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RESEARCH AND ANALYSIS

Life cycle assessment of emerging technologies at the lab scale

The case of nanowire-based solar cells

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Abstract

Nanomaterials are expected to play an important role in the development of sustainable products. The use of nanomaterials in solar cells has the potential to increase their conversion efficiency. In this study, we performed a life cycle assessment (LCA) for an emerging nanowire-based solar technology. Two lab-scale manufacturing routes for the production of nanowire-based solar cells have been compared—the direct growth of GaInP nanowires on silicon substrate and the growth of InP nanowires on native substrate, peel off, and transfer to silicon substrate. The analysis revealed critical raw materials and processes of the current lab-scale manufacturing routes such as the use of trifluoromethane (CHF₃), gold, and an InP wafer and a stamp, which are used and discarded. The environmental performance of the two production routes under different scenarios has been assessed. The scenarios include the use of an alternative process to reduce the gold requirements—electroplating instead of metallization, recovery of gold, and reuse of the InP wafer and the stamp. A number of suggestions, based on the LCA results—including minimization of the use of gold and further exploration for upscaling of the electroplating process, the increase in the lifetimes of the wafer and the stamp, and the use of fluorine-free etching materials—have been communicated to the researchers in order to improve the environmental performance of the technology. Finally, the usefulness and limitations of lab-scale LCA as a tool to guide the sustainable development of emerging technologies are discussed.

KEYWORDS

industrial ecology, life cycle assessment (LCA), life cycle inventory (LCI), nanotechnology, photovoltaic, sustainability

1 | INTRODUCTION

The demand for safer, greener, and more sustainable products and services has evolved rapidly in the past years (Franklin, 2015). Engineered nanomaterials are expected to play an important role in the development of such products in a wide variety of applications ranging from energy, transport, and healthcare to packaging, biomedicine, and textile sectors (European Commission, 2015).

An important application of nanomaterials is in the solar sector. Next generation photovoltaic (PV) architectures can use nanostructures to improve light trapping, thus increasing the conversion efficiency¹ of the cell (Wallentin et al., 2013). Examples of such technologies are the multijunction solar cells that consist of multiple (nano) layers in which every layer is responsible for capturing a different part of the light spectrum. Multijunction technologies that can reach conversion efficiencies close to 45% have already been developed (Dimroth et al., 2014). In this study,

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¹ Conversion efficiency of a solar cell is the percentage of energy from sunlight that is converted into electricity.

we focus on the recently emerged indium-phosphide (InP) and gallium-indium-phosphide (GaInP) nanowire-based solar cells (nanowires that combine different III-V materials). This technology can be used in a tandem formation—two-junction solar cells—in which the bottom junction is a silicon solar cell and the top junction is a nanowire solar cell. In our previous study (Pallas, Peijnenburg, Guinée, Heijungs, & Vijver, 2018), we have shown that when taking the whole life cycle of nano-based products into account, many challenges need to be addressed in order for the nanotechnological products to perform better compared to existing technologies, in terms of greenhouse gas emissions and energy consumption. The main reasons for the poor performance of nano-based technologies are, in most applications assessed, the energy-intensive processes needed for the production of nanomaterials.

To address the environmental concerns related to nanomaterials and nano-based technologies development, a holistic evaluation of their environmental performance over the entire nanoproduct's life cycle needs to be performed. Life cycle assessment (LCA) has been suggested to be the key tool in such comprehensive assessments for nanotechnologies (Bauer et al., 2008; Franklin, 2015; Guinée, Heijungs, Vijver, & Peijnenburg, 2017; Klöpffer et al., 2007). The nanowire-based solar cell technology assessed in this study is an emerging technology, which is under development at the lab scale. Concerns regarding nanomaterial development need to be tackled at this early stage of research and development (R&D). Jeswiet and Hauschild (2005) showed that about 70% of the final costs and impacts on the environment are based on decisions that are made in the early development phase of a technology. Thus, technological improvements at this early development phase can be of high importance for the future environmental performance of the technology.

Two past studies from Meijer, Huijbregts, Schermer, and Reijnders (2003) and Mohr, Schermer, Huijbregts, Meijer, and Reijnders (2007) have assessed the environmental impact of thin-film GaInP/multicrystalline silicon (GaInP/mc-Si) and GaInP/gallium-arsenide (GaInP/GaAs) tandem modules. Both these studies assess thin-film tandem technologies based on aggregated production processes using ten year old data. In our study, we assess the environmental impact of two novel lab-scale production routes for nanowire-based tandem solar cells at an early R&D stage. In addition, several past studies have focused on the so-called prospective or ex-ante LCA to study the future impact of lab-scale technologies by developing upscaling scenarios (Roes & Patel, 2011; Villares, Işildar, Mendoza Beltran, & Guinee, 2016; Walser et al., 2011). The goal of ex-ante LCA studies is to identify the impacts of a new technology in the early stage of R&D in order to prevent future unintentional environmental consequences (Arvidsson et al., 2017). In this study, we investigate whether we can use lab-scale LCA results to gain valuable insights and guide the sustainable development of emerging technologies, and we discuss how lab-scale LCA fits into the context of ex-ante LCA.

To that end, we firstly aim to investigate the potential environmental impacts and hotspots of two different lab-scale manufacturing routes of nanowire-based tandem solar cells. Thus, we perform LCA of the development of nanowire solar cells for the two manufacturing routes and identify critical hotspots in the production chain. Secondly, we aim to explore the usefulness of early-stage lab-scale LCA as a sustainability advisory tool for technology developers. Lastly, we inform the technology developers on potential system improvements, based on the outcomes of the hotspot analysis, in order to guide further sustainable development of the production of the two versions of the nanowire-based solar technology.

After this introduction, the methodology section describes the systems assessed in detail, including how the LCA was applied at the lab scale and the related scenarios that were identified. Then, results of the environmental performance of the two different production routes of the nanowire-based technology under different scenarios are presented. In addition, environmental hotspots and main contributors to environmental impacts are identified. Next, we discuss our results, draft suggestions to the technology developers for systems improvements, and discuss the usefulness of lab-scale LCA as an advisory tool to guide the sustainable development of emerging technologies. Moreover, a discussion on the uncertainties, limitations, and other issues encountered in our analysis is presented. Finally, conclusions on the insights gained from the results of the research are presented in the last section.

