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Comparative alternative materials assessment to screen toxicity hazards in the life cycle of CIGS thin film photovoltaics

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HIGHLIGHTS

- Comparative alternatives assessment of thin film manufacturing technologies.
- Development of chemical alternatives assessment in a life cycle context.
- Screening of manufacturing and solar cell hazardous substances simultaneously.

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ABSTRACT

Copper–indium–gallium–selenium–sulfide (CIGS) thin film photovoltaics are increasingly penetrating the market supply for consumer solar panels. Although CIGS is attractive for producing less greenhouse gas emissions than fossil-fuel based energy sources, CIGS manufacturing processes and solar cell devices use hazardous materials that should be carefully considered in evaluating and comparing net environmental benefits of energy products. Through this research, we present a case study on the toxicity hazards associated with alternative materials selection for CIGS manufacturing. We applied two numeric models, The Green Screen for Safer Chemicals™ and the Toxic Potential Indicator. To improve the sensitivity of the model outputs, we developed a novel, life cycle thinking based hazard assessment method that facilitates the projection of hazards throughout material life cycles. Our results show that the least hazardous CIGS solar cell device and manufacturing protocol consist of a titanium substrate, molybdenum metal back electrode, $CuInS_2$ p-type absorber deposited by spray pyrolysis, ZnS buffer deposited by spray ion layer gas reduction, ZnO:Ga transparent conducting oxide (TCO) deposited by sputtering, and the encapsulant polydimethylsiloxane.

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1. Introduction

Policy makers and manufacturers advocate photovoltaic (solar) panels as a sustainable alternative to fossil fuel-based energy sources [1]. Energy conversion efficiencies for copper–indium–gallium–selenium–sulfide (CIGS) solar cells (found within solar panels) of greater than 19% have already been achieved, making CIGS a feasible solar material for future industrial competition with the incumbent mono- and polycrystalline silicon-based solar cell technologies [2,3]. CIGS solar cells are comprised of nanometer to micrometer thick layers of materials deposited during manufacture. Each layer provides a specific function, where their combination creates a semiconductor that converts light to energy. The relative thickness and material content of each layer varies among manufacturers. Six different layers are used in CIGS solar cells, as illustrated in Table 1: substrate, metal back electrode, p-type absorber, buffer, transparent conducting oxide (TCO) (also referred to in the literature as an n-type window), and encapsulant [4]. The layered nature of CIGS solar cells allows for significant variation in material composition and manufacturing processing between solar cells. This, compounded with the search for new materials and processes that improve CIGS solar cell efficiency, mechanical properties, economic viability, and sustainability [3], creates a wide diversity of CIGS manufacturing processing and solar cell material composition options.

The recent European Union directive on the Restriction on the Use of Certain Hazardous Substances in Electrical and Electronic Equipment (RoHS) [5], and the impending Safer Consumer Products Law in the State of California are examples of legislative initiatives that motivate for the removal of toxic substances from fabricated

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Table 1
Material compositions of selected commercial CIGS solar cells from Niki et al. [4].

CIGS solar cells	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
TCO	ZnO:Al	ZnO:Al	ZnO:B	ZnO:Al	ZnO:Al	ZnO:Al
Buffer	CdS	CdS	$Zn(S,OH)_x$	CdS	CdS	InS
P-type absorber	$Cu(In,Ga)Se_2$	$Cu(In,Ga)(S,Se)_2$	$Cu(In,Ga)(S,Se)_2$ $Cu(In,Ga)Se_2$	$Cu(In,Ga)Se_2$	$CuInS_2$	$Cu(In,Ga)Se_2$
Metal back electrode	Mo	Barrier Mo	Barrier Mo	Barrier Mo	Mo	Mo
Substrate	SLG	SLG	SLG	Stainless steel foil	SLG	SLG

Notes: TCO, transparent conducting oxide; SLG, soda-lime glass.
Cells with multiple entries are comprised of more than one material.

products [6]. Both pieces of legislation focus on the substances in products and neglect the potential toxic effects of the process chemicals used in their manufacture. This creates a situation that may increase the overall use of toxic substances, because the material composition of a product is the artifact of transformative chemical reactions – the use of toxic substances in manufacturing does not necessarily create a toxic product and vice versa. For CIGS solar cells, various toxic substances can be identified in both manufacturing process chemicals and in the resulting solar cells. For example, known toxic substances SeO_2, H_2S, and $CdCl_2$ are used in manufacturing while different toxic substances, such as CdS, are found within CIGS solar cells [7,8]. Because manufacturing process chemicals and solar cell material compositions are inherently linked, it is necessary to evaluate them concurrently in order to identify a less toxic process/product combination. At present, a wide variety of manufacturing process methods and CIGS solar cell material compositions are in development at the laboratory stage. The purpose of this work is to provide systematic and transparent classification of the lower hazard process/product combinations before extensive commercialization of laboratory scale technologies takes place.

