



Metallurgical infrastructure and technology criticality: the link between photovoltaics, sustainability, and the metals industry

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Abstract

Various high-purity metals endow renewable energy technologies with specific functionalities. These become heavily intertwined in products, complicating end-of-life treatment. To counteract downcycling and resource depletion, maximising both quantities and qualities of materials recovered during production and recycling processes should be prioritised in the pursuit of sustainable circular economy. To do this well requires metallurgical infrastructure systems that maximise resource efficiency. To illustrate the concept, digital twins of two photovoltaic (PV) module technologies were created using process simulation. The models comprise integrated metallurgical systems that produce, among others, cadmium, tellurium, zinc, copper, and silicon, all of which are required for PV modules. System-wide resource efficiency, environmental impacts, and technoeconomic performance were assessed using exergy analysis, life cycle assessment, and cost models, respectively. High-detail simulation of complete life cycles allows for the system-wide effects of various production, recycling, and residue exchange scenarios to be evaluated to maximise overall sustainability and simplify the distribution of impacts in multiple-output production systems. This paper expands on previous studies and demonstrates the key importance of metallurgy in achieving Circular Economy, not only by means of reactors, but via systems and complete supply chains—not only the criticality of elements, but also the criticality of available metallurgical processing and other infrastructure in the supply chain should be addressed. The important role of energy grid compositions, and the resulting location-based variations in supply chain footprints, in maximising energy output per unit of embodied carbon footprint for complete systems is highlighted.

Keywords Circular economy · Sustainability · Process simulation · CdTe and Silicon photovoltaics · Life cycle assessment (LCA) · Technoeconomics

Introduction

Metals, their production, and system interactions

Technologies that enable the harnessing of renewable energy contain various metals that facilitate specific functionalities.

These include a number of precious and special metals/metalloids, often in miniscule—but essential—quantities. Most of the minor metals are only produced as co-products of their carrier metals (Bleiwas 2010), thereby drawing all associated carrier metal value chains, including the associated infrastructure, into the life cycle. As demand for some of these metals is on the increase (UNEP 2013), several of them have been classified as *critical raw materials* (CRMs) because of the combination of their economic importance, supply disruption risk, and the resource intensity associated with their extraction from lower-grade deposits (Frenzel et al. 2017; Nassar and Fortier 2021). Not all critical materials are necessarily scarce—in some cases, supply risk can be alleviated by having and keeping the right infrastructure in the right locations. Without the associated critical infrastructure, however, critical materials cannot be produced.

Manufacturing processes cause pure metals and other materials to become heavily intertwined, the degree to

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which directly impacts the effectiveness of recycling—in terms of quantity and quality—and thus circularity potential. Upon entering the end-of-life stage, devices collected for recycling become complex urban minerals in which no elements are present in pure form. As with the extraction of valuable metals from primary geological minerals, urban mineral beneficiation and extraction processes need to be designed to run at their thermodynamic limits, so optimising resource efficiency and consumption. This complexity has been visualised in the Metal Wheel, which can be found in various publications, e.g. Reuter et al. (2019) and Verhoef et al. (2004). Negative impacts on sustainability, i.e. the environmental, economy, and society, need to be minimised at the same time, while still increasing economic welfare for the stakeholders operating in the life cycle. Before such optimisation can be performed, all material and energy flows (losses and entropy creation included), and potential environmental, economic, and social impacts need to be quantified for the entire system (Reuter et al. 2019). Of particular importance is also the location of infrastructure in the supply chain, as it strongly affects sustainability—environmental impacts related to power consumption can change dramatically depending on the combination of fossil- and non-fossil energy sources in the local electricity grid. Production and recycling costs and social impacts can also change significantly between locations. With this information in hand, the potentially many trade-offs in this complex optimisation problem can be identified and quantified.

Good separation of the multitude of intertwined materials, compounds, alloys, and others usually cannot be achieved in only one reactor, but rather in a system of reactors (i.e. a plant) or a system of plants and processes which then form part of the circular economy. It is self-evident that the production and recycling of metals are not only about the technology but how best to manipulate the exchange of materials between different phases in individual reactors, between different reactors, and between systems of reactors (Reuter 2016; Reuter et al. 2021). To achieve this, mass and heat transfer between different phases in a reactor, process kinetics and dynamics, chemistry, and thermodynamics need to be understood well. Furthermore, it is about the exchange of information between life cycle stages, e.g. making available recycling data to facilitate design-for-recycling, and financial exchanges to keep the life cycle going. Two PV technologies, cadmium-telluride (CdTe) and monocrystalline Si (mono-Si) PV, will be presented to illustrate these concepts. This paper demonstrates the benefits of simulating these large life cycle systems at the process level, and linking simulations with environmental assessment and cost models, and provides insights on their sustainability and circular economy potential. For the results presented here, the authors expanded the methodologies presented in previous publications, in which the resource consumption (RC),

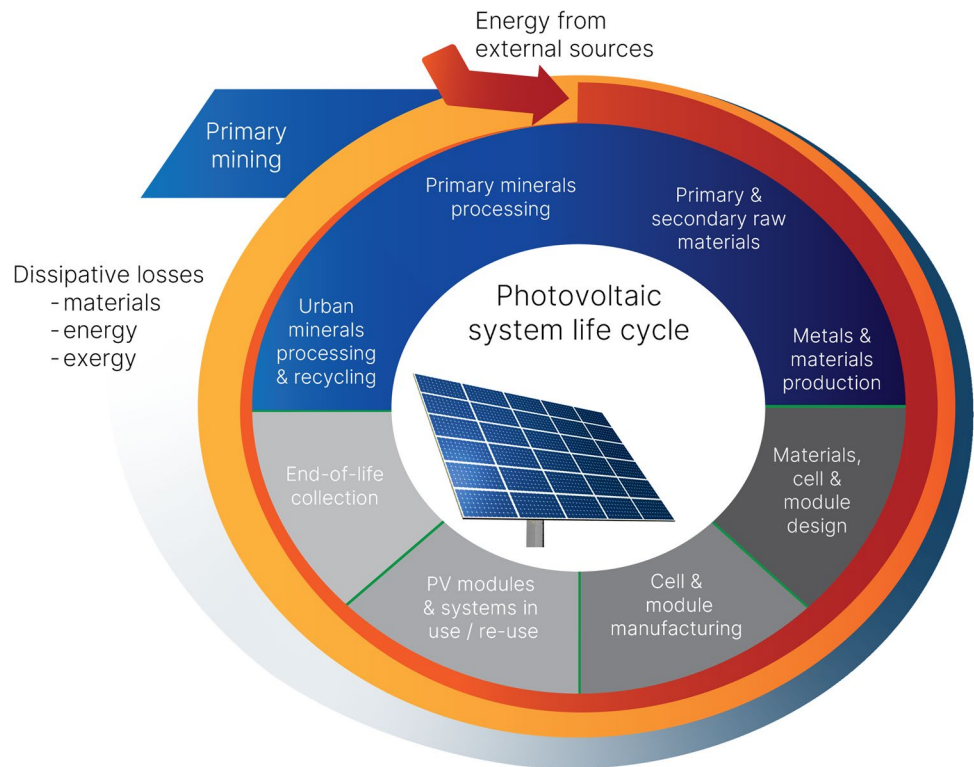
resource efficiency (RE), and environmental impacts of the CdTe (Bartie et al. 2020) and mono-Si (Bartie et al. 2021a) PV module life cycles were assessed.

The role of metals in photovoltaics

Dominant PV technologies include first-generation wafer-based crystalline silicon (c-Si) and second-generation CdTe and copper-indium-gallium-diselenide (CIGS) thin-film cells in which several semiconductor and other metal layers are deposited onto sub- or superstrates and laminated into modules with another layer of glass polymer sheet as backing. Between these three technologies, the metals and other elements needed include Ag, Al, Au, B, Cd, Cu, Ga, In, Mg, Mo, Ni, P, Pb, Se, Si, Sn, Te, Ti, Zn, and others in various combinations. Between the CRM lists of the USA and Europe, more than half of these are considered critical (European Commission 2020; Graedel et al. 2022). Significant research and development are also underway to further develop tandem modules, which consist of combinations of these and new third-generation technologies that utilise, e.g. Pb-based perovskites to maximise power conversion efficiency (PCE) (Lal et al. 2017; Mohammad Bagher et al. 2015). As the production of tandem modules effectively combines the life cycles of two different PV technologies, the resulting step changes in PCE come with increased life cycle complexity, resource requirements, losses, and impacts. Therefore, it is important to analyse PV life cycles at a detail level that enables the identification and optimisation of relevant sustainability and CE-related hotspots and trade-offs. This is important for the PV industry, to be able to assess resource and recycling requirements in the long run, and to optimise and strategise accordingly (e.g. Haegel et al. 2019).