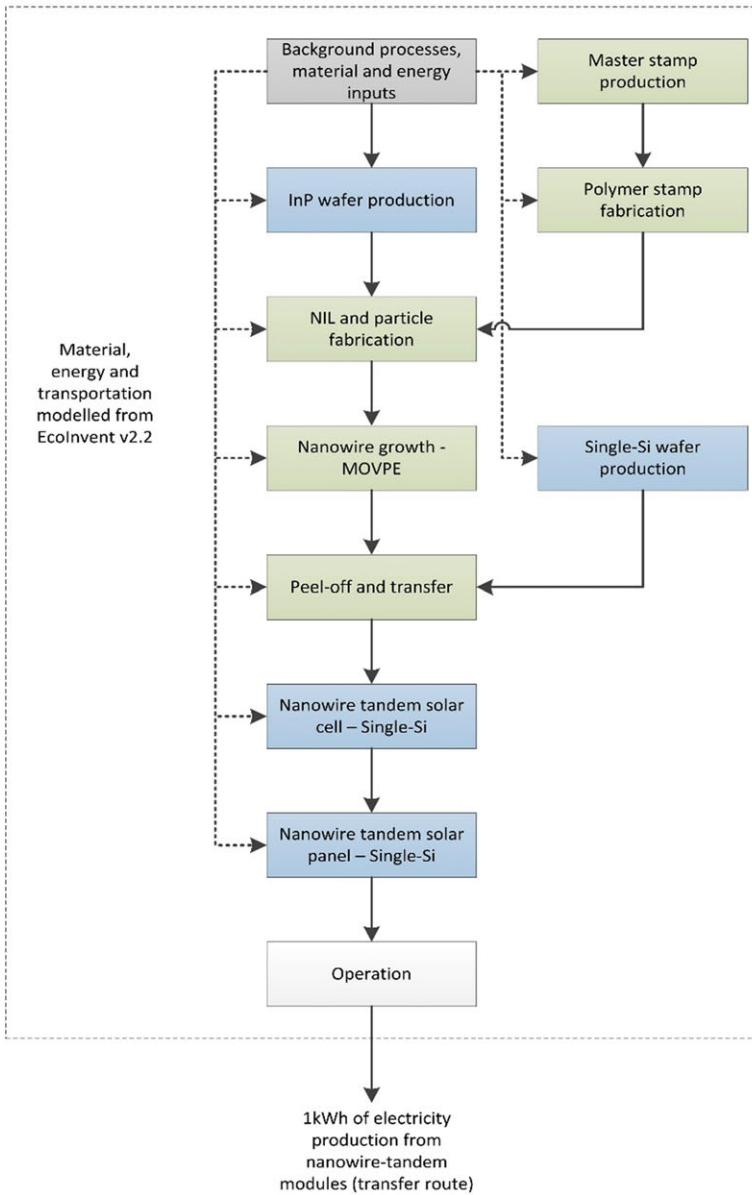
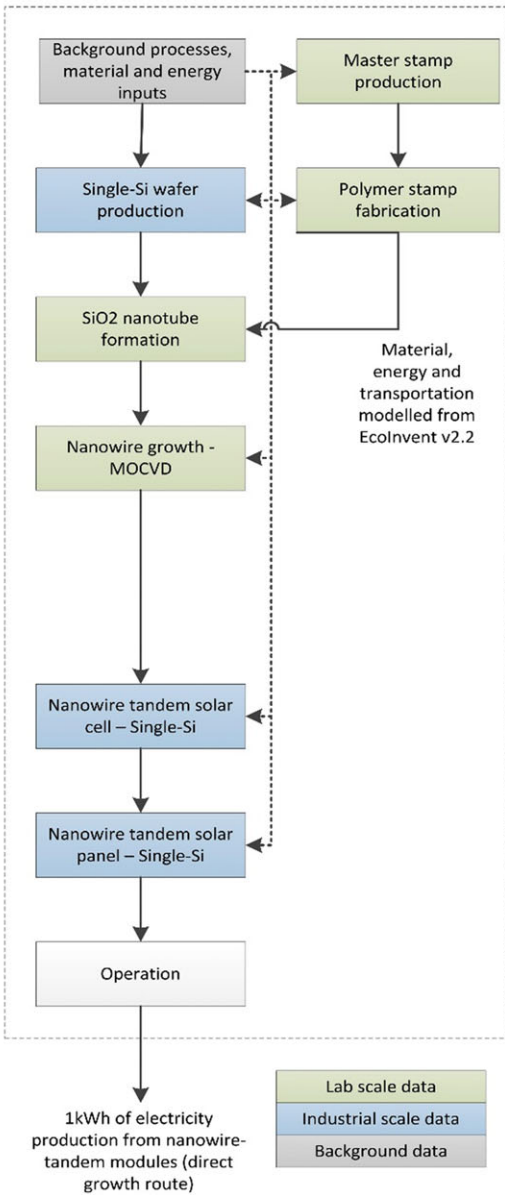
2 | METHODOLOGY

2.1 | System description: Nanowire growth, manufacturing of solar cell, and module

Two laboratory-scale production routes for nanowire growth are modeled and assessed in this study. The two production routes are:

- Direct growth route: direct growth of nanowires on a silicon wafer with metal organic chemical vapor deposition (MOCVD) using SiO₂ nanotube template assistance,
- Transfer route: metal organic vapor phase epitaxy (MOVPE) growth of nanowires on a III-V substrate, peel off, and transfer to silicon wafer (Borgström et al., 2018).

The two lab systems have some important differences. In the transfer route, nanowires are grown on InP substrate before they are transferred to silicon. In addition, there is demand for gold that is deposited on the InP wafer. On the other hand, the direct growth requires many process steps for the formation of the SiO₂ nanotube template that is used to assist the growth of nanowires directly on silicon. Details can be found in the supporting information available on the journal's website (Sections S1 and S2).

a) System Boundary
Transfer route

b) System Boundary
Direct growth route


Lab scale data
Industrial scale data
Background data

FIGURE 1 Product systems of nanowire tandem single-Si solar panels for the transfer route (System A—left) and the direct growth (System B—right) route. Lab-scale processes are represented with green color; industrial-scale processes using data from the literature are represented with blue color; background processes modeled from EcoInvent v2.2 are represented with grey color. See more detailed information for the lab-scale routes in the supporting information on the Web (Sections S1 and S2)

The laboratory system production routes for the growth of nanowires are part of the bigger system for the production of solar cell and modules. The nanowire layer together with the silicon substrate forms a tandem structure. Both routes—the direct growth and transfer—are assumed to use the most common commercial p-n junction Si solar cell as a bottom cell (Fraunhofer ISE, personal communication, 2016). In a p-n junction Si solar cell, the bottom part of the Si substrate is positively charged (p-type) and the top part is negatively charged (n-type). Together, they form the p-n junction, which allows the flow of electricity in the cell.

The supply chain for the production of silicon crystalline cells and PV modules has been very well described in past studies (Frischknecht et al., 2015; Jungbluth, Stucki, Flury, Frischknecht, & Büsser, 2012). It includes raw material extraction, purification of metallurgical-grade silicon to electronic-grade silicon and solar grade silicon, Czochralski (CZ) single-Si crystallization and wafer production, cell production, and module production. Detailed information on the supply chain for the production of crystalline silicon solar modules can be found in the supporting information on the Web (Section S3). Unit process data for the production of the single-Si solar panel can also be found in the supporting information on the Web (Tables S4–S7). Since both routes are assumed to use single-Si as a bottom cell, the differences lay in the production of nanowires. The flowchart for the production of the nanowire tandem solar modules, which presents the differences among the production routes, is shown in Figure 1.

The two manufacturing routes have their own advantages and challenges. The transfer route has the advantage that high-quality nanowire solar cells have already been demonstrated on a III-V substrate and it has a large growth parameter window (Wallentin et al., 2013). Moreover, efficient production of nanowires that are embedded in polymer and peeled off from the III-V substrate has also been demonstrated (Anttu et al., 2014). The direct growth on silicon route offers the advantage of a monolithic approach for the direct growth of nanowires to silicon substrates, provides a viable path towards scalability, and does not require an additional III-V substrate (Borg et al., 2014; Schmid et al., 2015). Challenges within the two production routes remain to be solved in order to achieve reliable functional solar devices.