For the purpose of this work, hazard is defined as the potential to cause damage, harm or an adverse effect to humans or the environment [9]. Chemicals exhibit select hazard traits that range from cancer causation to aquatic toxicity to flammability, as generally categorized into human health, environmental and physical hazards. For example, cadmium, beryllium, arsenic and vinyl chloride are known to cause cancer in humans [10]. In this context, these substances are considered to be hazardous to humans. The hazard evaluations herein do not consider fate, transport or exposure, but rather they focus solely on the human health, environmental and physical hazard traits of the substances evaluated. Furthermore, the evaluations do not account for material formulations or material quantity, in an effort to be conservative and to avoid the debate over the validity of hazard dilution [11].

The combined evaluation of the hazards associated with the substances used in manufacturing processes and the materials in the CIGS solar cells themselves into a single assessment requires life cycle thinking, but provides different guidance than a life cycle assessment (LCA). LCA is an assessment designed to quantify and combine the environmental impacts of material extraction, processing, use, and end-of-life stages of a product, process, or technology [12]. The focus of this work is to screen hazardous substances associated with the process chemicals in manufacturing and with the materials embodied in a CIGS solar cell, which correspond to hazardous impacts during the manufacture and end-of-life CIGS solar cell life cycle, respectively. Hazard is not of concern during the use stage if we assume the CIGS solar cell materials do not degrade during their lifetime. By considering the hazards of manufacture and end-of-life together, a certain degree of life-cycle thinking is applied, but this approach is not LCA for several reasons. Foremost, LCA assesses the entire product life cycle, where this assessment only considers the impacts associated with manufacture and end-of-life. In addition, LCA assesses a greater range of environmental impacts, such as global warming potential and land use. Although more impacts are considered, their classification requires the quantity of substances used at each life cycle stage, which is not available for many novel CIGS manufacturing processes or solar cells material compositions [13]. Furthermore, LCA does not consider important toxicity information for selecting low-hazard process/product combinations, such as government regulations and banned substance laws [14]. Thus, LCA is not used in this study.

Instead of LCA, we use chemical alternatives assessments (CAA) of manufacturing process chemicals and solar cell material compositions to create a focused assessment of human and environmental toxicity and hazard [15]. This hazard based CAA requires the application of scoring and screening tools that facilitate hazard comparison [15]. Hazard scoring or screening tools are methods that provide guidance for substance selection via the combination of regulatory and industry accepted hazard classification metrics and properties into scores. Each tool assesses individual chemicals and materials, and their scores can be combined to represent the hazard associated with a device or process that consists of multiple substances. The final score provides a normalized baseline for judging the relative hazard between a material and its alternatives. Such tools use a comprehensive ranking system that streamlines the comparison of materials with unrelated hazard characteristics (e.g., when comparing a compound with potential impact on aquatic life to one that is flammable). Hazard assessment tools are adaptable to make hazard comparisons for entire manufacturing processes or for products. Therefore, through a detailed case study approach, they can provide decision support for selecting the preferred manufacturing processes and solar cell material composition using hazard as a basis.

Combining both manufacturing processes and solar cell material composition CAAs requires the use of a novel life cycle thinking methodology. CAA is designed to identify the least hazardous manufacturing process and CIGS solar cell material compositions separately. However, we wish to identify the least hazardous combination of manufacturing process substances *and* solar cell materials composition. Such a connection creates a hypothetical CIGS solar cell with reduced hazard in *both* life cycle stages. Lavoie et al. [15] suggest using life cycle thinking with a CAA, but the authors do not present explicit methodologies for accomplishing this goal. To do this, we implement what we call life cycle hazard projection (LCHP).

LCHP consists initially of making a CAA at a single life cycle stage, and then utilizes the assessment to guide choices for the other stages. For example, after the hazard assessment of CIGS manufacturing processes, the combination of all essential, lowest-hazard processes can be used to make a specific CIGS solar cell. Because it may not exist, we refer to the theoretical solar cell as having a projected material composition. This theoretical solar cell can then be assessed in a separate CAA to determine its potential hazards based on its projected composition. This links both life cycle stages

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