Process simulation provides a platform for creating digital twins of systems of linked value chains and allows one to capture the detail level often missing from approaches that use aggregated input data (Jacquemin et al. 2012; Reuter 2016; Reuter et al. 2015) and often consider quantity, but not quality (Reuter et al. 2019). The work discussed in this paper has been realised using the HSC Chemistry (Metso:Outotec 2021) process simulation software. The complete supply chains have been mapped to consider all the complex non-linear combinations and chemistries in a large number of different reactors and systems. Following this approach permits calculating both energy and exergy flows (enthalpy and entropy of all streams) and linking them to power using a common unit, i.e. kW. Figure 1 shows the typical stages in a circular life cycle of a PV module with materials and energy also entering from outside the system to keep it functioning. The energy balance is represented by the orange ring, and the inevitable dissipation of exergy along the life cycle by the changing thickness of the red ring. Running the life cycle at its thermodynamic limits would minimise the thinning of this ring and reduce the amounts of external energy and

Fig. 1 PV module life cycle stages showing the consumption of external materials and energy, and their dissipation along the life cycle



materials that need to enter the system to slow down losses and keep value within the life cycle. Note that the resulting environmental and other impacts are strongly influenced by the location of each part of the complete CE infrastructure. This is discussed in Sects. 3.2.2 and 3.4.

High-detail simulations such as these facilitate simultaneous assessments of RC, RE, and potential environmental, social, and economic impacts using up-to-date operational data for existing technologies and relatively straightforward adaptation to create alternative datasets for the exploration of future scenarios. By linking these dimensions, the approach lends itself to design for sustainability and design for circularity by complementing design activities with relevant resource and sustainability information from the outset.

The Cd-Te PV system

The life cycle of a CdTe PV module is presented here as the first example of a system that encompasses several base and minor metal production chains. To manufacture a state-of-the-art CdTe PV cell, the metals needed include, among others, Al, Cd, Cu, Se, Sn, Te, and Zn. In this system, Cd is a co-product of Zn and Pb, while Te and Se are co-products of Cu (Bartie and Reuter 2021). A schematic diagram of the CdTe module life cycle is shown in Fig. 2. A thin-film PV module typically consists of a glass substrate onto which several semiconductor, metal contact, and other layers are

deposited. Apart from the encapsulant and back glass, all layers contain metals (First Solar 2020a, b).

As mentioned, Cd, Te, and Se are mainly produced as by-products, and therefore, the life cycle includes the production of their carrier metals, and not just finished semiconductors. By expanding the foreground system boundaries in this way, resource, environmental, and other hot spots can also be identified within individual processes in metal value chains, opening up more opportunities for improvement in sustainability throughout the value chain. Recycling closes the life cycle loop, albeit only partially due to material and energy inefficiencies and losses, and the creation of entropy.

The mono-Si PV system

Silicon PV technologies dominate the PV market and also rely on the availability of various materials. Despite its abundance in the earth's crust, Si metal itself is considered a critical raw material because of its economic importance and potentially increased supply risk (European Commission 2020). Continued research and development over the last decades have resulted in higher cell and module efficiencies and considerable decreases in the amount of solar grade Si (SG-Si) required to generate a Watt of power, reaching 3.6 g/W_{DC} in 2019, half of the consumption a decade prior (IEA-PVPS 2019). At the same time, however,

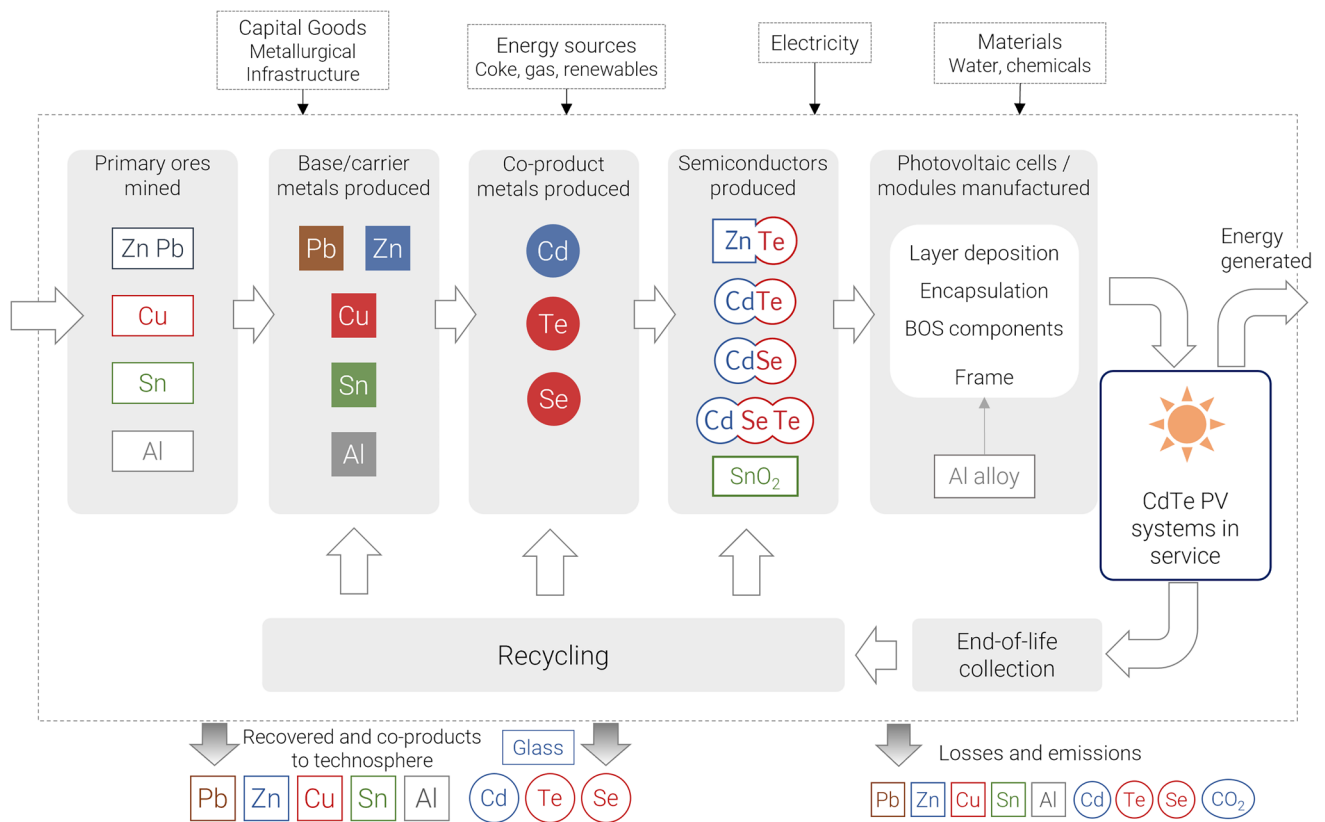


Fig. 2 Physical flows in the CdTe PV module life cycle (Bartie and Reuter 2021)

PV deployment is growing rapidly, the net effect being an increase in demand from 33 kt in 2015 to 235 kt in 2030 in the European PV industry (Gislev and Grohol 2018).

Opportunities are emerging to compensate, at least partially, for the net growth in demand from secondary resources. End-of-life (EOL) PV module quantities are expected to increase significantly between 2025 and 2030 with cumulative global PV waste quantities forecast to reach eight million tons by 2030 and almost 80 million tonnes by 2050 (IRENA and IEA-PVPS 2016). It is clear that design for circularity and sustainability and the development of complementary business models and high-quality recycling processes need to be prioritised.

The objective of recycling is to maximise RE by closing material loops. What cannot be ignored is that losses occur at every step along the way, meaning that these loops can only ever approach closure up to limits determined by life cycle design and the laws of nature. These losses cannot be designed out if they are not identified in the first place. Therefore, while EOL recycling is critically important, losses and inefficiencies need to be identified and minimised throughout the life cycle, in manufacturing processes as well as during product design. A block

flow diagram of the mono-Si system analysed is shown in Fig. 3.

Methods and approach

Digital twinning of the systems

To create a steady-state process model of the entire CdTe life cycle system shown in Fig. 2, Cu production was modelled as a sulphide flash smelting operation with electric furnace slag cleaning, Peirce Smith converting, and anode furnace refining followed by electrolytic refining to Cu cathode. Te and Se are produced through further treatment of anode slimes, and all Cu scrap is recycled internally. A combination of conventional roast-leach-electrowinning (RLE) and direct Zn smelting was used for Zn production, with Cd recovered from residues generated during RLE purification stages. Lead production was modelled as a direct smelting process with bullion refining through conventional Cu and sulphur dressing, the removal of As, Sn and Sb (and the recovery of Te from recycled semiconductor material) in the Harris process, desilvering in the Parkes process, and Zn removal by vacuum distillation.