2.2 | Life cycle assessment

LCA is a well-established method to quantify the potential environmental impacts of a product or technology system over its life cycle. LCA has been standardized through ISO Standards (ISO 14044, 2006) and according to these ISO Standards, four phases should be distinguished—goal and scope definition, life cycle inventory analysis, life cycle impact assessment (LCIA), and interpretation. The ISO standards do not provide practical methods, rather method requirements. Therefore, we adopted in this study the operational implementation of the ISO Standards by Guinée et al. (2002).

In this study, we performed two LCAs for the different manufacturing routes. Firstly, the laboratory processes of the two production routes for nanowire growth were modeled using primary data from lab experiments. Secondly, the industrial processes for the development of the silicon wafer, III-V wafer, silicon solar cell, and module fabrication were modeled. The data used in this stage were collected from the literature and from the ecoinvent database (version 2.2). Finally, a comparison of the environmental performance of nanowire-based solar panels for the two lab-scale manufacturing routes was performed. Environmental impacts and hotspots for the two production routes were identified and discussed.

2.2.1 | Goal and scope definition

The goal of the LCA at the laboratory scale is an investigation of the potential environmental impacts and hotspots for the two different production routes of nanowire tandem solar cells. The identification of environmental hotspots at the early stage of R&D is used as a guide for the sustainable design of the nanowire solar cell technology and provides a roadmap for the improvements that need to be considered for successful upscaling of the technology. The analysis of the environmental impact of the new solar cells is reported back to the developers of the technology to guide the sustainable development of the new technology. We do not perform a comparison to an existing commercial technology since lab-scale processes are not really comparable to industrial-scale processes. In industrial-scale processes, yields are optimized and the scale of difference between lab and industrial-scale processes can vary by many degrees of magnitude. We focus our analysis on identifying the processes and materials with better potential for upscaling, guiding the sustainable development of the technology.

The functional unit of the product system is 1 kWh of electricity production using nanowire tandem solar panels (Figure 1). The reference flows are defined as quantified flows that are linked to the use phase of the system providing the functional unit. The first alternative represents a GaInP nanowire tandem solar panel that has been developed with direct growth to a single-Si wafer. The second alternative is an InP nanowire tandem solar panel that has been grown on an InP substrate, has been peeled off, and transferred to a single-Si silicon wafer. The geographical scope of the study is assumed to be Southern Europe, with an insolation² of 1,700 kWh/m²/year.

2.2.2 | Life cycle inventory analysis

The product system analyzed includes the extraction of raw materials, wafer production, nanowire growth, cell manufacturing, module fabrication, and operation of the PV system. In this study, we have assumed the same module conversion efficiency, performance ratio (PR), and insolation (discussed below) of the nanowire tandem solar panels for both manufacturing routes, which results in the same module area. For that reason, the balance of system components (switches, wiring, inverter, and mounting system) that are related to the module area have not been included in our analysis. In addition, end-of-life (EOL) treatment has not been included in the product system due to lack of data regarding recycling of solar modules and regarding treatment and behavior of nanomaterials (nanowires) after they have been discarded. The EOL treatment of the module is not expected to show differences since both manufacturing routes are assumed to use the single-Si technology as a bottom cell and they have the same module area. Differences might occur due to the nanowire material composition. This is discussed in Section 4. The product system analyzed is linked to the background system processes of the ecoinvent v2.2 database. This linking is applied to material and energy requirements of our product system. The system boundary can be seen in the flowcharts for the production of the nanowire tandem solar panels, as presented in Figure 1. Different colors are used for the lab processes (green color) and the industrial processes (blue color). Lab system processes for the direct growth and transfer routes can be found in supporting information on the Web (Sections S1 and S2). The foreground input data linking to ecoinvent background processes are fully reported using the ecoinvent v2.2 IDs in order for the results to be reproducible and to contribute to the advancement of data transparency in the field of industrial ecology (Hertwich et al., 2018).

² Insolation is the solar radiation received on Earth. It is measured by solar energy per cm² per minute and similar units. It is affected by the angle of the Sun, daylight duration, and distance between the Earth and the Sun.

The laboratory data for the nanowire growth of the two routes are based on experimental values and energy estimations provided by the technology experts. To this end, the detailed system of processes and the material flows for the two production routes were identified (Fraunhofer ISE, personal communication, 2016; IBM Research—Zurich 2016; Lund University 2016). Lab-scale unit process data for the development of the nanowire layer for the two production routes can be found in the supporting information on the Web (Tables S1–S3). The data for the production of a single-Si wafer, cell, and PV module were based on the latest publication of Frischknecht et al. (2015) on behalf of the International Energy Agency. The ecoinvent v2.2 database has been used for the background material and energy data (Frischknecht et al., 2005). Insolation is assumed to be 1,700 kWh/m²/year, which corresponds to the Southern European countries' meteorological conditions and is a typical representation of the global average (Frischknecht et al., 2015). An 85% PR for today's PV system has been assumed, which includes losses in performance, for example due to heating of the cells (Fraunhofer ISE 2017). The typical life time of a solar module is 30 years (Fthenakis et al., 2011). For the nanowire/single-Si tandem solar cell, efficiency is assumed to be higher than 25%, which is the main objective of the EU Nano-Tandem project (EU H2020 - NanoTandem 2015). For that reason, we assume a 25% conversion efficiency for nanowire tandem modules. The module area has been calculated using the equation from Monteiro Lunardi, Ho-Baillie, Alvarez-Gaitan, Moore, and Corkish (2017). More detailed information can be found in the supporting information on the Web (Section S4).

2.3 | Additional requirements and parameters

An InP wafer is required for the transfer production route. The typical production methods for GaAs or InP wafers (wafers that consist of III-V materials) in order to achieve high pure single crystals are the liquid encapsulated Czochralski or the Bridgmann methods (Miles, Hynes, & Forbes, 2005). In this study, an InP wafer with a thickness of 350 μm is assumed to be produced by the CZ process. This is a process with high energy demand. The energy consumption of the processes has been derived on the basis of CZ single crystalline silicon and silicon wafer production from Frischknecht et al. (2015). For the InP wafer production, quantities of indium and phosphorous have been calculated using the mass of the wafer and the atomic weight of In and P (supporting information on the Web Section S5).

The metallization process for the deposition of gold is a very inefficient process. It requires about 170 times more gold than the process gold output (supporting information on the Web Section S6). Thereupon, about 90% of the remaining gold is lost in the solution after the lift-off process of the polymer layers. The metallization process can be replaced by another process called electroplating. This process reduces the gold requirements by about 300 times (Jafari Jam et al., 2014).

2.4 | Scenarios

For the transfer route, there are additional requirements compared to the direct growth route for the InP wafer production and the use of gold in the metallization process. A number of scenarios will be considered for these additional requirements. As a baseline case, we assume no reuse of wafer and stamp and no gold recovery. However, it might be feasible that both the wafer and the stamp can be used a limited number of times.

Scenario 1—reuse of wafer and stamp; the InP wafer is assumed to be used 10 times before it wears out. The stamp can be used approximately 100 times before it wears out (Tucher, Höhn, Hauser, Müller, & Bläsi, 2017). The reuse of stamp scenario is applied in both manufacturing routes.

Scenario 2—recovery of gold in the metallization process; with current practices, about 50% of the gold used in the lab is recovered (Jafari Jam et al., 2014). The gold recovery scenario is additional to the wafer and stamp reuse scenario.

