Chapter 1

General introduction

1.1. Six decades of photovoltaic technological development

In 1876, William Grylls Adams and Richard Evans Day made an astounding discovery: a solid material, selenium, could generate electricity when exposed to light. Despite the far-reaching consequences of this discovery, it was not until 1954 that the first photovoltaic (PV) cell was created at Bell Laboratories in the United States. This primordial solar cell was made of silicon and had a conversion efficiency of 4% which was later raised to 11%. At a cost-per-watt nearly 600 times higher than that of coal power plants, Bell Laboratories' silicon cell found only limited applications in miniature ship and airplane models and portable radios.[1,2]

It was the space race of the 1960s that put the solar cell as a front-runner technology to power earth-orbiting satellites, where they easily outperformed competing chemical and nuclear power alternatives.[3] While cost was not a limiting factor to put solar cells in space, it presented a very difficult barrier to making them competitive back on Earth. Solar would have to wait until the next millennium to see an enormous drop in price, enough to make them a serious alternative for terrestrial applications (Figure 1-1).

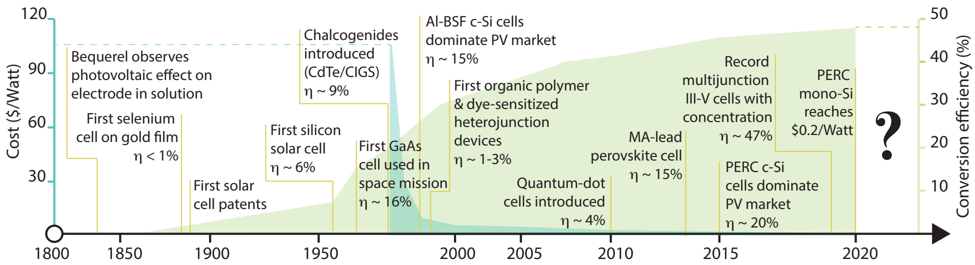

Figure 1-1 Timeline of developments in PV designs overlayed on increases in conversion efficiency and decrease in cost (in 2015 U.S. dollars). Sources: NREL[4], IEA[5].

1.2. A sunny future

There is almost no doubt that in the coming decades PV will take a leading role in energy systems across the world. Hundreds of PV growth projections have been proposed by leading experts from multiple disciplines, including the Intergovernmental Panel on Climate Change (IPCC), academic and research institutions, energy corporations, financial consultants, governments, and NGOs. The average of these projections for the compounded annual growth rate in global PV capacity deployment by the year 2050 is 10.6%, and the interquartile range is 8.6-13.6% for 1,488 scenarios evaluated (Figure 1-2).[6]

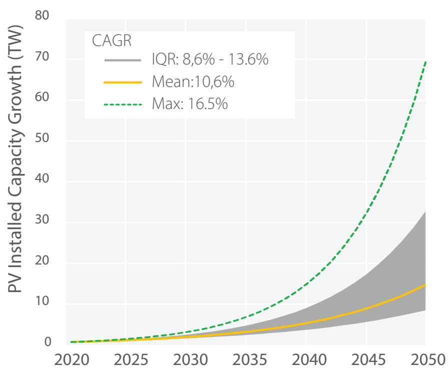

Figure 1-2 Global PV growth projections

The most optimistic scenarios see a total installed PV capacity of 70 TW by the year 2050 (and there is reason to look towards the most optimistic scenarios since most scenarios proposed to date have fallen short of actual PV growth[7]). Such a sharp increase in installed capacity could represent an impressive market share of 35% of the projected total primary energy demand. Taking an average panel conversion efficiency of 20% and a PV cell size of 156.75 x 156.75 mm, such a deployment could require 14 trillion PV cells to be installed on ca. 340 billion square meters of space (roughly 0.2% of the Earth's total land area). For a typical aluminium-glass framed PV panel weight of 11 kg/m^2, this translates to ca. 3.8 billion tonnes of installed materials, mostly glass and aluminium by weight.

1.3. Environmental benefits and trade-offs

For a long time, the environmental benefits of PV remained largely unquestioned. PV is emission-free during operation, which gives it a very strong advantage vs. combustion of fossil fuels that release carbon dioxide and methane as well as other toxic gases and particulate matter to the atmosphere. In addition to this, the PV cells and modules are mostly made of elements that have negligible adverse ecological effects when released into the environment. This means that even when landfilled at their end-of-life (EOL), PV modules are mostly inert. The massive success of the last decade and the expected growth in PV deployment, however, have evoked a closer look at potential environmental pitfalls. Insofar as conventional crystalline silicon cells (c-Si) go, these have been related to land use, the energy intensity of the silicon supply chain, and waste volumes.[8] Some additional concerns have been raised regarding the use of lead for the soldering of the PV module frames. And more recently, concerns have been raised regarding the availability/criticality of materials[9], with pure silicon being included in the EU list of critical raw materials along with other elements such as indium required in more recent PV technologies.