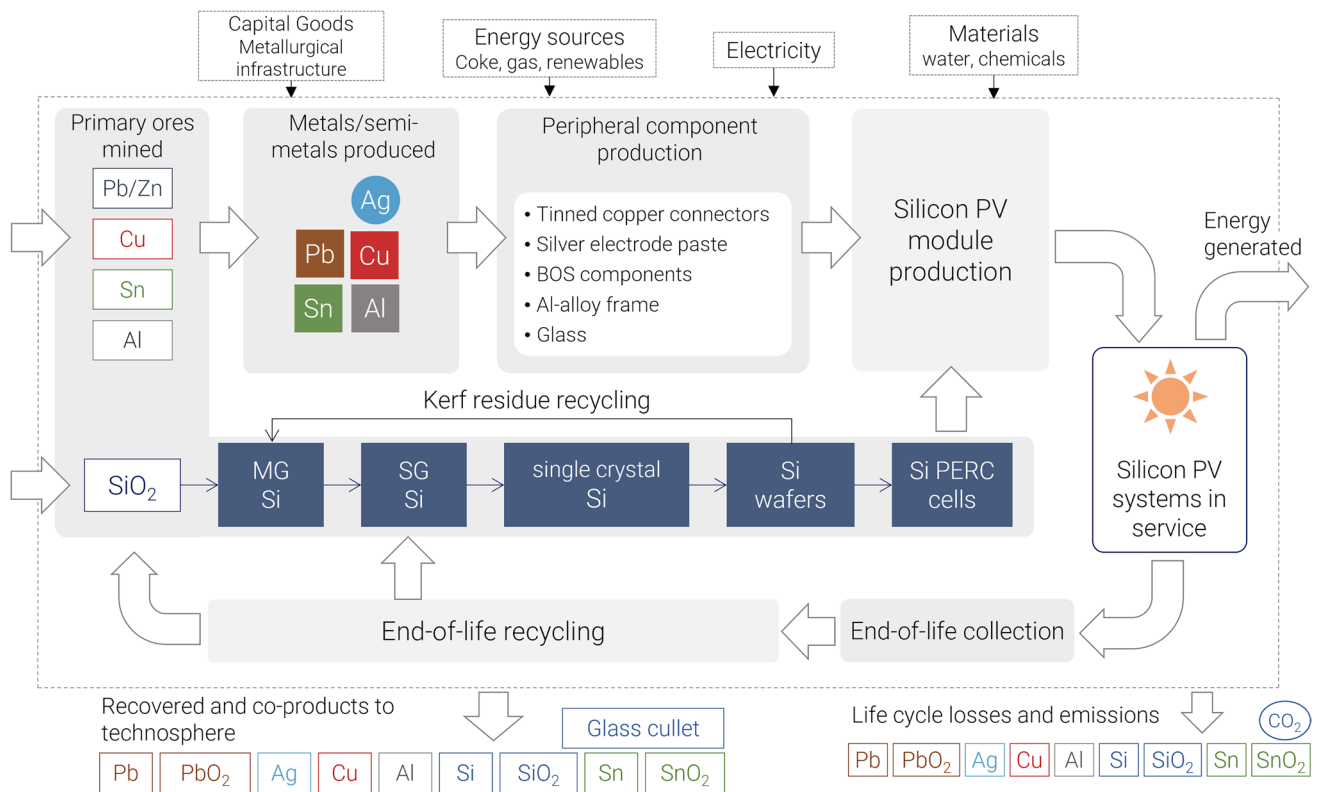


Fig. 3 Physical flows in the mono-Si PERC PV module life cycle system where PERC refers to passivated emitter and rear cell, the current industry-standard Si cell configuration (VDMA 2021)

The manufacturing and recycling of CdTe solar cells were modelled using process descriptions and data from published literature (e.g. Fthenakis 2004; Sinha et al. 2012; Wade 2013) and product specifications from the largest producer of CdTe PV technology (First Solar 2020b). Processes were linked through the exchange of compatible residues, so creating a closed loop integrated metallurgical production system that aims to minimise untreated residues and waste, and to maximise the quantities and qualities of products. Detailed descriptions of this model and all included process flowsheets can be found in previous publications (see Abadías-Llamas et al. 2019, 2020; Bartie et al. 2020). Models for the production of Pb, Zn, and Cd, and the production and recycling of CdTe PV modules are available online (Heibeck et al. 2020; Bartie and Heibeck 2020).

The same approach was used to create a detailed digital depiction of the mono-Si PV life cycle system shown in Fig. 3 to assess its RE, carbon footprint, and techno-economic performance. As with the CdTe system, the process units in each of the process blocks were modelled separately and connected to create a model for that process. The processes were then connected to create the life cycle system, and material loops closed as far as possible by means of recycling. In this simulation, metallurgical grade Si (MG-Si) is produced via the carbothermic reduction in quartz with

ladle refining for impurity removal. Solar grade Si (SG-Si) is produced with the Siemens process and monocrystalline Si (mono-Si) with the Czochralski method. Diamond wire sawing is used for the cutting of Si wafers, which then proceed to PV cell production. It is assumed that the residue that forms during wire sawing, the so-called kerf residue, is recycled to the SG-Si production process as MG-Si. For the recovery of metals and SG-Si from used wafers, a process developed by Huang et al. (2017) was simulated.

The simulation models capture the complexity of the processes and systems by considering relevant physical relationships, chemical reactions, thermodynamics, and process constants that define their response to changes in inputs or other process parameters. Results were compared with published operating points and known industrial reality for validation. Using this approach, the dependence on aggregated models for the foreground system is significantly reduced.

The Si PV simulation was expanded to include capabilities beyond that of the CdTe system simulation. These included the ability to predict the life cycle system's response to changes in wafer thickness and two recycling rates—kerf residue as MG-Si and EOL wafers as SG-Si. By additionally linking simulation results and a bottom-up cost model, the effects of recycling and a potential carbon tax

on the PV module minimum sustainable price (MSP) and levelised cost of energy (LCOE) were estimated.

To improve computational efficiency for carrying out parameter studies, which, in this case, involved the simultaneous variation in three independent variables (wafer thickness and the two recycling rates), neural networks were created as surrogate functions that represent the process simulation output. Neural networks allow for generalised nonlinear process modelling without the need to predefine regression equations (Reuter et al. 1992). To achieve this, the simulation model was run several thousand times using uniformly distributed random combinations of the three independent variables as inputs. Subsequently, a large dataset containing the corresponding simulation results for all relevant dependent variables was created. MATLAB's neural network tool was used to generate the code that initiated, trained, tested, and validated the networks using this dataset. The neural networks then allowed for the individual and simultaneous effects of EOL and kerf recycling rates, and wafer thickness throughout the system to be evaluated in a fraction of the time it would have required using only the simulation model.

Resource consumption and efficiency

The production and recycling of metals and PV modules come at a cost. Resource throughput and efficiency are often quantified separately for material and energy streams using the laws of conservation. These indicators are important but do not capture changes that may have occurred in the utility of these streams (Göbbling-Reisemann 2008). Applying the second law of thermodynamics using exergy analysis provides a way to track resource quality and its inevitable degradation along life cycles. While mass and energy always balance, exergy does not and this imbalance (i.e. irreversibility) over any process represents its degradation of the thermodynamic quality of materials and energy combined, due to the creation of entropy (refer to Fig. 1). In the approach presented here, exergy cost—the cumulative irreversibility associated with the product of interest (Szargut 2007)—serves as a proxy for resource consumption. Exergy efficiency is taken to represent the thermodynamic resource efficiency of a process. As mentioned, the advantage of exergy as an indicator is that material and energy streams are combined, and all expressed in units of measure for energy (Ayres 1998).

Environmental impact

Life Cycle Assessment (LCA) is the standardised and well-established method for assessing environmental impact (ISO 2006; ILCD 2010, 2011) and was used to estimate Global warming potential (GWP) and Acidification

potential (AP) for the CdTe system using GaBi LCA software (sphera 2020). Total carbon emissions for the mono-Si system were determined as the sum of CO₂ generated directly in each process step (Scope 1 emissions) that associated with power consumption (Scope 2 emissions), and published values for the glass, Al alloy frames, mountings, cables, and connectors (Scope 3 emissions) (de Wild-Scholten 2013; Frischknecht et al. 2015). Direct CO₂ emissions remain constant for a given production configuration, but Scope 2 and 3 emissions depend on the composition of the energy mix at the production location.

In multi-product systems such as the carrier/co-product systems described earlier, substitution cannot be applied to avoid having to allocate overall impacts to products (ISO 2006), as many of the co-products cannot be produced in alternative, standalone processes that can be used to estimate their individual impacts. According to the standard, allocation should be based on physical relationships as far as possible. In the metals industry, however, economic allocation is applied frequently. It is a hotly debated topic (e.g. Finnveden et al. 2009; Heijungs et al. 2021), especially when there are large differences between the products' economic values (Valero et al. 2015). For comparison and to highlight some of the challenges, the distribution of impacts between products in the CdTe system was calculated using mass, exergy cost, exergy content, and economic value as allocation factors.

