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Design issues for improved environmental performance of dye-sensitized and organic nanoparticulate solar cells

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ABSTRACT

Though environmental improvement has been claimed for the application of nanotechnology to solar cells, several characteristics of the fullerene-based organic, and the dye-sensitized nanoparticulate, solar cell are not conducive to such improvement. These include relatively high energy and materials inputs in the production of nanoparticles, a relatively low solar radiation to electricity conversion efficiency, a relatively short service life, the use of relatively scarce metals and relatively poor recyclability, if compared with the multicrystalline Si solar cell which currently is the market leader. Moreover, the lack of data and the inability of current methods to handle hazards of nanoparticles generate problems in conducting comparative life cycle assessment of nanoparticulate solar cells. So far, the claimed environmental advantage can not be substantiated for fullerene-based and dye-sensitized nanoparticulate solar cells. There are options for the environmental improvement of these nanoparticulate solar cells, but actual development does not seem to focus on environmental improvement.

1. Introduction

It has been argued that the application of nanotechnology holds a promise for much improved environmental performance [1–5]. This promise has also been argued to apply to photovoltaic or solar cells [1–5]. Photovoltaic cells currently predominantly employ Si crystals which have a much larger than 100 nm diameter [6]. Among current Si-based solar cells the market leader is multcrystalline (mcSi), employing solar grade Si (which can be produced from primary metallurgical grade Si) [6]. The production process for mcSi solar cells may change in the near future due to the introduction of ribbon Si, which lowers the life cycle energy input (and costs) [6].

To look at the environmental performance of photovoltaic cells using nanotechnology, solar cells will be considered here which exploit nanoparticles (<100 nm) for power generation. Many types of nanoparticles are considered for application in solar cells, including nanocrystalline Si, C nanoparticles such as fullerenes (usually C_{60} or C_{61} and their derivatives) and a variety of metal, metal oxide, sulphide (S), arsenide (As), telluride (Te) and selenide (Se) nanoparticles [7–12]. Frontrunners among nanoparticulate photovoltaic cells are the dye-sensitized solar cells (also DS(S)C or Grätzel cells), which use TiO_2 nanoparticles [12], and fullerene-based organic solar cells [9,11]. These cells are frontrunners because they are the object of relatively much research and development work and some commercialization. DS(S)Cs are marketed by companies such as 3G Solar, G24 Innovations, Solarprint and Dyesol, and fullerene-based organic solar cells by Konarka Technologies. Both DS(S)C and fullerene-based organic solar cells will be considered here.

The DS(S)C consists of a nano-TiO_2 photo electrode, an organometallic or organic dye (sensitizer), an electrolyte and a counter electrode. Between the electrodes of an organic solar cell is usually a 'bulk heterojunction' layer of fullerenes and polymers. A buffer layer for the electrode of e.g. TiO_2 or LiF may also be included.

The TiO_2 of the DS(S)C may be on a layer containing In (indium) and/or Sn (tin), and the electrodes of nanoparticulate cells may contain the same metals (In, Sn), Pt (platinum), Au (gold), Cr (chromium) or Al (aluminum).

This paper will discuss major determinants of the 'cradle to grave' or life cycle environmental performance of the DS(S)C and the fullerene-based organic solar cells which serve the electricity grid for 25 years and options for their environmental improvement. A comparison will be made with mcSi cells which serve the electricity grid and do not employ nanoparticles, on the basis of the production of the same amount of kilowatt-hours (kWh).

Claims about the environmental advantage of solar cells employing nanoparticles can be traced back to the much lower

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input of materials in the solar cells themselves, which (ceteris paribus) has a favorable impact on environmental performance in life cycle assessment [4,8,12]: 'less is better'.

On the other hand, there may also be characteristics of nanoparticulate solar cells which may have (ceteris paribus) the opposite effect of increasing life cycle environmental impact or burden.

The following characteristics of current dye-sensitized and fullerene-based nanoparticulate solar cells come to mind [14–21]:

- producing nanoparticles may require much larger inputs of energy (in practice fossil fuels) and materials than the production of the same mass of larger-sized materials [13],
- a relatively low efficiency in converting solar irradiation into electricity, if compared with mcSi cells [14,20,21],
- a relatively short service life [15–19],
- relatively poor recyclability of nanoparticle-based solar cells,
- the use of metals derived from relatively scarce natural resources, such as Pt, Au, Sn, In and Ru (ruthenium).

