G.A. Norris, D.W. Pennington, T. McKone, J. Ind. Ecol. 6, 3-4 (2003)
3. O. G. Griffiths, J.P. O'Byrne, L. Torrente-Murciano, M.D. Jones, D. Mattia., M. C. McManus, J. Clean Prod. 42, (2013)
4. O. Jolliet, A. Brent, M. Goedkoop, N. Itsubo, R. Mueller-Wenk, et al. Final report of the LCIA definition study. (2003)
5. ISO 14044: 2006, Environmental management - Life cycle assessment Requirements and guidelines, International Standardisation Organisation (2006)
6. R. Heijungs, J. Guinée, R. Kleijn, V. Rovers, Int. J. Life Cycle Assess. **12**, 4 (2007)
7. P.B. Shantheyanda. Characterization of aluminum doped zinc oxide thin films for photovoltaic applications, Master Thesis, University of Central Florida, Orlando, Florida, (2009)
8. R. Hischier, S. Hellweg, C. Capello, A. Primas, Int. J. Life Cycle Assess. 10, 1 (2005)