Technoeconomic assessment (carbon pricing, MSP, and LCOE)

Technoeconomic assessments were carried out for the mono-Si system to investigate the combined effects of circularity and a hypothetical carbon tax on module cost and LCOE. A bottom-up cost model, with assumptions partly adopted from Liu et al. (2020) and Sofia et al. (2019), was utilised to estimate the effects of recycling rates, wafer thickness, and carbon taxation on MSP and LCOE. MSP, the minimum module price at which manufacturers can meet investment return expectations, was calculated using discounted cash flow analysis—the MSP is iteratively calculated as the price at which the sum of the present values of all projected future cash flows breaks even with the initial investment, i.e. the price at which the so-called net present value (NPV) is zero (Zweifel et al. 2017). LCOE, the ratio of total energy generated and total cost, was calculated for a system lifetime of 30 years, a power conversion efficiency of 21.7% (Sofia et al. 2019), an average annual irradiation of 1,500 kWh/(m².year), and an annual degradation rate of 0.5%. To create a link between the process simulation and the cost model, MG-Si and SG-Si

prices were updated based on recycling rates under the assumption that the prices of secondary Si (SG-Si from EOL wafers and MG-Si from recycled kerf) are two thirds of that produced from primary raw materials. Life cycle carbon taxes of 50 and 100 \$/tonne CO₂-equivalent (\$/tCO₂e) were considered.

Results and discussion

Resource consumption and efficiency

Resource flows in carrier/co-product metal systems for CdTe raw material production

The CdTe system is a good example of a system in which the key raw materials are produced as by-products of other systems. Approximately 40% of Te produced in the world today is used in CdTe PV applications (USGS 2021). To produce the Te and Cd, the prior production of Cu, Zn, and Pb cannot be avoided. The Cu system is required for Te production and the Zn system for Cd production. The Zn and Pb systems are linked, and the Pb system is also needed for the recycling of Te. The quantities and overall recoveries for relevant metals produced in the system to manufacture one CdTe module, as predicted using the simulation model, are shown in Table 1.

Table 1 shows that, to produce the CdTe needed for one PV module, also taking into account Cd and Te needed for non-PV uses, the system represented by this simulation would automatically also produce 104 kg Cu, 74 kg of Zn, and 35 kg of Pb due to the interconnectedness of the metal production systems. Without production infrastructure for the carrier metals, it would not be possible to bring PV modules to market. With the strong forecast growth in PV deployment (IRENA 2019), carrier- and co-metal production requirements could be challenging to meet. For CdTe PV, it has been shown that meeting even conservative demand forecasts would be limited by the periodic availability of Te, rather than its scarcity, which is strongly dependent on

the supply chain and production methods of Cu (Fthenakis 2012; Bustamante and Gaustad 2014).

Resource flows and efficiencies in the mono-Si system

Figure 4 shows a Sankey diagram representing the closed, steady state Si balance for the system, with line widths proportional to the elemental Si content of each stream. It provides a visualisation of the locations and relative magnitudes of Si-containing streams, including losses, in the life cycle for a case in which 50% of the kerf residue and 95% of EOL wafers are recycled.

Considering the streams exiting the wafer cutting process, the magnitude of the loss of high-grade, expensive SG-Si as kerf becomes clear and highlights the opportunity to increase material efficiency through kerf recycling at MG-Si quality. A second option, the vertical line between wafering and the Czochralski process, is shown for recycling kerf at the higher SG-Si quality. This option will be highlighted again in the carbon footprint analysis. Based on the configuration of our simulation, considerable amounts of Si also leave the system as microsilica, a useful byproduct used as an additive in refractories and concrete (Ciftja et al. 2008), and in residues from various other processes. By identifying and quantifying losses throughout the life cycle, a more realistic view of RE is obtained.

For the scenario shown in Fig. 4, the recoveries of materials as a percentage of the quantity entering the assumed recycling process are 86.9% Si from wafers, 70.3% Ag, 82.2% Cu, 98.9% Al (including module frames), 94.1% Sn (as SnO₂), and 94.0% Pb (as PbO₂). Note that these values have been updated from a previous version (Bartie et al. 2021a)—we have removed the assumption that 10% of recycled Si wafers can be re-used directly, and have included Al recovery from module frames.

Effects of closed-loop Si recycling on PV power potential in the mono-Si system

The use of NNs as surrogates for the simulation model allows for the effects of parameter ranges to be analysed relatively easily. Figure 5 shows the combined effects of closed-loop EOL and kerf Si recycling, at constant primary quartzite consumption, on the nominal PV power that could be generated from all the Si available in the system at a PCE of 21.7%. As one would intuitively expect, increased circularity increases power generation potential without the need for increased primary resource consumption. As described in Sect. 2.1, this effect can be quantified realistically using the thermodynamic process simulation approach. Three scenarios are shown as points in Fig. 5 at a constant quartzite consumption of 100 kt—the reference scenario with no recycling, a 95% EOL recycling scenario, and one in which

Table 1 Total mass and recovery of metals produced

| Product | Quantity produced | Recovery (%) |
|-----------------|-------------------|--------------|
| Zinc | 74 kg | 90.8 |
| Copper | 104 kg | 95.5 |
| Lead | 35 kg | 94.1 |
| Cadmium | 267 kg | 79.4 |
| Tellurium | 55 kg | 86.9 |
| CdTe PV modules | 1 unit | |

updated from Bartie and Reuter (2021) for material flows that produce one PV module

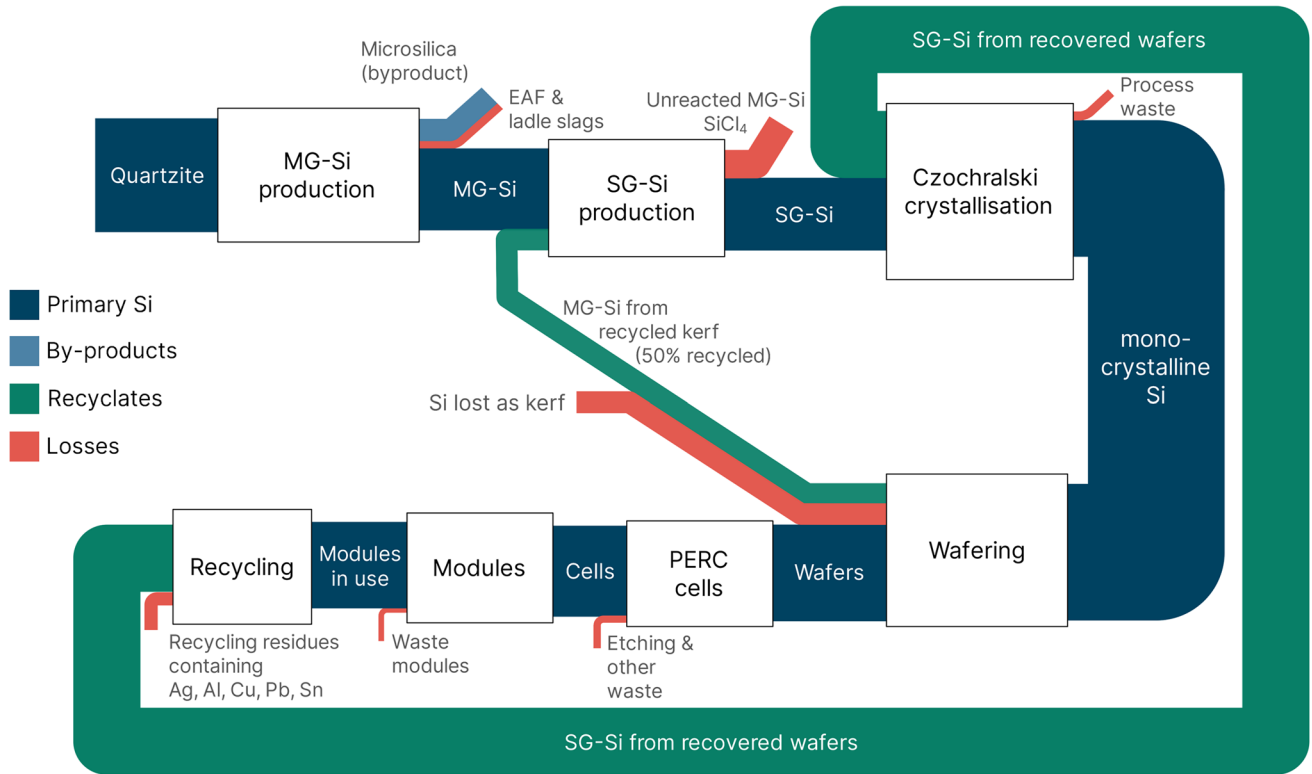
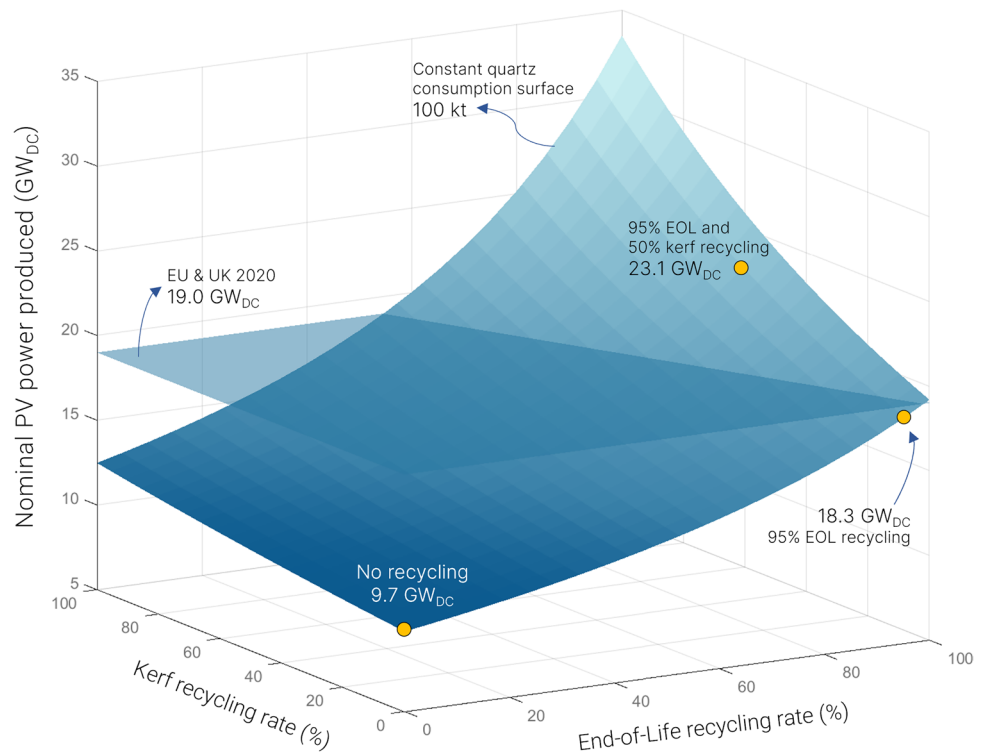