The combined effect of these aspects may well be substantial. Analyses of the life cycle CO_2 emission kW h^{-1} of current DS(S)Cs show a relatively high emission, if compared to current mcSi cells [12,20,21]. Similarly, present life cycle CO_2 emissions per kWh from fullerene-based cells exceed those of mcSi cells [22]. Raugei and Franckl have suggested a relatively high life cycle CO_2 emission kW h^{-1} for future DS(S)C, if compared with solar cells based on ribbon Si [6].

The aspects of nanoparticle-based photovoltaic cells which can have a negative impact on environmental performance are not only important because of their weight in assessing the life cycle environmental impact. Also they may provide a focus for environmentally improved design of nanoparticulate cells.

It should be noted though, that with currently available data and methods, there are problems for comparative studies concerning the nanoparticulate cells discussed here. Nanoparticulate solar cells may use materials for which available life cycle assessment databases contain no, or insufficient, data to allow for proper environmental assessment, e.g. [22] and the implications of improvement options regarding DS(S)Cs and fullerene-based solar cells for life cycle inputs of energy and materials are often uncertain. Also, current life cycle assessment methodology is unable to properly handle the hazard of mineral nanoparticles [23].

In Section 2, aspects of nanoparticulate cells which can add to the environmental burden will be discussed in turn. In Section 3 the lack of data and proper methodology will be discussed. This will be followed in Section 4 by suggestions for environmental improvement. Section 5 will summarize the conclusions from this paper.

2. Aspects of nanoparticlulate solar cells which are not conducive to environmental improvement

2.1. Relatively high inputs in the production of nanoparticles

The nanoparticulate solar cells considered here, are characterized by lower direct inputs of materials and a lower life cycle energy input than mcSi cells [12,22]. The environmental advantage of nanoparticulate solar cells is however limited by the relatively high input of energy and materials in the production of TiO_2 and fullerene nanoparticles, if compared with larger-sized TiO_2 and C particles [13,22,24]. TiO_2.nanoparticles may require at least a 3–4 times larger input of energy than conventional TiO_2 particles, whereas on a kg for kg basis the input of precursor may be increased by a factor 1.5–3.9 [13,24]. The production of fullerenes is energy intensive and is estimated [21] to require between 25 and 129 GJ of primary energy per kg C_{60}. C_{60} production can also be highly material intensive. For instance, an estimated 385 kg of benzene is currently needed as feedstock for the production of 1 kg C_{60} by combustion [22].

2.2. Relatively low conversion efficiency

The nanoparticulate photovoltaic cells considered here, have as yet a lower solar radiation to electricity conversion efficiency than mcSi solar cells. The reported maximal efficiencies for the DS(S)C and single junction fullerene-based organic cells are ~11.2% and 5.4%, respectively [14]. The maximum reported efficiency for standard multicrystalline Si cells is 18.7% [14], whereas mass-produced commercial mcSi cells have a conversion efficiency of about 14.4% [20].

The current difference in efficiency between nanoparticulate and mcSi cells may partly be due to differences in technological learning. The current mcSi solar cells are further on the learning curve than the nanoparticle-based solar cells considered here, which are under development since the late 1980s and early 1990s, whereas Si-based cells are under development since the 1950s [12,15,25,26]. However, there are estimates of the potential for further efficiency improvement of the nanoparticulate solar cells considered here. For fullerene-based organic solar cells, it has been argued that practicable maximum conversion efficiency may be in the order of 10–11%, when not in tandem [27–29]. For DS(S)C the maximum achievable efficiency has been estimated at 12% [12]. Thus, it would seem likely that with similar technological learning the conversion efficiency of DS(S)C and fullerene-based organic solar cells may still be poorer than in case of mcSi solar cells (also [6]).

2.3. Relatively short service life

On solar irradiation, photovoltaic cells are subject to demanding conditions [15–19]. McSi photovoltaic cells, serving the electricity grid, have in these conditions a useful lifetime (service life) of 25–30 years [15,20]. During this time the solar radiation to electricity conversion efficiency of the cells remains over 80% of the original value.

Experiments with DS(S)C have shown that they are relatively vulnerable to the harsh conditions, under which solar cells have to operate. Intrusion of O_2 and H_2O leads to rapid deterioration of DS(S)C performance [19]. Performance may also be reduced by high temperatures and ultraviolet irradiation [18,19]. Leakage and degradation of DS(S)C liquid electrolyte have been shown to be problems too [12,18,19,30].