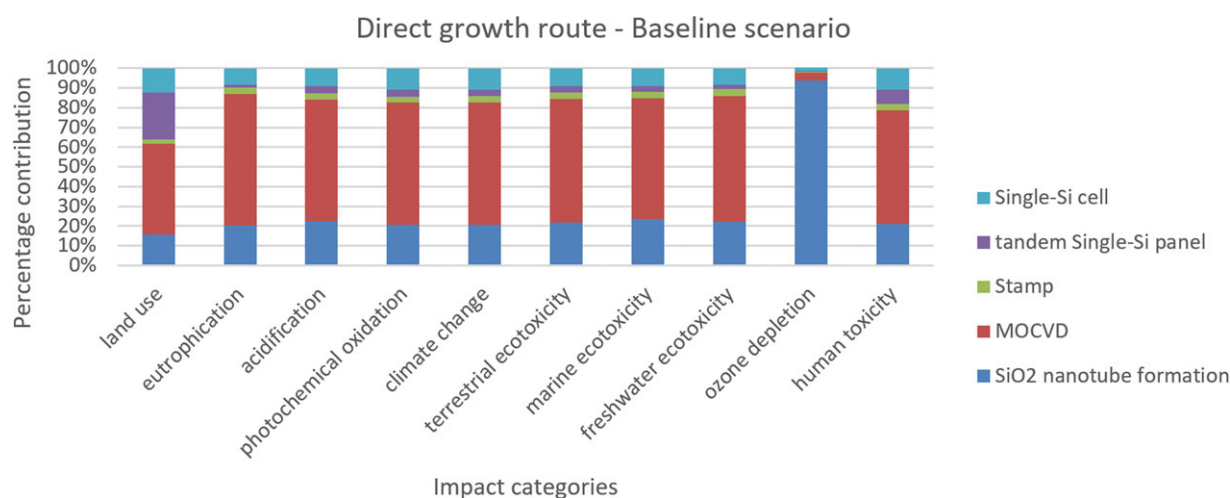
Scenario 3—replacement of the metallization process with an electroplating process; in the metallization process, gold is heated in high temperatures and evaporates. During evaporation, gold is deposited on the polymer layer at the top of the wafer. However, at the same time, most of the gold is lost on the side walls of the evaporation chamber. This process can be replaced by electroplating, in which gold particles are deposited on the wafer with the use of an anode and a cathode for the creation of an electric current and 24 karats pure gold solution. In this process, which is also called electrodeposition, there are no gold losses and the process is feasible only when the gold content in the solution is kept above a specific value. If gold is depleted below this specific value, a commercial replenisher can be used to replenish the gold solution. We recall that by replacing the metallization process with electroplating, the demand for gold can be reduced by a factor of 300. However, in this process, an additional layer of a SiN mask has to be deposited on the surface of the wafer using a plasma-enhanced chemical vapor deposition process. Additional material and energy inputs can be found in the supporting information on the Web (Table S2).

3 | RESULTS

For the LCA, CMLCA software version 5.2 beta has been used. The CML 2001 impact assessment method has been used for the LCIA (Guinée et al., 2002). The following 10 impact categories were assessed: land use, eutrophication, acidification, photochemical oxidation, climate change, terrestrial ecotoxicity, marine ecotoxicity, freshwater ecotoxicity, ozone depletion, and human toxicity.

TABLE 1 Characterization results for the direct growth and transfer routes. The difference in performance is expressed by dividing the results for the transfer route by the results for the direct growth route

Impact category	Direct growth route—baseline (Dg)	Transfer route—baseline (Tr)	Unit	Difference between routes (Tr/Dg)
Land use	2.99E-03	1.59E-02	m ² a	5.33
Eutrophication	4.50E-04	5.57E-03	kg PO ₄ -Eq	12.37
Acidification	6.30E-04	1.57E-03	kg SO ₂ -Eq	2.49
Photochemical oxidation	2.76E-05	5.61E-05	kg ethylene-Eq	2.03
Climate change	1.39E-01	2.26E-01	kg CO ₂ -Eq	1.63
Terrestrial ecotoxicity	6.17E-04	4.75E-03	kg 1,4-DCB-Eq	7.70
Marine ecotoxicity	2.22E+02	3.84E+03	kg 1,4-DCB-Eq	17.27
Freshwater ecotoxicity	6.83E-02	1.35E+00	kg 1,4-DCB-Eq	19.78
Ozone depletion	9.96E-08	1.59E-08	kg CFC-11-Eq	0.16
Human toxicity	7.37E-02	1.95E+00	kg 1,4-DCB-Eq	26.39

**FIGURE 2** Contribution (%) of the direct growth processes to various per impact categories—baseline scenario

3.1 | Direct growth route and transfer route—Baseline scenario

The carbon footprint for the production of 1 kWh of electricity is about 0.14 kg of CO₂-eq for the direct growth route and 0.22 kg of CO₂-eq for the transfer route. The direct growth route performs better in all the impact categories assessed but one—ozone depletion (Table 1). The reason for the higher ozone depletion impact is the use of trifluoromethane (CHF₃) in reactive ion etching processes. The reactive ion etching processes in the case of direct growth are used to etch away the SiO₂ layer.

On the other hand, the reason that the transfer route performs worse compared to the direct growth route is mainly due to the inefficient gold metallization process, followed by the additional need for the InP wafer that is used for the nanowire growth. It can also be noticed that for land use, eutrophication, terrestrial/marine/freshwater ecotoxicity, and human toxicity impact categories, the transfer route performs significantly worse compared to the direct growth route. For example, the human toxicity impact is more than 26 times higher for the transfer route than for the direct growth route (Table 1). The main reason behind this finding is again the deposition of gold in the metallization process. Gold particles are required for the growth of nanowires. The yield of the metallization process—which is a type of evaporation process—is very low and, in addition to that, the process is very energy intensive. The deposition of a 15 nm gold layer on a 4-inch wafer requires about 280 mg of gold. From that amount, only 1.63 mg is deposited on the wafer; the rest of the gold is lost on the walls of the chamber. In contrast, in the direct growth route, no gold is required, which explains the big difference on the toxicity impacts for the two routes, as we will see in the contribution analysis below.

3.2 | Contribution analysis of impacts

3.2.1 | Direct growth route

The contributions to the characterization results for the direct growth route are shown in Figure 2. The main driver of climate change is the MOCVD process. It contributes about 60% to the climate change impact due to its high energy demand. The MOCVD process is also the biggest contributor