Fig. 4 Sankey diagram of the balanced flows of Si through the life cycle with 95% EOL recycling and 50% kerf recycling (Bartie et al. 2021b)

Fig. 5 Combined effects of EOL and kerf recycling on nominal PV power production at constant primary quartzite consumption (updated from Bartie et al. (2021a): PCE changed from 23% to 21.7% for consistency in this paper and actual annual PV deployed updated to 2020; underlying data can be found in the Supporting Information)



50% of the kerf residue is additionally recycled. While the simulation model allows for the curved surface to be generated for any quantity of quartzite consumption, 100 kt is used in Fig. 5 to allow for a horizontal surface representing the total nominal PV power generation capacity deployed by the EU and UK in 2020 (IEA 2021), to be shown as a tangible reference.

For the consumption of 100 kt of quartzite with no recycling, the equivalent nominal PV power generation potential is 9.7 GW_{DC}. With 95% EOL recycling, this value increases by 88%, less than 95% because of accounting for losses in the system. Adding the 50% kerf recycling results in a 137% increase from the reference scenario. In this simulation, an increase greater than 100% is achieved because primary quartzite consumption is not displaced by the equivalent amount of recycled Si but is added to the available Si in the system, representing growth in PV deployment. The 16.7 GW_{DC} of nominal PV power reference can be achieved via any combination of raw material consumption, EOL recycling rate, and kerf recycling rate on the horizontal plane at that value. However, potential trade-offs with environmental impact and economic viability must also be evaluated. More detailed results can be found in Bartie et al. (2021a).

Using exergy to identify sources of resource inefficiency

The exergy flows that occur during CdTe and mono-Si PV manufacturing are shown in Fig. 6. Of the exergy inputs (material and energy streams combined), 41% and 24% are lost irreversibly in the CdTe and mono-Si systems, respectively, which equate to specific exergy dissipations of 19.5

and 15.5 kWh/m² of these modules produced, respectively. Module sizes are based on the specifications of commercial units—0.72 m² for CdTe (First Solar 2018) and 1.96 m² for Si (Frischknecht et al. 2015). Reducing the amounts of Al used for module frames (assumed for both systems) or producing frameless modules, reducing the use of adhesives and polymer foils, and the incorporation of more renewable energy sources into electricity grid mixes are highlighted as potential opportunities for RE optimisation under the operating conditions specified in the models presented here.

This type of analysis can be done for any process or combination of processes in the life cycle. In the CdTe system, for example, a Zn fuming furnace was introduced to connect the Pb and secondary Cu systems and this resulted in a 4% increase (from 53 to 57%) in overall system exergy efficiency (Bartie et al. 2020). At the same time, however, this resulted in a 7% increase in GWP and a 9% increase in AP, highlighting the interaction and trade-offs between RE and environmental impacts that need to be optimised. It should be noted that although this system is based on best available techniques, it has not yet been optimised. Therefore, there is a high probability that efficiencies could be further improved through innovation while also reducing the magnitudes of any trade-offs. Figure 7 shows the contribution of subsystems to the total exergy cost for the production of Te and Cd. Exergy cost is expressed as exergy (in kWh) dissipated per tonne of metal produced.

For both Te and Cd, more than half of the total exergy dissipation originates from energy-intensive electrochemical refining processes. When electricity is used, its exergy (which equals its energy) is completely dissipated, regardless

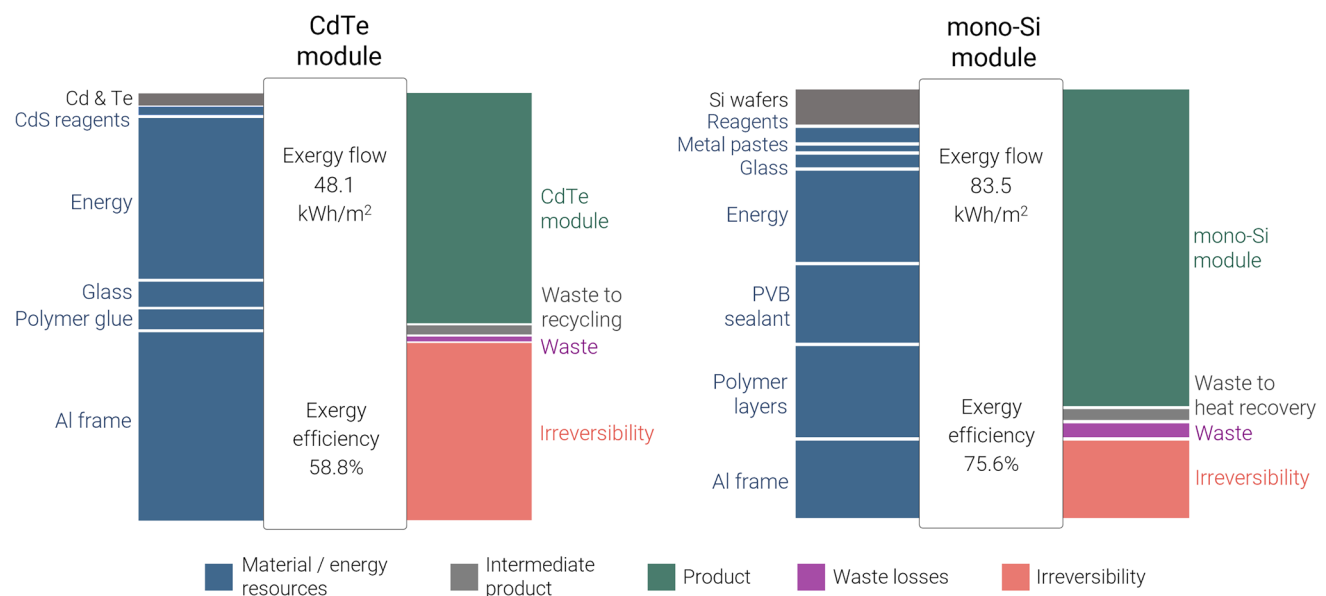


Fig. 6 Exergy flow, irreversibility, and efficiency for CdTe and mono-Si PV module manufacturing (underlying data can be found in the Supporting Information)