Damage to organic constituents due to the intrusion of O_2 and H_2O is also a matter of concern for the fullerene-based solar cells [27–29,31–35]. Electrode material reactions with the rest of the cell and damage to organic cells at high temperatures tend to be larger for organic solar cells than in the case of mcSi cells [15]. Furthermore, partial oxidation of electron contact material has been shown to negatively affect cell performance over time. Instability of morphology due to phase separation has also been shown to be a problem [9]. Enveloping solar cells in a way that minimizes the intrusion of O_2 and H_2O has been shown to extend the service life of organic solar cells [15,29,32–34]. However, current enveloping materials (usually synthetic polymers) are subject to degradation when exposed to solar radiation [15]. Their use is associated with an expected service life which is still well below 10 years and considerably adds to material inputs in the production of solar cells [9,15,33–35].

There is great uncertainty about the service life achievable by mass-produced nanoparticulate solar cells, but as yet it would seem to be substantially shorter than for standard Si cells. It has been suggested, that for the DS(S)C a useful lifetime of 10 years is 'within reach' [19], but this as yet would not seem the case for organic solar cells [15,22,28,31–35].

2.4. Poor recyclability

Recyclability is important to reduce the cradle to grave environmental burden of products. When recycling takes place and if the environmental burden thereof, including transport, is relatively low, the initial environmental burden of solar cell production can partly be distributed over the original and the recycled products and this tends to lower the environmental burden of the original product [36,37]. McSi cells can be recycled into high quality secondary products at a relatively low cost [38,39]. Si from discarded mcSi solar cells can be used as a resource for the production of new solar cells, and this has a substantial environmental benefit (when not corrected for differences in transport between discarded cells and virgin resources) [38,39].

Recycling of nanoparticulate solar cells has not drawn a major research effort so far. However experience with post-consumption recycling of waste from electrical equipment has shown that, when substantial amounts are present, the metals in nanoparticulate cells can in all probability be recycled into products with high quality applications [40–43]. But beyond metals, recyclability seems low. In part, the design of nanoparticulate solar cell uses the interpenetration of substances (C_{60} and polymer, TiO_2 and dye) and this is not conducive to recycling [44]. Recycling of composite polymeric materials (which are a major constituent of organic solar cells and may be important in DS(S)C with a relatively long service life) has turned out to be a problem [44]. Only low quality applications of secondary composites have been found, and in practice such composites often end up being incinerated or landfilled [44]. Recycling of non-composite synthetic polymers, which can be enveloping materials for nanoparticulate solar cells [15,22,33–35], is more attractive [44]. However, when such materials are substantially degraded, as is likely to occur during a long service life [15], only low quality applications would still be possible [44]. Thus it would seem likely that, given present cell design, unlike in the case of mcSi cells, only a very limited part of the nanoparticulate solar cells can be recycled into high quality applications (at acceptable cost). This negatively affects their environmental performance, if compared with mcSi cells.

2.5. The use of metals derived from relatively scarce natural resources

Depletion of natural resources is often viewed as an aspect of life cycle environmental assessment which contributes to the environmental burden, e.g. [20]. Because Si is the second most abundant element in the earth's crust [25], the environmental burden of Si use due to resource depletion is very low. On the other hand, the use of metals derived from relatively scarce natural resources, corresponds with a relatively heavy environmental burden. In the category of such compounds come Au, Ru and Pt (applied in DS(S)C), and In and Sn (applied in DS(S)C and organic nanoparticulate cells) [9–12,45–47].

Using depletion of natural resources in life cycle assessment has been criticized, e.g. in the case of metals, because dissipation and disposal rather than depletion is problematical [48]. If this line of reasoning is followed, this aspect of the environmental burden will be largely determined by the degree of recycling that is achieved (see Section 2.4).

3. Missing data for life cycle assessment

Though current databases include adequate data for the life cycle assessment of mcSi cells [20,49], this is quite different for nanoparticulate cells [6,12,21,22]. As yet, standard methodologies for life cycle assessment do not allow for the inclusion of nanoparticle hazard [23]. This problem is not easily remedied. Hazard is usually handled by life cycle assessment on the basis of weight of the substances released into the environment. However the hazard of mineral nanoparticles such as TiO_2 is rather determined by number, surface area, nature of the surface and structure [50]. Also, information about several non-nanoparticulate components in nanoparticulate solar cells, such as a variety of polymers and dyes, is largely missing in databases currently used for life cycle assessment of solar cells and this also seems to hold for dyes and polymers that are currently used in efforts to improve conversion efficiency and service life ([6,12,21,22] and Section 4). This holds for energy input and related CO_2 emissions, but even more for other aspects of environmental impact such as depletion of natural resources, (eco)toxicity, acidification, eutrophication and impact on the ozone layer.