1.4. Multijunction III-V/silicon tandem solar cells

To date, c-Si cells have dominated the PV market due to the availability and stability of silicon and the decades of research and development (R&D) behind the technology. The current commercially available c-Si cells can convert energy from the sun with ca. 21% efficiency, while the record-holding lab prototype exceeded 26% in 2021.[4] The c-Si design has already capitalized from economies of scale (cumulative installed capacity in 2020 was 760 GW[10], provided by billions of panels) and the average cost of a c-Si module was US\$0.20/W_p in April 2020.[11] As marginal increases in c-Si efficiency now come at increasing manufacturing prices, c-Si's market dominance in the long term may be challenged if much higher efficiencies at smaller price premiums can be achieved by competing designs, leading to a lower cost per watt. Multijunction IIII-V/silicon tandem cells[12] (III-V/Si) is one emerging concept which combines c-Si bottom cells with top III-V layer absorbers to reach conversion efficiencies beyond c-Si's theoretical limit of 29.4%.[13] With significantly less time and resources invested in research and development, III-V/Si cell efficiencies above 35% have already been demonstrated at lab-scale.[14] If deployed at large scale, III-V/Si could allow for significant savings of land area, material consumption and waste generation from PV systems.

From May 2017 until April 2021, the SiTaSol project consortium[15] led by Fraunhofer ISE, and including leading industrial partners and research institutes in the field of photovoltaics, worked on developing solutions to bring the high-efficiency but very high-cost III-V/Si technology closer to commercialization. SiTaSol sought to further develop processes which could eventually meet challenging cost targets in order to improve the economic feasibility of such solar cells at large scale. The key priorities of the project were the development of a new metalorganic vapour phase epitaxy (MOVPE) reactor with an efficient use of the precursor gases, enhanced waste treatment, recycling of metals and low-cost preparation of the c-Si growth substrate. The project consortium was also tasked with evaluating the environmental impacts and risks of the technology if it were deployed at large scale. The data generated within the SiTaSol R&D program were used to inform the assessments conducted in this thesis.

1.5. *Ex-ante* environmental assessment

As innovative PV designs such as III-V/Si strive to achieve lower cost-to-output ratios ($/kWh), they become increasingly complex by introducing new materials in different configurations for which the interactions with the environment are less well-known. And yet if an innovation in PV design achieves a competitive ratio, it has a higher chance of being introduced into the market at an accelerated rate. This means it will be propagated across very large-scale production, consumption, and recycling/disposal systems across the globe. Therefore, it is imperative to better understand the environmental implications of newer designs before these large-scale systems are deployed. Once these systems are in place, it is much more difficult to modify the technology's design. This dilemma has been clearly presented by Collingridge[16] and discussed by various authors in the context of sustainability[17–19] (see Figure 1-3 and Box 1-1).

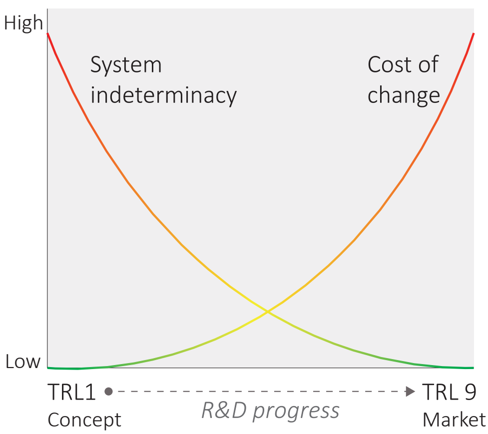

Figure 1-3 The Collingridge Dilemma (TRL: Technology Readiness Level)

In recent years, the recognition of the need for an *ex-ante* environmental assessment approach has shaped a growing sub-discipline with increasing numbers of publications and dedicated working groups across the U.S. and the European Union.[20] Perhaps the strongest backing for *ex-ante* assessments has come from the European Union, whose Horizon 2020 investment framework often requires them to grant funding for proposed R&D programs.