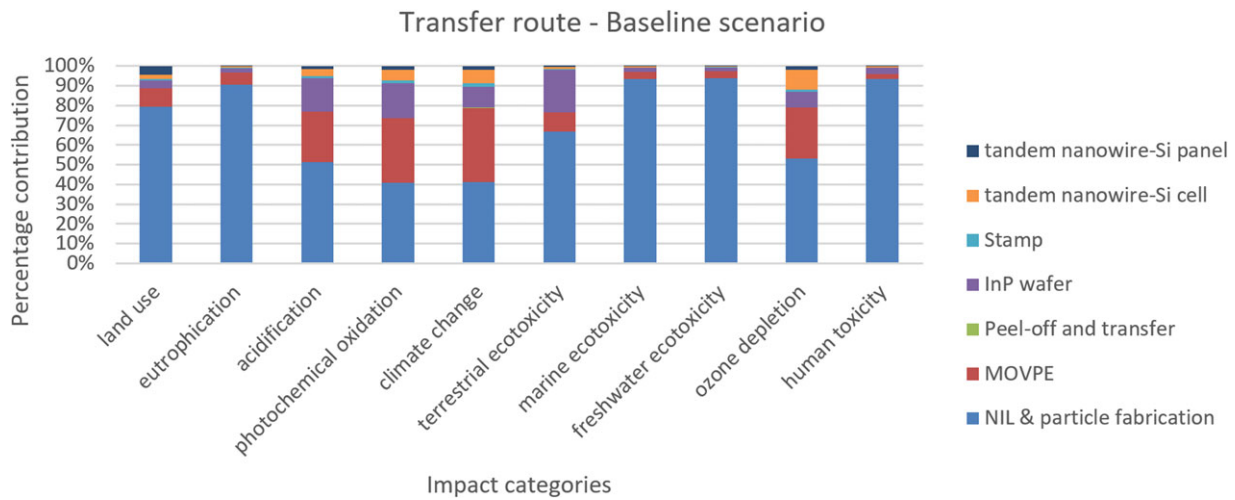


FIGURE 3 Contribution (%) of transfer route processes to various impact categories—baseline scenario

in all the impact categories assessed but one—the ozone depletion. The biggest contributors in ozone depletion are the reactive ion etching processes that are within the SiO₂ nanotube formation step (detailed results can be found in supporting information on the Web Section S8).

A more careful look at the upstream contributions to the characterization results shows that the biggest contributor to ozone depletion is the production of trichloromethane (CHCl₃). In the ecoinvent database, CHF₃ is produced from CHCl₃ and hydrogen fluoride. The production of CHCl₃ results in emissions of tetrachloromethane (CCl₄)—also known as carbon tetrachloride—to air. CCl₄, which is a long-lived substance that can stay in the atmosphere for many years, belongs to the gases responsible for stratospheric ozone depletion (Liang, Strahan, & Fleming, 2017). CCl₄ is a by-product of the production of CHCl₃, which is used as feedstock for the production of hydrochlorofluorocarbons (Fraser et al., 2014; Han, Li, Tang, & Liu, 2012) or hydrofluorocarbons and yields small emissions (Montzka et al., 2011). Even though CCl₄ is controlled by the Montreal protocol, the concentrations in the atmosphere are declining at a slower pace than expected (Liang et al., 2017), most likely due to larger unidentified or underestimated emissions (Fraser et al., 2014).

For the climate change impact, the processes related to electricity generation are the main contributors—lignite burned at the power plant, hard coal burned at the power plant, and other processes related to electricity production. They are part of the European electricity mix that has been assumed in our analysis.

3.2.2 | Transfer route

For the transfer route, the main driver of climate change is the metallization process, which is within the nano-imprint lithography (NIL) and particle fabrication step, followed by the epitaxial nanowire growth in the MOVPE process (Figure 3). For the other impact categories assessed, the main driver is the metallization process due to the use of gold (detailed results can be found in supporting information on the Web Section S8). We can also notice that the InP wafer appears to have a big contribution to terrestrial ecotoxicity, photochemical oxidation, acidification, and climate change.

The biggest upstream contributions to the characterization results of the product system originate in different background industries. For climate change, the biggest contributors are diesel burned in the building machine from the gold refinement process, followed by natural gas burned in the industrial furnace from the gold refinement and hard coal burned at the power plant and other industries related to electricity production. The outcome is different for land use, eutrophication, marine/freshwater ecotoxicity, and human toxicity. The biggest contributor to these characterization results is the disposal of sulfidic tailings off-site from the production of the gold used in the metallization process. For terrestrial ecotoxicity, the biggest contributor is the background process of gold at the refinery due to emissions of mercury into the air.

3.3 | Impact results under different scenarios

We present the characterization results for the different scenarios for two selected/representative impact categories—climate change and freshwater ecotoxicity (Figure 4). The results for the other impact categories can be found in the supporting information on the Web (Section S7).

In the first scenario, we have modeled the reuse of the wafer and the stamp. Reuse of the stamp is applied to both manufacturing routes, while reuse of the wafer is applied only to the transfer route. InP wafer and stamp reuse is feasible for a limited number of times. In our scenario, we have assumed 10 times reuse of the wafer and 100 times reuse of the stamp before it wears off. For the transfer route, reuse of the wafer results in 10% improvement in climate change and 2% improvement in freshwater ecotoxicity. Reuse of the stamp results in further slight improvement of about 2% in climate change, which gives a total of 12% improvement in climate change by the reuse of the wafer and the stamp. For the direct growth

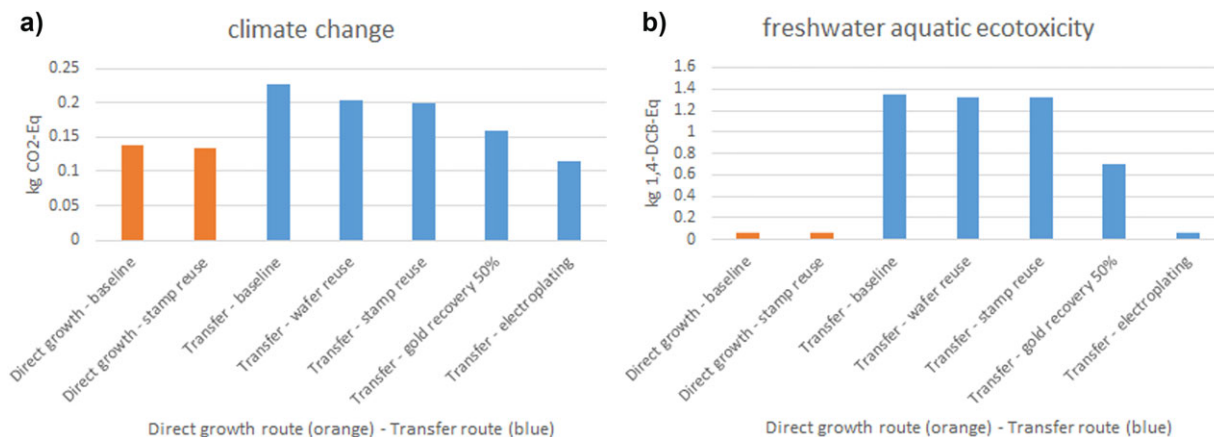


FIGURE 4 Characterization results under different scenarios: (a) climate change, (b) freshwater aquatic ecotoxicity. The direct growth route is presented by means of orange color and the transfer route is presented by means of blue color

route, reuse of the stamp results in a small 3% improvement in both climate change and freshwater ecotoxicity impacts. Stamp reuse does not appear to result in considerable change. However, since impacts in both routes are driven by other energy intensive processes or specific materials, which should be optimized when up-scaled, it is suggested that stamp reuse might have a more important role to play in an upscaled system. Finally, it is important to mention that reuse of the stamp has no impact on ozone depletion due to the fact that this is driven mostly by the use of the CHF₃ gas in the reactive ion etching processes. Results are summarized in Figure 4 and in the supporting information on the Web (Section S7).

For the gold losses during the metallization process, we have considered a second scenario in which 50% of the gold is recovered. This scenario has been modeled in addition to the reuse of the substrate and the stamp. By applying the gold recovery scenario, we see a significant improvement in the environmental performance. The climate change result is reduced by 30% and the freshwater ecotoxicity result is reduced by 48% compared to the baseline scenario (Figure 4).