4. Options for the improvement of environmental performance of nanoparticulate solar cells

If one takes an overall view, the environmental advantage of lower direct material inputs in the nanoparticulate solar cells considered here, is counterbalanced by relatively high inputs of energy and materials in nanomaterial production, additional inputs of materials for enveloping cells to prevent deterioration, poorer conversion efficiency, lower useful service life, use of metals from relatively scarce natural resources and/or poorer recyclability. Currently this leads to a relatively low life cycle emission of CO_2 $kW\,h^{-1}$ for mcSi cells if compared with dye-sensitized and fullerene-based solar cells (see Table 1).

As pointed out in the Introduction, disadvantages of the nanoparticulate solar cells considered here may in the future lead to a relatively high life cycle CO_2 emission $kW\,h^{-1}$, if compared with solar cells based on ribbon Si. Thus, in the further development of nanoparticle-based photovoltaic cells, the aspects that negatively affect environmental performance are issues to preferentially address.

So far, environmental improvement of nanoparticulate cells has not been the object of a systematic research effort. Nevertheless, a number of suggestions for improvement of the solar cells

Table 1
Environmental attributes of multicrystalline Si (mcSi) versus dye-sensitized and fullerene-based nanoparticulate solar cells

Relative advantage of dye-sensitized and fullerene-based nanoparticulate solar cells, relevant to environmental performance	Relative advantage of mcSi solar cells relevant to environmental performance	Current overall environmental performance
- Low direct input of materials in nano particulate cells - Low life cycle energy input in nanoparticulate cells, though nanoparticle production is relatively energy intensive	- Longer service life of mcSi cells - Higher conversion of solar energy to electricity by mcSi cells - Better recyclability of mcSi cells - More abundant natural resources for materials for mcSi cells	Relatively low life cycle CO_2 emission kWh^{-1} for mcSi cells, if compared with the nano particulate cells considered here

considered here can be made. One is the reduction of the life cycle input of materials in nanoparticle production, and more generally: reduction of the life cycle materials input of nanoparticulate solar cells. Reduction of the life cycle input of materials has been important in improving the environmental performance of mcSi solar cells [6,39] and may also be significant in improving the environmental performance of nanoparticulate cells. For instance, Kato et al. [21] have shown that reduced life cycle inputs of acetone and isopropanol could substantially decrease the life cycle CO_2 emission of the DS(S)C which they studied.

Other suggestions for environmental improvement of the nanoparticulate solar cells considered here will be discussed in the following. This discussion includes matters relevant to the environmental impact of those suggestions.

4.1. Improving energy efficiency

An obvious target for improvement is increasing the solar radiation to electricity conversion and lowering energy input in the production of nanoparticles to be included in photovoltaic cells. The former is the object of much development work, e.g. [12,27–29,51–53]. As pointed out in Section 2.2 the best reported performance of DS(S)C is not far from its achievable maximum. This is different for fullerene-based organic cells but here recent conversion efficiency improvement seems slow, e.g. [51].

Remarkably, in efforts to improve conversion efficiency there is little attention to the life cycle environmental impact of materials suggested in this context. For instance, the use of pyridine derivatives, such benzimidazole compounds, has been suggested as an option to improve the efficiency of polymeric DS(S)C. Because pyridine derivatives may have substantial biological activity [54,55], their potential release during the product life cycle and the impact thereof should be considered in assessing the environmental performance of DS(S)C which include such compounds.

As to the input of energy in nanoparticle production, there may be various ways to generate specific nanoparticles with strongly varying energy inputs [13,24]. This allows for the selection of relatively energy-efficient production processes, which in turn can be improved by technological learning [6].

4.2. Substituting compounds derived from scarce natural resources and improving recycling

Substituting compounds derived from relatively scarce natural resources by substances derived from more abundant resources may lead to environmental improvement, when it is assumed that this depletion adds to the environmental burden. It has been proposed that Ru-compounds may be substituted by organic dyes, e.g. [45]. However, when considering such substitution one should be aware of side effects that may have an upward effect on the environmental burden. For instance, Burke et al. [45] have argued that the replacement of ruthenium compounds by planar organic dyes may necessitate the employment of an additional TiO_2 layer. Also electrodes of aluminum, which is relatively abundant in the earth' crust, to replace rarer metals have been shown to be easily photocorroded when applied in organic cells; this may strongly reduce service life [4,45].