Several authors have attempted to provide methods or guidance frameworks for *ex-ante* assessment, particularly in LCA[21–24].

Box 1-1: Predicting the environmental performance of a future technology

The innovation process in many ways resembles the crossing of a fuzzy maze, where the pathways in close vicinity of the research topic are numerous but easily distinguishable, while the ones farther away are also numerous but evolving in time and thus harder to anticipate (Figure 1-4). Developing a commercially successful technology requires extensive trial-and-error, and backward steps are commonplace. Furthermore, technologies are often made of different components which are developed separately and then have to work together. At the same time, extrinsic drivers in the socioeconomic and environmental landscapes evolve constantly, while also being determinant of the future environmental implications of the technology.

To illustrate this situation, we can think of a researcher who is trying to come up with a revolutionary design for the car of the future. At any point in time throughout the R&D process, the researcher will face many unknowns. Some of them will be intrinsic to the technology, e.g., will plutonium fuel be sufficiently stable? Or, what will be the consumption of plutonium per km? Others will be extrinsic, e.g., will the price of plutonium be too high in the future? Or, will the global reserves of plutonium deplete and make the technology non-viable? Will social concerns or environmental regulations become too strict for radioactive fuels in commercial vehicles? A technology that enters the R&D process at TRL 1 will be subject to many changes by the time it enters the market at TRL 9. These changes are likely to have profound implications on the environmental performance of the technology. The decision of when, and under which assumptions to make an *ex-ante* assessment such as an LCA or a risk assessment (RA) is not trivial.

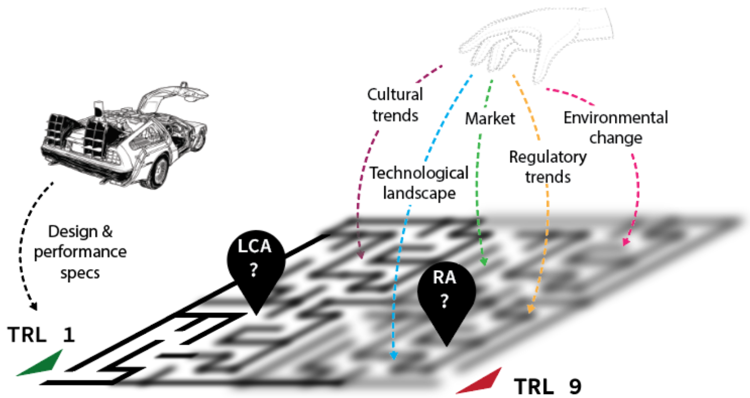

Figure 1-4 The dynamic and uncertain journey of an R&D project

On the central question of how to forecast the evolving and not fully-known future technological configurations and their behaviour in the environment, few of these proposals have placed quantitative uncertainty analysis and global sensitivity analysis[25] (GSA) at the centre of the frameworks.* Rather they have largely relied on scenario analysis and technological roadmaps[26] to explore the implications of different possible futures. One

* Throughout this work we will generally refer to uncertainty as it is considered in the modeling domain. Uncertainty is then an expression of model indeterminacy[29]. Saltelli at al.[25] define uncertainty analysis as "quantifying uncertainty in model output", and sensitivity analysis as "the study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input".

noteworthy exception is the work of Ravikumar et al.[27], who proposed the use of GSA to guide prioritization of research in "anticipatory" LCA. In the subsequent chapters of this thesis, uncertainty and sensitivity analysis take an increasingly important role until it they are placed at the centre of the *ex-ante* exercise. As will be demonstrated towards the end of this work, this will expand the capabilities of *ex-ante* assessments, enabling them to answer different questions that can better guide the R&D processes towards safer and more sustainable designs.

1.6. Research aim

The aim of this research is two-fold. On the one hand, it investigates the emerging III-V/Si cell design and the production-consumption systems in which it would be embedded, in order to determine the potential environmental impacts and risks the technology may pose when deployed at a large scale. On the other hand, it adapts and further develops existing *ex-ante* environmental assessment methods to make them more suitable to provide early guidance for the sustainable and safe design of emerging technologies. Five main research questions are posed and answered in this study:

I. What are the environmental hotspots in the emerging PV technologies landscape and what is the magnitude of the variabilities in the life cycle impacts?

II. What are the life-cycle environmental impacts of III-V/Si cells compared to c-Si cells and what are the key opportunities for improvement?

III. What are the potential ecological risks introduced by III-V/Si cells throughout their life cycles?

IV. How can unresolved technological pathways in the development of III-V/Si cells be incorporated in *ex-ante* environmental assessments?