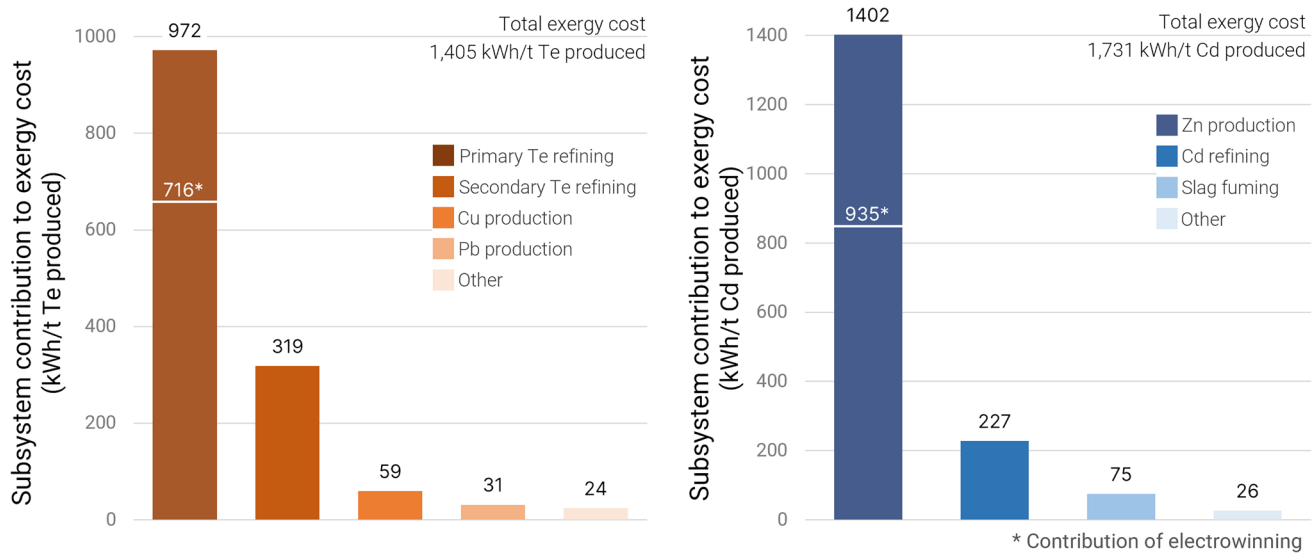


Fig. 7 Subsystem contributions to exergy cost for the production of Te (left) and Cd (right), all values determined within the process simulation model (Heibeck et al. 2020)

of how it was produced. However, its embodied environmental impact is strongly influenced by *how* it was produced (e.g. the mix of fossil and non-fossil resources used), which depends strongly on *where* it was produced. Therefore, the most effective way to improve the net sustainability of these processes would be to locate them where electricity grid mixes are made up of predominantly renewable energy sources and not in locations where carbon-based electricity grids are still the norm. This is discussed further in Sect. 3.4.

Environmental impact

Impacts and allocation challenges in the CdTe system

To produce all the quantities in Table 1, the total system GWP has been estimated at 733 kg CO₂-equivalent (kgCO₂e) and the total AP at 7.7 mol H⁺ equivalent (mol

H⁺-eq.) using the ILCD midpoint v1.09 (ILCD 2011) life cycle impact assessment method. To be able to state the environmental impact associated with individual products in this large system, the overall impacts need to be distributed in an appropriate way. As mentioned, LCA guidelines recommend that, if it cannot be avoided, allocation should be based on physical relationships between the products and their environmental impacts or on economic value, the former the preferred option. In multi-metal systems such as that presented here, allocation cannot be avoided as subdivision of the production processes is not possible (Ekvall and Finnveden 2001). Following these guidelines, the distributions of overall impacts to the system's products were calculated by quantity produced, exergy cost, exergy content, and economic value for comparison (see Table 2).

As is evident from Table 2, the results are generally inconsistent—it is difficult to decide which set of distributed

Table 2 Total emission distribution between outputs by mass, exergy cost, exergy content, and value of system products

| System output | Allocation parameter | | | |
|-----------------|--|-------------|----------------|-------------------|
| | Mass | Exergy Cost | Exergy Content | Economic value* |
| | Percentage of total impact allocated to output | | | |
| Copper | 41.7 | 38.0 | 24.0 | 62.9 |
| Zinc | 29.7 | 19.2 | 43.3 | 16.4 |
| Lead | 14.0 | 6.8 | 4.9 | 6.2 |
| Cadmium | 0.097 | 0.033 | 0.071 | 0.055 |
| Tellurium | 0.011 | 0.017 | 0.0078 | 0.22 |
| CdTe PV modules | 14.4 | 35.8 | 27.7 | 14.1 [#] |

*Based on average commodity prices for 2020 (statista.com)

[#] Based on average selling price (\$0.345/W) for 2019 (seekingalpha.com)

impacts is most likely to be representative of reality. Similar challenges have been reported by others (e.g. Stamp et al. 2013; Bigum et al. 2012). Furthermore, various additional calculation approaches are recommended in LCA guidelines to account for EOL impacts (i.e. cut-off/recycled content, EOL recycling/avoided burden), which are applied differently for open loop and closed loop recycling, and in attributional and consequential LCAs (Nordelöf et al. 2019). Detailed descriptions are beyond the scope of this paper but suffice it to say that these add further complexity and can be counterintuitive (Guinée and Heijungs 2021). Difficulties also arise when attempting to compare results with those of other researchers, as the studied systems are often not directly comparable (Farjana et al. 2019). In this study, only some of the allocated values agree with those published by e.g. Nuss and Eckelman (2014), Van Genderen et al. (2016), and Ekman Nilsson et al. (2017), and only if mixed allocation methods are used. A hybrid allocation method could, therefore, be implemented in some way, but would likely have to be based on somewhat arbitrary and subjective assumptions.

For the current system, as defined in the simulation: the price of Cd is only 3% of that of Te. To produce the CdTe semiconductor, however, Cd is clearly just as important as Te. In this case, mass-based allocation would be more appropriate. Looking at the overall system in which much larger amounts of Cu, Zn, and Pb are produced with Cd and Te for applications other than PV, value-based allocation would probably make more sense as the producer's objective would be to maximise profit. Because Te is significantly more expensive than all the other metals, a portion of the environmental impact would be allocated to it—in this case an order of magnitude more than with the other allocation factors. Such a small quantity is produced; however, that its impact is virtually negligible relative to that of the system (0.2% based on economic allocation). Similarly, and even though eleven times more Cd than Te leaves the system as a product, its allocated impact is even smaller (less than 0.1% for mass, exergy, and economic allocation). Allocation based on exergy cost gives impacts several orders of magnitude higher for both Cd and Te, but it is unclear how a sensible choice between the allocation factors would be made. Subjective or arbitrary decisions would have to be made in this scenario to generate an uncertain result that would likely carry low credibility.

The simplest and clearest way to avoid having to choose between various EOL and allocation methods and/or combinations of them is to make use of detailed process models such as those presented here and in other recent work (Abadías-Llamas et al. 2019; Bartie et al. 2020; Hannula et al. 2020; Fernandes et al. 2020). The flowsheet models contain all the necessary detail to determine the absolute emissions from every process in the system as and when they really occur, eliminating the need to divide the overall emission between outputs.

Effects of circularity on carbon footprint in the mono-Si system

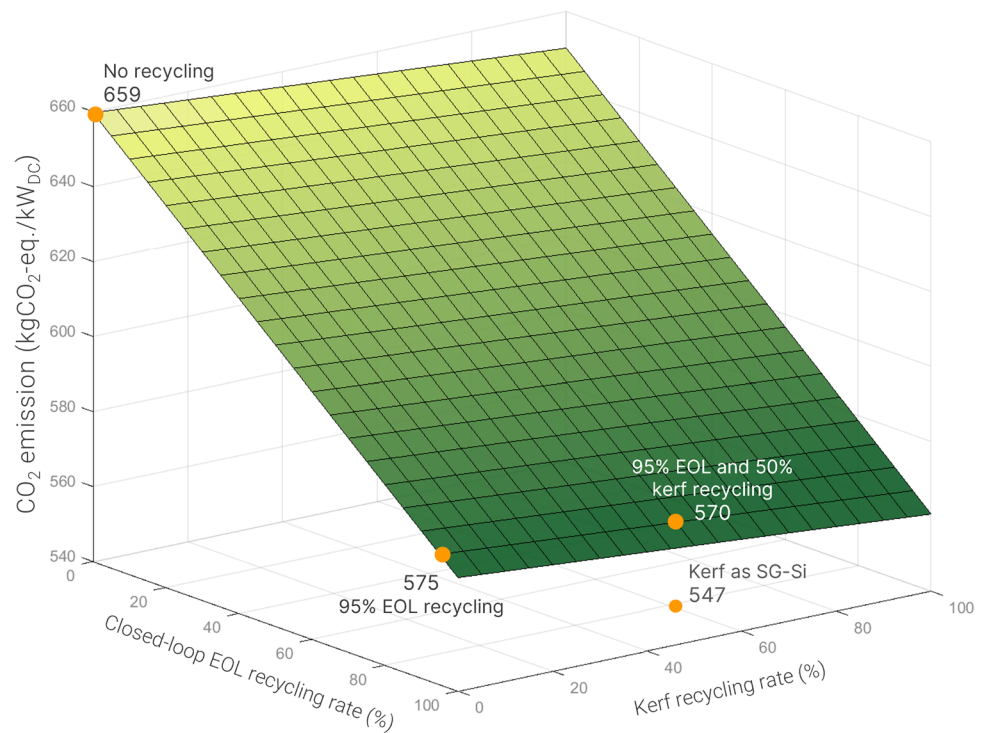
Following the same approach as for nominal power generation, Fig. 8 shows the CO₂-equivalent emissions per nominal kW power generated for the German electricity mix and quantifies how increased circularity could increase sustainability. With no recycling, emissions amount to 659 kgCO₂e/kW_{DC} based on the assumptions in our simulation, decreasing by 13% with 95% EOL recycling and an additional 1% by adding 50% kerf recycling. The decreases are mainly due to reductions in Scope 2 emissions—in the system as defined here, EOL recycling bypasses the Siemens process, which is the most energy-intensive process in the life cycle, while kerf recycling only bypasses MG-Si production. An additional 3% decrease in emissions could be achieved by recycling kerf at SG-Si quality, in which case the recyclate would also bypass the Siemens process (see Fig. 4). This analysis highlights and quantifies the effects of recyclate quality on sustainability and the potential benefits innovation and development of high-quality recycling processes could bring, albeit that the potential environmental footprint of such upcycling processes has not been considered here.