In the third scenario, we model the alternative electroplating process. By replacing the metallization process with the electroplating process, requirements of gold can be reduced by a factor of 300. That results in vast improvements in most impact categories. Climate change impact is reduced by 49% and freshwater ecotoxicity impact is reduced by 95% compared to the baseline case (Figure 4). More information can be found in the supporting information on the Web (Sections S7 and S8).

4 | DISCUSSION

4.1 | Scenario analysis

In the study, a number of different scenarios have been applied for the transfer route. We showed that reuse of the wafer and stamp results in 12% reductions in climate change. However, since industrial-scale data have been used for wafer production, we should expect wafer reuse to have a more important role in a future upscaled system. It is therefore important that the technology developers find solutions to increase the lifetime of these products. In addition, the contribution analysis showed that gold use in the metallization process in the transfer route has a large impact on most impact categories and especially on land use, eutrophication, terrestrial/marine/freshwater ecotoxicity, and human toxicity. Recovery of gold with a 50% yield can significantly reduce the impacts (by in between 30% and 53% for all impact categories—see supporting information on the Web Section S7). However, by applying the electroplating method instead of metallization, the environmental performance improves even further, despite the additional materials and energy requirements of the SiN mask. The scale of improvement in some impact categories is huge (eg, reduction by 96% for human toxicity impact—see supporting information on the Web Section S7). The reason is that gold requirements are significantly reduced by the use of the electroplating process, which affects the overall impact of the transfer route. Minimization of gold use is therefore the most important driver for impact reductions. Electrodeposition can therefore be a key technology with high potential for upscaling at an industrial scale.

In the case of the direct growth route, the application of the stamp reuse scenario does not result in considerable change. In an upscaled version of the system, where process efficiencies have been achieved, reuse of the stamp might result in larger improvements in the overall impact. For the ozone depletion result—which is mainly driven by the use of CHF₃ gas due to production of CHCl₃ and emissions of CCl₄ upstream in the value chain—a different setup might be considered for future upscaling in order to reduce the ozone depletion impact. Alternative materials, such as fluorine-free etching materials (Abdolhad, Nilchi, & Mohajerzadeh, 2010), or developing an etching process optimized towards lower CHF₃ consumption are suggested to be explored for the reactive ion etching processes.

4.2 | System consistency

The definition of the system boundaries and the functional unit creates some inconsistencies in the product system. We recall that the data for the nanowire growth in the two production routes—direct growth and transfer—are provided directly from lab experiments and estimations. On the other hand, the data related to InP wafer production, single-Si wafer production, single-Si solar cell, and panel fabrication are based on industrial-scale processes. In addition, background processes and material and energy estimates provided from the ecoinvent v2.2 database are also industrial-scale data that are used as inputs in our lab system. Priority was given to the completeness of the product system in order to provide its function for the comparison of the two manufacturing routes.

4.3 | Summary of key suggestions to technology developers

The insights gained from the environmental hotspot analysis at this early stage of development are summarized in the following sections.

4.3.1 | Transfer route

- The use of gold is responsible for the high impact, in all impact categories assessed, especially in the terrestrial/marine/freshwater ecotoxicity, human toxicity, eutrophication, and land-use impact categories. It is suggested that the use of other materials—for example, silver—is explored.
- The electroplating process can replace the metallization process and is likely to provide a far better environmental performance in all impact categories due to significant reductions in the use of gold, despite the additional material and energy requirements for the SiN mask. Since the use of gold is such an important contributor to the environmental impact, the electroplating process is recommended for further research regarding upscaling.
- Reuse of stamp and wafer results in considerable improvements, for example 12% reduction in climate change impacts (10% comes from wafer reuse). Further research is thus recommended, in order to lengthen the lifetimes of the stamp and the wafer. Options on recycling/recovery of the materials contained in the wafer and stamp after their EOL are recommended to be explored.

4.3.2 | Direct growth route

- Reuse of the stamp does not result in considerable change. However, in a future upscaled technology when process efficiencies have been achieved, stamp reuse might have a more significant role. Research in increasing the stamp's lifetime is therefore suggested.
- The use of CHF_3 gas in the reactive ion etching processes results in high ozone depletion impact due to the production of CHCl_3 upstream. It is suggested that alternative materials, such as fluorine-free etching materials, or minimization of the use of CHF_3 by designing an optimized etching process, are explored.

4.4 | Validity of lab-scale results when upscaling

It is common that lab-scale technologies do not perform well compared to industrial-scale technologies. Future improvements in the production yields should be expected when scaling up a technology (Frischknecht, Büsser, & Krewitt, 2009). For example, the lab epitaxial process we modeled in this study—used to deposit III-V materials—takes place in a single reactor that can handle one wafer and requires about an hour of processing time. On the other hand, a commercial chemical vapor deposition tool for crystalline silicon solar cells can handle thousands of wafers per hour. The difference in size and throughput between lab-scale and industrial-scale processes can be huge. Moreover, in lab technology, processes such as wet etching can be done manually by scientists, while an industrial wet etching tool can handle thousands of wafers per hour. In addition, previous studies have also shown that the difference in environmental performance between a lab- and an industrial-scale technology can be very large (Villares et al., 2016; Walser, Demou, Lang, & Hellweg, 2011). Thus, no valuable insights can be gained by comparing lab-scale technology with commercial technology, except that the environmental performance of incumbent commercial technology can at least set the benchmark for the future performance of the novel technology. The aim of the lab-scale LCA is therefore not to find the most efficient technology; rather, it is to identify dominating hotspots for the development of the new technology.

Our suggestions are therefore a result of the use of lab-scale LCA to gain insights on the dominating hotspots. More specifically, the underlying commercial single-Si technology is already modeled in our product system—the single-Si wafer, cell, and module manufacturing (Figure 1). Thus, all the material and energy requirements for the development of nanomaterials are additional to the existing technology. Secondly, the contribution analysis showed that the use of CHF_3 and gold are dominating hotspots, accounting for more than 90% for some impact categories (Figures 2 and 3). In addition, the InP wafer production and the energy requirements of the epitaxial processes are also important hotspots. The epitaxial process (MOVPE or MOCVD) is expected to be significantly more efficient when it is scaled up. For that reason, there were no suggestions derived regarding the epitaxial process. On the other hand, the quantities of CHF_3 and gold required for the lab-scale production will not be significantly affected when scaling up the technology. Moreover, in an upscaled version, when other process efficiencies have been taken into account for all system processes—for example, decreased energy requirements of the scaled-up processes—the CHF_3 and gold use will likely have an even more

significant role in driving the overall impacts, if scientists will not be able to further improve their efficiency. Lastly, by modeling alternative processes for the deposition of gold, we showed that the technology scientists need to focus their attention on is the electroplating process instead of metallization; or alternatively, they could look into eliminating the use of gold by the application of different materials or processes. Similarly for the use of CHF_3 , they also need to look into alternative etching materials.