In the case of mcSi solar cells, recycling (not corrected for differences in transport of discarded solar cells and virgin materials) has been found to substantially reduce the life cycle environmental burden [38,39]. One might expect the improvement to be less in the case of the nanoparticulate cells considered here, because recycling would probably be restricted to metals and perhaps non-composite polymers, as pointed out in Section 2.4.

4.3. Extension of service life

Extension of service life may much improve the environmental performance of nanoparticulate cells. For instance it has been estimated that increasing service life of organic cells on glass to 10–20 years may make such cells environmentally competitive with current mcSi cells, whereas for their plastic counterparts a service life of 1–5 years may suffice, when the extension of service life does not require the additional input of materials and energy [22].

There are options for the extension of service life of both DS(S)C and organic cells.

Options to improve stability by improved enveloping of cells have been outlined in Section 2.3. These are subject to environmental trade-offs because they tend to imply increased life cycle materials intensity.

Leakage from DS(S)C is linked to the use of a liquid electrolyte which may vary in volatility. Replacement of the liquid electrolyte by a solid one (in practice by an organic polymer) can eliminate leakage of electrolyte by DS(S)C [56,57]. However, the polymeric electrolytes may be subject to relatively rapid degradation mediated by TiO_2, when there is intrusion of oxygen and water [15,58]. Addition of radical scavengers may limit such degradation [59]. Moreover, the solar radiation to electricity conversion efficiency tends to be reduced when the liquid polymer is substituted by a solid polymer [56,57]. Another option is the use of a semi-solid state gel as electrolyte. Many of the gels investigated thus far have a lowered conversion efficiency, but a gel polymer incorporating TiO_2 nanoparticles has been reported to have a conversion efficiency similar to DS(S)Cs with liquid electrolyte [60–65]. However, it may well be that incorporation of TiO_2 nanoparticles reduces cell stability, when there is intrusion of oxygen and water [58], which again may be counteracted to some extent by the inclusion of radical scavengers [59]. A variety of suggestions have been made to increase the oxidation resistance, and the chemical and morphological stability of polymers which in turn may extend the service life of solar cells, including more rigid structures, cross-linking of polymer chains, the use of p–n block polymers and the use of a variety of conjugated polymers, e.g. [9,66]. So far there are no evaluations of the life cycle environmental impacts of such polymers, which may confer improved stability. A fullerene variety has been proposed that has much improved photostability, but its application as yet leads to a much reduced conversion efficiency [66]. The problems with oxidation of electron contact material in organic cells may be reduced by the inclusion of high stability metals [17,46,47,67], which are however derived form relatively scarce natural resources. There can be environmental trade-offs for the expansion of service life, but there is no focus on optimizing such trade-offs in actual development.

4.4. Selecting options for environmental improvement

Options which reduce the life cycle input of materials, while at least maintaining the service life and conversion efficiency of nanoparticulate solar cells, would seem interesting environmental improvement options, e.g. [21]. Beyond that, selecting the best short-term options for environmental improvement is difficult with currently available data. For instance, increasing service life and efficiency are at first sight attractive options, e.g. [22], but it is not clear whether they would be achievable without increasing the current life cycle environmental burden, as is supposed in available studies, e.g. [22].

5. Conclusion

Though environmental improvement has been claimed for the application of nanotechnology to solar cells [1–5], several characteristics of the nanoparticulate solar cells considered here are not conducive to such improvement (see also Table 1). These include relatively high inputs of energy and materials in the production of nanoparticles, a relatively low solar radiation to electricity efficiency, a relatively short service life, the need for enveloping materials to limit the intrusion of H_2O and O_2, the use of relatively scarce natural resources and/or relatively poor recyclability if compared with mcSi solar cells. Also, missing data and the inability to handle nanoparticle hazard generate problems for proper comparative life cycle assessment of nanoparticulate cells. So far, the claimed environmental advantage of the nanoparticulate solar cells considered here can not be substantiated. If one aims at environmental improvement of nanoparticulate solar cells, the relatively high inputs of energy and materials in the production of nanoparticles, the overall life cycle inputs of materials, the relatively low solar radiation to electricity conversion, the relatively short service life and the use of more abundant natural resources and/or improved recyclability are objects for improved process and product design. However, in actual development work there seems to be no focus on achieving (net) environmental improvement. This is at variance with the attention to environmental improvement in the development of other types of solar cells, e.g. [20,39,49].

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