The locations of the energy-intensive processes have a strong influence on emissions. Although it is assumed in Fig. 8 that the entire life cycle is co-located on the German electricity grid, it is instructive to point out that moving it to Australia, for example, would result in a 32% increase in overall CO₂-equivalent emissions, while moving it to Brazil would result in a 26% decrease. There are, of course, other factors at play, such as where material resources are geographically located, production costs at different locations, transport costs, trade regulations, etc. No one conclusion should be viewed in isolation, but rather as part of the overall system that needs to be optimised.

Combined effects of Si wafer thickness and EOL recycling on carbon footprint in the mono-Si system

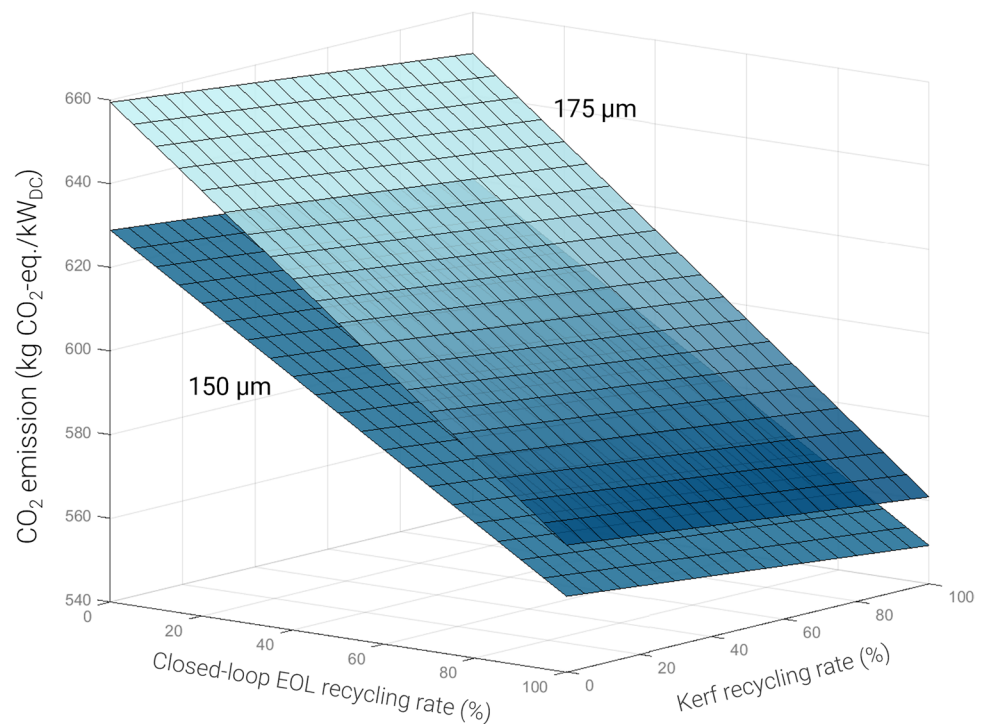
Over the last decade, improvements in cell and module efficiencies have resulted in a 50% reduction in the amount of Si needed to generate a Watt of power and this trend is expected to continue. The average thickness of the most frequently used Si wafers is currently between 170 and 175 μm, accounting for about 72% of the weight of a standard mono-Si cell (VDMA 2021). This value is expected to decrease to between 150 and 160 μm by 2031 (VDMA 2021), further reducing the consumption of Si for PV systems. Figure 9 shows the variation in CO₂-equivalent emissions with EOL and kerf recycling rate for wafer thicknesses of 150 and 175 μm. The reduction from 175 to 150 μm (without recycling) results in a 5% reduction in emissions. However, combined with an EOL recycling rate of 95%, emissions decrease by 15%. Compared to recycling alone (Fig. 8), the contribution of a 25 μm

Fig. 8 CO₂-equivalent emissions per nominal kW of power generated for module production on the German electricity grid (updated from Bartie et al. (2021a) for a PCE of 21.7% and an electricity supply emission factor of 0.558 kgCO₂e/kWh (Treyer 2021); underlying data can be found in the Supporting Information)



reduction in wafer thickness to decreasing carbon footprint is relatively small. This analysis of the effects of wafer thickness highlights one of the advantages of the process simulation approach—the ability to change process parameters and generate new process inventory data to assess the impacts of expected technology developments.

Fig. 9 Variation in CO₂ emissions with EOL and kerf recycling rate for wafer thicknesses of 150 and 175 μm (for a PCE of 21.7% and an electricity supply emission factor of 0.558 kgCO₂e/kWh (Treyer 2021); underlying data can be found in the Supporting Information)



Technoeconomic assessment and the effects of carbon taxation in the mono-Si system

Figure 10 shows the impacts carbon taxation on MSP and how it is influenced by closed-loop recycling. A carbon tax of \$100/tCO₂e increases MSP by 24% (from \$67/m² to \$83/m²) when no closed-loop EOL recycling takes

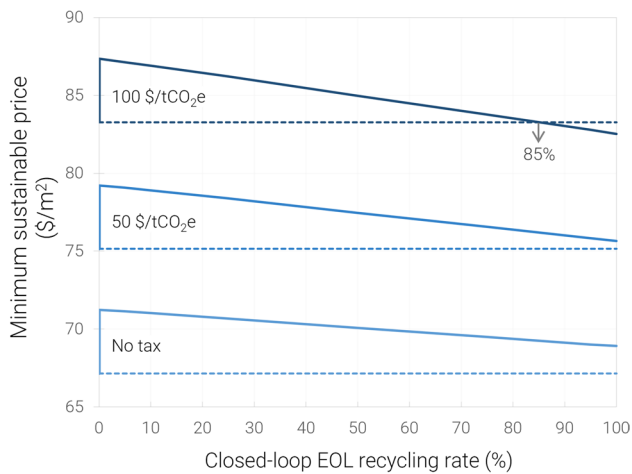


Fig. 10 Variation in manufacturing cost with EOL recycling rate at hypothetical carbon tax rates of 0, 50, and 100 \$/tCO₂e emitted (adapted from Bartie et al. 2021b; underlying data can be found in the Supporting Information)

place, and by 20% at a 95% recycling rate. As soon as recycling is introduced, an upwards step change in MSP occurs due to the fixed costs of the recycling process. As recycling rate then increases, MSP decreases but can only break even with the original MSP when the carbon tax is higher than approximately \$75/tCO₂e. Below this level, recycling cannot compensate fully for its cost. At a tax level of \$100/tCO₂e, however, the minimum recycling rate needed to break even is a relatively high 85%. These effects follow the same pattern for the LCOE, but are less significant. A \$100/tCO₂e tax results in a 6.6% increase in LCOE, from 7.81 to 8.33 c/kWh. However, the effects of balance-of-system items such as land, concrete, support structures, and others on the overall carbon footprint have not been included in our LCOE calculations yet. With these included, the effect of carbon tax on LCOE would be larger.

Both recycling and carbon taxation aim to reduce environmental impacts and lead to increased cost. The linking of process, environmental, and technoeconomic models allows for analyses such as this; however, that shows that there are conditions under which increased recycling could reduce costs to below their original values despite the carbon tax.