The role of lab-scale LCA as an advisory tool can fit into the context of prospective LCA in the sense that it essentially offers an identification of hotspots in the early phase of development. Such information is valuable because the freedom of altering the technology development is high in the early R&D stage, even though knowledge about the technology is limited. At a future phase of the technology and when industrial-scale investments take place, the knowledge will be more widespread, but the degrees of freedom in altering the technology will be very low. This is the so called “design paradox” or “Collingridge dilemma” (Arvidsson et al., 2017; Collingridge, 1981). Thus, the suggestions derived from our analysis lie at the center of the main reasoning for applying an LCA at an early R&D stage. Technology developers have the capability of altering the technology in order to eliminate the dominating hotspots of the use of CHF_3 and gold, due to the high degree of freedom for technology modifications that is provided at the early stage of development. It will of course be beneficial to continue performing LCAs on all the changes proposed on the basis of the lab-scale results, and to thus continue guiding the technology developers with information on the environmental performance of the developing system.

4.5 | Uncertainty

The unit process data provided in the supporting information on the Web are measurements from the lab experiments that embody inherent measurement uncertainty. However, far more major uncertainties may be attached to the technology system itself, as it is still under development. In some cases, scientists might even abandon a whole process/material and replace it with a new one. These changes cannot be captured in an early stage of LCA. For that reason, any major changes in the product system should be reflected back into the LCA model and a new analysis should take place.

The uncertainties of likely changes in the unit process data can be handled by the LCA practitioners by remaining consistent among the lab product systems compared and by understanding the overall picture. For instance, when the process time for a dry etching process is 15 min in the first lab production route and 10 min in the second lab production route, it does not mean that the etching process is more efficient in the second route. It rather reflects the specific parameters regarding the material scientists try to explore or the different tools they use. One way to address that is to select an average from these two values and apply it in both lab product systems, because this process will essentially be the same when upscaling the system for both manufacturing routes. Uncertainties of lab data measurements could be estimated in Monte Carlo simulations, for example. However, this currently has little value since it would suggest a certain quality of the results that does not exist because of the technology system changes that could still occur and cannot be included (yet) in such an uncertainty analysis. Again, the lesson from this is that the purpose of lab-scale LCA is not so much the numerical result (for example the characterization results); it rather is the identification of hotspots such as CHF_3 and gold.

For example, in the case of gold use—even if we consider upscaling—the electroplating process will always perform much better compared to the metallization process (even in the case that 50% of the gold is recovered). That is, as we showed, due to the fact that the electroplating process requires 300 times less gold compared to the metallization process. This big difference is valid in both a lab and an industrial-scale system. Similarly, the use of CHF_3 in the reactive ion etching process results in multiple times higher ozone depletion results. Moreover, in the contribution analysis presented in Figure 2, it is shown that the reactive ion etching (RIE) processes in the SiO_2 nanotube formation step contribute to more than 95% of the ozone depletion impact. Since the quantity of CHF_3 required is not expected to significantly change for the upscaled technology, it is an important hotspot that needs to be addressed at the current early R&D stage, and in the future for further development of this technology. An uncertainty analysis will not provide any additional information at this stage.

4.6 | Toxicity data

In this study, nano-specific toxicity as an environmental impact is not accounted for. The development of characterization factors (fate as well as effect factors) for nanomaterials is extremely immature. Even when scientific articles report LCA studies of products and systems based on nanotechnology, this ecotoxicity is not included, as we showed in the review study covering five different technological sectors (Pallas et al., 2018). We acknowledge that it would be of high importance to evaluate whether different material candidates for the nanowire composition are more toxic than others, in order to identify which combination of materials has the best potential for upscaling in terms of environmental performance. That type of study will be done in the future and is currently beyond the scope of this study. Nonetheless, for the same reasons as described previously, not accounting for toxicity as an impact in this lab-scale LCA between different manufacturing routes should not affect the validity of our outcomes. In particular, both manufacturing routes will have the same nanowire material composition when upscaled and the same synthesis process. Thus, the release and behavior of nanowires after their EOL should be considered the same in both routes.

5 | CONCLUSIONS

In the present study, we compared the environmental performance of two lab-scale manufacturing routes of the emerging nanowire tandem solar cells. The analysis showed that the use of CHF_3 and gold are important hotspots that need to be tackled in this early R&D stage, together with the additional impacts from the III-V wafer and stamp production. The analysis also showed that an alternative electroplating process for the gold deposition performs significantly better compared to the metallization process. A number of suggestions were proposed for the technology developers on how to deal with the environmental hotspots. Finally, we showed that, as an initial step in the early R&D stage and before upscaling the emerging technology, lab-scale LCA can play the role of an advisory tool for sustainable development by providing identification of environmental hotspots that stand out.

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CONFLICTS OF INTEREST

The authors have no conflicts of interest to declare.

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REFERENCES

- Abdolahad, M., Nilchi, J. N., & Mohajerzadeh, S. (2010). Fluorine-free high-resolution selective plasma etching of silicon-oxide layers on silicon substrates. *Journal of Physics D: Applied Physics*, 43(39), 395-402.
- Anttu, N., Abrand, A., Asoli, D., Heurlin, M., Åberg, I., Samuelson, L., & Borgström, M. (2014). Absorption of light in InP nanowire arrays. *Nano Research*, 7(6), 816-823.
- Arvidsson, R., Tillman, A.-M., Sandén, B. A., Janssen, M., Nordelöf, A., Kushnir, D., & Molander, S. (2017). Environmental assessment of emerging technologies: Recommendations for prospective LCA. *Journal of Industrial Ecology*. Retrieved from <https://doi.org/10.1111/jiec.12690>
- Bauer, C., Buchgeister, J., Hischer, R., Poganietz, W. R., Schebek, L., & Warsen, J. (2008). Towards a framework for life cycle thinking in the assessment of nanotechnology. *Journal of Cleaner Production*, 16(8-9), 910-926.
- Borg, M., Schmid, H., Moselund, K. E., Signorello, G., Gignac, L., Bruley, J., ... Riel, H. (2014). Vertical III-V nanowire device integration on Si (100). *Nano Letters*, 14(4), 1914-1920.
- Borgström, M. T., Magnusson, M. H., Dimroth, F., Siefer, G., Höhn, O., Riel, H., ... Åberg, I. (2018). Towards nanowire tandem junction solar cells on silicon. *IEEE Journal of Photovoltaics*, 8(3), 733-740.
- Collingridge, D. (1981). *The social control of technology*. New York: St. Martin's Press; London: Pinter.
- Dimroth, F., Grave, M., Beutel, P., Fiedeler, U., Karcher, C., Tibbits, T. N. D., ... Wekkeli, A. (2014). Wafer bonded four-junction GaInP/GaAs/GaInAsP/GaInAs concentrator solar cells with 44.7% efficiency. *Progress in Photovoltaics: Research and Applications*, 22(3), 277-282.
- EU H2020—NanoTandem. (2015). EU H2020 - NanoTandem project. Retrieved from <https://nano-tandem.ftf.lth.se/>
- European Commission. (2015). Horizon 2020 work programme 2016-2017. 5.ii. Nanotechnologies, advanced materials, biotechnology and advanced manufacturing and processing.
- Franklin, C. (2015). Chasing hazards: Toxicity, sustainability, and the hazard paradox. *Natural Resources & Environment*, 29, 39.
- Fraser, P. J., Dunse, B. L., Manning, A. J., Walsh, S., Wang, R. H. J., Krummel, P. B., ... O'Doherty, S. (2014). Australian carbon tetrachloride emissions in a global context. *Environmental Chemistry*, 11(1), 77-88.
- Fraunhofer ISE. (2016). Personal communication. Fraunhofer Institute for Solar Energy Systems ISE. Materials - Solar Cells and Technology MST.
- Fraunhofer ISE. (2017). Photovoltaics report. Fraunhofer ISE, Freiburg.
- Frischknecht, R., Büsser, S., & Krewitt, W. (2009). Environmental assessment of future technologies: How to trim LCA to fit this goal? *The International Journal of Life Cycle Assessment*, 14(6), 584-588. Retrieved from <http://link.springer.com/10.1007/s11367-009-0120-6>
- Frischknecht, R., Itten, R., Sinha, P., de Wild-Scholten, M., Zhang, J., Fthenakis, V., ... Stucki, M. (2015). Life cycle inventories and life cycle assessment of photovoltaic systems. International Energy Agency (IEA) PVPS Task, 12(9).
- Frischknecht, R., Jungbluth, N., Althaus, H.-J., Doka, G., Dones, R., Heck, T., ... Rebitzer, G. (2005). The ecoinvent database: Overview and methodological framework (7 pp). *The International Journal of Life Cycle Assessment*, 10(1), 3-9.
- Fthenakis, V., Frischknecht, R., Raugei, M., Kim, H. C., Alsema, E., Held, M., & de Wild-Scholten, M. (2011). Methodology guidelines on life cycle assessment of photovoltaic electricity. IEA PVPS Task, 12.