V. How can uncertainty analysis and global sensitivity analysis be used to prioritize research directions towards safer and more sustainable design of III-V/Si tandem technologies?

1.7. Outline of this thesis

Chapter 2 takes a high-level look at the environmental performance of the emerging PV landscape by conducting a systematic review and meta-analysis of LCAs of emerging PV designs. The analysis identifies environmental hotspots and trends across the different technology types and evaluates the magnitude of the variabilities in different impact scores compared to the incumbent silicon PV modules. As the title indicates, the main question answered is whether research and innovation in PV are heading in a positive direction in terms of life cycle environmental impacts. Chapter 2 also introduces an exploratory methodological novelty in that a Random Effects Model[28] is adapted and applied to a meta-analysis of LCA studies. To adapt the model we considered the incumbent technology (c-Si) as the control group, and the emerging PV technologies as the intervention group. Design innovations such as the incorporation of different absorbent materials (e.g. perovskites, III-V elements, CdTe) are thus seen as "interventions" that can influence the life cycle impact score of PV electricity. The model allows an investigation of variation in the effect of interventions within and between studies and technology types.

Chapter 3 focuses on the III-V/Si technology and conducts an LCA with a high level of resolution. Primary data obtained from lab and pilot tests within the SiTaSol project are used and extrapolated in a first attempt to resemble industrial-scale production as much as possible. A local sensitivity analysis is used to explore the implications of future improvements in the key contributing processes such as MOVPE energy efficiency, hazardous waste treatment and recycling, as well as changes in the background energy supply.

Chapter 4 addresses perhaps the most important learning from the first full-scale LCA conducted in Chapter 3: the unresolved design choices and unknown background system parameters are too numerous so that they cannot be solved and interpreted adequately with a local sensitivity analysis or scenario analysis. While parametric uncertainty (e.g., in the energy consumption of a manufacturing process) can be easily propagated in LCA models, scenario uncertainty (e.g., whether one material or manufacturing method is chosen over another for a given component) is more challenging. We demonstrate how this problem can be overcome by introducing binomial and multinomially distributed factors in the model, which can trigger discrete events stochastically based on their expected chances of success. This allows combining an unlimited number of technological choices or pathways in a single analysis and propagating this uncertainty of process or material selection along with other parametric uncertainties.

GSA is then used to understand which of the uncertain factors contribute the most to uncertainty in the impact scores. Here, two additional novelties are introduced; for the first time, GSA is applied to such a high-dimensional model with tens of thousands of uncertain model inputs (including uncertainty in the background LCA database). This is made possible by introducing a pre-filtering step which leaves non-contributing flows out of the analysis. Second, GSA is applied for the first time to a full-scale LCA model that combines parametric with scenario uncertainties. While the analysis focuses on one component of the technology (the front metal contacts of the PV cell), it establishes the building blocks for a straightforward extrapolation to larger systems and to other types of technologies.

Chapter 5 takes the insights from the technology and the methods obtained in Chapters 3 and 4 and applies them to a different framework, that of ecological risk assessment. Chapter 5 sets out to answer what is seemingly a simple question -*what are the risks posed by III-V material emissions from III-V/silicon tandem PV modules throughout their life cycles?* However, as the common phrase goes, "the dose makes the poison". To understand what the dose is, an integration of mass flow analysis with fate and exposure assessment models is required. Furthermore, these models must be probabilistic, prospective, and dynamic to appropriately reflect the ecological risks that may be potentially introduced by the technology. Compared to LCA models, risk assessment models are more sensitive to temporal and spatial determinations which introduce an even broader range of uncertainties and variabilities. Risk assessment thus presents a more demanding test for the applicability and usefulness of the uncertainty analysis and global sensitivity analysis methods proposed in previous chapters.

Chapter 6 lays out a framework that encompasses all the methodological developments of the previous chapters, placing quantitative uncertainty analysis and global sensitivity analysis at the forefront of *ex-ante* assessment, and presenting its full potential towards guiding safer and more sustainable technological designs. Having understood the diversity and magnitude of uncertainties and variabilities that can be encountered, it is also recognized that most of the data required to characterize these uncertainties will be unavailable. A Bayesian approach to probability is presented as the most suitable one for defining and characterizing uncertainty, given the largely subjective nature and reliance on expert knowledge. The Bayesian approach completes the puzzle by providing tools and mathematical underpinning to the characterization of uncertainty and its updating with subsequent iterations that fit very naturally the R&D process.

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