The location dependence of the embodied carbon footprint of PV energy in the mono-Si system

As highlighted throughout this paper, infrastructure location plays a pivotal role in life cycle sustainability. Figure 11 shows the ratio of power generated over the lifetime of a mono-Si PV system and its manufacturing carbon footprint as a function of closed-loop EOL recycling rate for different locations. It is

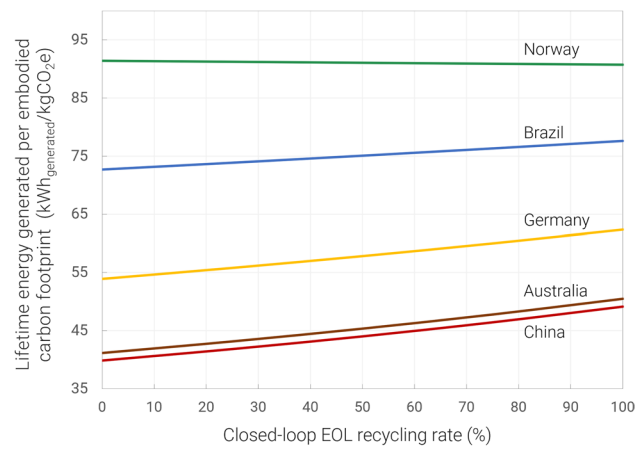


Fig. 11 Ratio of lifetime PV energy generated and its manufacturing carbon footprint as a function of EOL recycling rate (underlying data and electricity supply emission factors can be found in the Supporting Information)

assumed that manufacturing takes place in the country indicated that the PV system has a 30-year lifetime with a 0.5%/year degradation rate and a PCE of 21.7%. The average annual insolation is assumed to be 1,500 kWh/(m².year).

Figure 11 clearly shows how manufacturing location influences carbon footprint. Moving manufacturing from China or Australia to Germany, for example, would have a positive effect by increasing the ratio of energy generated and CO₂ emitted by more than 30% in the case without recycling. In China and Australia, 71% and 77% of electricity were generated from fossil resources in 2020, respectively (IEA 2022). Countries like Brazil and Norway, on the other hand, respectively, generated 75% and 98% of their electricity using wind, solar PV, and hydropower in the same year (IEA 2022). To maximise energy output per embodied carbon footprint, it is clear that infrastructure development should occur away from countries still largely dependent on fossil fuels for power generation.

Increased circularity lowers the embodied carbon footprint of PV energy, but this effect is weaker the lower the carbon intensity of the relevant electricity grid. The reason is that the strongest effect of Si recycling is its contribution to avoiding electricity consumption in energy-intensive processes and hence avoiding Scope 2 emissions. The carbon intensity of Norway's electricity grid is an order of magnitude lower than those of the other countries, and as a result, this life cycle's Scope 2 emissions are lower than its Scope 1 emissions, the latter constant regardless of location. In this case, the increase in Scope 1 emissions brought about by increased recycling is higher than the simultaneous decrease in Scope 2 emissions (explained in Sect. 3.2.2), resulting in a slightly negative slope for Norway in Fig. 11. To take full advantage of the Si circularity effect, it would make sense

to focus on using secondary Si in locations where electricity grids are most carbon-intensive.

These comparisons are based on recently published emission factors for the *generation, supply, and distribution* of electricity from the ecoinvent (version 3.8, 2021) database (Wernet et al. 2016). It should be noted that these are higher than the carbon intensities of electricity *generation* reported by the European Energy Agency (EEA) and the International Energy Agency (IEA), among others. The EEA reports a carbon intensity of 0.311 kgCO_{2e}/kWh for Germany (EEA 2021), for example, compared to the 0.558 kgCO_{2e}/kWh from the ecoinvent database (Treyer 2021). While the former is more recent (2020 vs. 2018), it does not include emissions associated with supply chains and electricity losses during transmission across networks. As a result of the time lag, the values used to generate the results presented here (and used for environmental impact assessments in general) may not fully reflect recent progress in reducing the carbon intensities of electricity consumption.

Conclusions and outlook

This paper discussed the links between the metals and PV industries with specific reference to the CdTe and mono-Si PV life cycles. The approach presented here allows for evaluation of complex systems in terms of resources, environmental impact, technoeconomic performance, and their interactions simultaneously. The use of a physics-based foundation of inventory data on a process simulation platform ensures consistency in assessments of these dimensions, so facilitating rigorous life cycle sustainability assessment. Simulation results identify system configurations that enhance RC and RE and reveal the system-wide effects of changes in these on environmental impact and technoeconomic performance, so quantifying the positive impacts of increased circularity—therefore, CE—on the system’s sustainability. The following conclusions are drawn from the work to date:

- Of the minor metals needed for CdTe and other PV module manufacturing, most are co-products of other production systems and many are CRMs. Their availability must be ensured by designing and building the necessary infrastructure without delay. The location of the infrastructure plays a decisive role in life cycle sustainability.
- In the CdTe system, an increase in overall RE was achieved by linking the Pb and Cu production subsystems by means of additional metallurgical infrastructure. The increased efficiency, however, resulted in increased environmental impact. Introducing the other dimensions of sustainability (society, economy) as well as other system improvements creates various trade-offs that need to be optimised for overall sustainability and CE.
- The analysis of recycling in the mono-Si system, of both the internal kerf residue and EOL wafers, quantified how circularity and the quality of recycled Si influence RE and carbon footprint. Both kerf and EOL wafer recycling increase the potential to generate PV power without additional consumption of the primary mineral resource. At the same time, the overall carbon footprint per module is reduced, and more so when the recyclates are of higher purity. Si recovered from wafers at SG-Si quality bypass the primary production of both MG-Si and SG-Si, resulting in significant reductions in Scope 2 (i.e. power consumption-related) emissions. For Si recovered from kerf at MG-Si quality, this effect is smaller as only the MG-Si production process is bypassed. This highlights the benefits of keeping recycling loops in the life cycle as small as possible and the importance of innovation and investment in recycling infrastructure capable of producing high-purity secondary resources for sustainable CE.
- Analysis of the combined effects of recycling and a hypothetical carbon tax in the mono-Si PV system showed that increased recycling alone is unlikely to be successful at balancing the increase in MSP caused by such a tax. Recycling itself initially increases cost, which then decreases as recycling rate increases. However, it only breaks even with the original cost at high recycling rates and high taxes. As intended with such a tax, the best remedy would be to avoid emissions in the first place, so increasing sustainability. The follow-on effect on LCOE is smaller due to other costs over and above that of the modules.
- As also reported by others, the sensible allocation of environmental impacts to products in multi-output systems remains challenging. The clearest and most efficient solution is to use process simulations that give the real emissions for every process from which impacts can be calculated directly instead of having to distribute overall emissions between products, so avoiding allocation altogether, even for very complex systems. For cases that include EOL treatment, the simulation approach provides the same clarity as recycling is modelled in the foreground system, negating the need for assumptions about what might be occurring in the background system.
- While numerous factors are at play, real RC and RE can only be quantified if entropy creation (i.e. exergy dissipation) is also accounted for. This “hidden” dissipative energy flow is usually where costs are incurred and, if not accounted for rigorously, may result in faulty policy and economic models.
- This work also suggests that supply chains for PV systems should be positioned in low environmental impact energy infrastructures to ensure that the embodied footprint of the system, including recycling, is as low as possible and enhances the performance of the system as

a whole, i.e. to maximise the ratio of energy delivered by the PV system over its lifetime and its embodied carbon emissions.

In summary, the infrastructure needed to enable the circular economy and to power sustainability is as critical as the critical materials it needs to produce from primary and secondary resources. It needs to facilitate the running of the life cycle shown in Fig. 1 at its thermodynamic limits—at the highest possible efficiency and lowest possible footprint—within prevailing social and economic constraints. It is envisaged that optimisation frameworks and results from this work would contribute to guiding strategy and policy in the renewable energy arena. Specifically, it also clearly shows quantitatively that the system, including recycling, must be positioned in energy landscapes with the lowest possible impact to ensure that the footprint of the system itself is as low as possible. The presented approach is not limited to the analysis of PV systems and can be applied to any product life cycle.

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Author contributions *Neill Bartie* involved in conceptualisation, methodology, software, validation, formal analysis, investigation, writing—original draft, visualisation; *Lucero Cobos-Becerra* took part in conceptualisation, validation, investigation, project administration; *Magnus Fröhling* involved in conceptualisation, validation, writing—review & editing, supervision; *Rutger Schlatmann* took part in conceptualisation, methodology, validation, writing—review & editing, supervision; *Markus Reuter* involved in conceptualisation, methodology, software, validation, writing—original draft, review & editing, supervision.

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Data availability The underlying data for Figs. 5 to 11 can be found in the Supporting Information.

Code availability As mentioned and cited in Sect. 2.1, two simulation models are available online (Heibeck et al. 2020; Bartie and Heibeck 2020).

Declarations

Conflicts of interest/Competing interests Not applicable.

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