- Guinée, J. B., Gorrae, M., Heijungs, R., Huppes, G., Kleijn, R., de Koning, A., ... van Oers, L. (2002). Handbook on life cycle assessment. Operational guide to the ISO standards. *The International Journal of Life Cycle Assessment*, 7, 311.
- Guinée, J. B., Heijungs, R., Vijver, M. G., & Peijnenburg, W. J. G. M. (2017). Setting the stage for debating the roles of risk assessment and life-cycle assessment of engineered nanomaterials. *Nature Nanotechnology*, 12(8), 727–733. <https://doi.org/10.1038/nnano.2017.135>
- Han, W., Li, Y., Tang, H., & Liu, H. (2012). Treatment of the potent greenhouse gas, CHF₃—An overview. *Journal of Fluorine Chemistry*, 140, 7–16.
- Hertwich, E., Heeren, N., Kuczenski, B., Majeau-Bettez, G., Myers, R. J., Pauliuk, S., ... Lifset, R. (2018). Nullius in verba: Advancing data transparency in industrial ecology. *Journal of Industrial Ecology*, 22(1), 6–17.
- IBM Research—Zurich. (2016). Personal communication. IBM Research—Zurich. Science & Technology Department.
- Jafari Jam, R., Heurlin, M., Jain, V., Kvennefors, A., Graczyk, M., Maximov, I., ... Samuelson, L. (2014). III–V nanowire synthesis by use of electrodeposited gold particles. *Nano Letters*, 15(1), 134–138.
- Jeswiet, J., & Hauschild, M. (2005). EcoDesign and future environmental impacts. *Materials & Design*, 26(7), 629–634.
- Jungbluth, N., Stucki, M., Flury, K., Frischknecht, R., & Büsser, S. (2012). Life cycle inventories of photovoltaics. ESU-Services Ltd., Uster, CH, Retrieved from www.esu-services.ch
- Klöppfer, W., Curran, M. A., Frankl, P., Heijungs, R., Köhler, A., & Olsen, S. I. (2007). *Nanotechnology and life cycle assessment. A systems approach to nanotechnology and the environment: Synthesis of results obtained at a workshop, Washington, DC 2–3 October 2006*. European Commission, DG Research, jointly with the Woodrow Wilson International Center for Scholars.
- Liang, Q., Strahan, S. E., & Fleming, E. L. (2017). Concerns for ozone recovery. *Science*, 358(6368), 1257–1258. Retrieved from <http://science.sciencemag.org/content/358/6368/1257.abstract>
- Lund University. (2016). Personal communication. Lund University. Solid State Physics Department.
- Meijer, A., Huijbregts, M. A. J., Schermer, J. J., & Reijnders, L. (2003). Life-cycle assessment of photovoltaic modules: Comparison of mc-Si, InGaP and InGaP/mc-Si solar modules. *Progress in Photovoltaics: Research and Applications*, 11, 275–287.
- Miles, R. W., Hynes, K. M., & Forbes, I. (2005). Photovoltaic solar cells: An overview of state-of-the-art cell development and environmental issues. *Progress in Crystal Growth and Characterization of Materials*, 51(1), 1–42.
- Mohr, N. J., Schermer, J. J., Huijbregts, M. A. J., Meijer, A., & Reijnders, L. (2007). Life cycle assessment of thin-film GaAs and GaInP/GaAs solar modules. *Progress in Photovoltaics: Research and Application*, 15, 63–79.
- Monteiro Lunardi, M., Ho-Baillie, A. W. Y., Alvarez-Gaitan, J. P., Moore, S., & Corkish, R. (2017). A life cycle assessment of perovskite/silicon tandem solar cells. *Progress in Photovoltaics: Research and Applications*, 25, 679–669.
- Montzka, S. A., Reimann, S., Engel, A., Kruger, K., Sturges, W. T., Blake, D., ... Jucks, K. (2011). Scientific assessment of ozone depletion: 2010—Ozone-depleting substances and related chemicals. Global Ozone Research and Monitoring Project-Report No. 52—World Meteorological Organization.
- Organización Internacional de Normalización. (2006). ISO 14044: environmental management, life cycle assessment, requirements and guidelines. ISO.
- Pallas, G., Peijnenburg, W., Guinée, J., Heijungs, R., & Vijver, M. (2018). Green and clean: Reviewing the justification of claims for nanomaterials from a sustainability point of view. *Sustainability*, 10(3), 689. Retrieved from <http://www.mdpi.com/269112>
- Roes, A. L., & Patel, M. K. (2011). Ex-ante environmental assessments of novel technologies—improved caprolactam catalysis and hydrogen storage. *Journal of Cleaner Production*, 19(14), 1659–1667. <https://doi.org/10.1016/j.jclepro.2011.05.010>
- Schmid, H., Borg, M., Moselund, K., Gignac, L., Breslin, C. M., Bruley, J., ... Riel, H. (2015). Template-assisted selective epitaxy of III–V nanoscale devices for co-planar heterogeneous integration with Si. *Applied Physics Letters*, 106(23), 233101.
- Tucher, N., Höhn, O., Hauser, H., Müller, C., & Bläsi, B. (2017). Characterizing the degradation of PDMS stamps in nanoimprint lithography. *Microelectronic Engineering*, 180, 40–44.
- Villares, M., Işildar, A., Mendoza Beltran, A., & Guinee, J. (2016). Applying an ex-ante life cycle perspective to metal recovery from e-waste using bioleaching. *Journal of Cleaner Production*, 129, 315–328. Retrieved from <http://www.sciencedirect.com/science/article/pii/S0959652616303341>
- Wallentin, J., Anttu, N., Asoli, D., Huffman, M., Åberg, I., Magnusson, M. H., ... Witzigmann, B. (2013). InP nanowire array solar cells achieving 13.8% efficiency by exceeding the ray optics limit. *Science*, 339(6123), 1057–1060.
- Walser, T., Demou, E., Lang, D. J., & Hellweg, S. (2011). Prospective environmental life cycle assessment of nanosilver T-shirts. *Environmental Science and Technology*, 45(10), 4570–4578.

SUPPORTING INFORMATION

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