Optoelectronic Modeling of Graded-Bandgap Thin-Film Solar Cells

F. Ahmad, A. Lakhtakia, P. B. Monk, and B. J. Civiletti

Affectionately dedicated to the memory of Prof. Ninoslav D. Stojadinović

Abstract— Thin-film solar cells are cheap and easy to manufacture but require improvements as their efficiencies are low compared to that of the commercially dominant crystalline-silicon solar cells. A coupled optoelectronic model was formulated and implemented along with the differential evolution algorithm to assess the efficacy of grading the bandgap of the absorber layer in three thin-film solar cells. Optimal grading was predicted to yield efficiency of 27.7% with a 2200-nm- thick CIGS absorber layer for the CIGS solar cell, 21.74% with a 870-nm-thick CZTSSe layer for the CZTSSe solar cell, and 34.5% with a 2000-nm-thick AlGaAs layer for the AlGaAs solar cell. For a solar cell with two bandgapgraded absorber layers, an efficiency of 34.45% was predicted with a 300-nm-thick CIGS layer and a 870-nmthick CZTSSe layer. For colored solar cells, efficiency loss was predicted from 10% to 20%, depending upon the percentage of incoming solar photons rejected.

I. Introduction

As the worldwide demand for eco-responsible sources of cheap energy continues to increase for the betterment of an ever-increasing fraction of the human population, the cost of traditional crystalline-silicon (c-Si) solar cells continues to drop. While this is a laudable development, small-scale photovoltaic generation of energy must become ubiquitous for human progress to become truly unconstrained by energy economics [1]. Also, concerns regarding global warming grow more severe with every passing day. As the global meteorological patterns change, the annually averaged global temperature continues to rise, indicating a grave threat to life on our planet. Hence, cutting the consumption of carbonaceous fossil fuels is the prime need of the time.

Thin-film solar cells are a viable option in addition to c-Si solar cells due to low cost and ease of manufacturing. Other benefits of thin-film solar cells include: less material use in absorbing layers made of materials with higher optical absorption compared to c-Si, flexibility of some thin-film solar cells, and control over the composition of a material.

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Currently, thin-film solar cells containing absorber layers made of either CIGS or CdTe are commercially dominant. However, there are serious concerns about the planetwide availability of indium and tellurium, both needed for CIGS and CdTe solar cells. Furthermore, both indium and cadmium are toxic, leading to environmental concerns about their impact following disposal after use. Thin-film solar cells must be made from materials that are abundant on our planet; moreover, the materials of choice must be those that can be extracted, processed, and discarded with low environmental impact. Another primary concern regarding potential Earth-abundant and non-toxic thin-film solar cells is regarding their low power-conversion efficiencies compared to CIGS and CdTe, e.g., the 12.6% efficiency of CZTSSe solar cells is considerably lower than the \sim 22% efficiency of CIGS and CdTe solar cells.

To tackle the problem of material scarcity, thinning of the absorber layer is desirable, all the more so because it will reduce material usage and enhance manufacturing throughput concomitantly. However, a thinner absorber layer will reduce the absorption of incident solar photons. Back-end modifications such as back-surface passivation and periodic corrugation of the backreflector are commonly researched techniques to overcome these problems. Another method to increase efficiency is spatial grading of the bandgap of the absorber layer by controlling the compositional ratio to allow photon absorption over a wider frequency range. However, suboptimal bandgap grading cannot guarantee improved power-conversion efficiency. Optimal strategies are required to find the best-performing thin-film designs based on bandgap grading, absorber-layer thinning, and back-end modifications.

II. INVESTIGATIONS AND RESULTS

A series of theoretical investigations were performed to tackle the problem of material scarcity as well as to enhance power-conversion efficiency of thin-film solar cells by thinning the absorber layer, grading the bandgap in the absorber layer, and modifying the back end. Three different types of thin-film solar cells were considered: CIGS [2], CZTSSe [3], and AlGaAs [4]. The bandgap of the absorber layer was graded either sinusoidally or linearly. The thickness of the absorber layer was allowed to vary from 100 nm to 2200 nm. Back-end modifications incorporating a periodically corrugated

backreflector and a back-surface passivation layer were considered as well. An anti-reflection coating and a top passivation layer were also incorporated in the design, as shown schematically in Fig. 1.

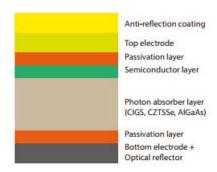


Fig. 1. Schematic of a thin-film solar cell.

A coupled optoelectronic model [5] was used along with the differential evolution algorithm [6] to maximize the efficiency in relation to geometric and bandgap-grading parameters. Furthermore, as colored solar cells can promote large-scale adoption of rooftop solar cells, efficiency loss due to color-rejection filters was estimated [7].

The coupled optoelectronic optimization predicted that tailored bandgap grading could significantly improve efficiency for all three considered thin-film solar cells. For CIGS solar cells with a 2200 nm-thick absorber layer, an efficiency of 27.7% was predicted with a sinusoidally graded bandgap absorber layer along with back-end modifications in comparison to 22\% efficiency achieved experimentally with a homogeneous CIGS absorber layer [2]. An efficiency of 21.7% was predicted with sinusoidal grading of a 870-nm-thick absorber CZTSSe layer in comparison to 12.6% efficiency achieved experimentally with a 2200-nm-thick homogeneous CZTSSe layer [3]. Similarly, an efficiency of 34.5% was predicted through optoelectronic optimization of AlGaAs solar cells with a sinusoidally graded bandgap absorber layer along with back-end modifications in comparison to 27.6% efficiency achieved experimentally with a homogeneous AlGaAs absorber layer

A thin-film solar cell with two absorber layers (instead of only one), with bandgap energy graded in both, can capture solar photons in a wider spectral range. With a 300-nm-thick CIGS absorber layer and an 870-nm-thick CZTSSe absorber layer, an efficiency of 34.45% was predicted by the coupled optoelectronic model, provided that bandgap grading is optimal in both absorber layers [8].

The efficiency enhancements can be further increased by concentrating the illuminating sunlight, according to ongoing investigations. Details will be reported in due course of time. For colored thin-film solar cells, calculations show that on average, the efficiency of a typical solar cell will be reduced by about 9% if 50% red photons are reflected or by about 13% if 50% blue-green photons are reflected. The efficiency reduction increases to about 18% if all red photons are reflected or about 26% if all blue-green photons are reflected. Thus, optoelectronic optimization by bandgap grading and back-end modifications is more than enough to overcome efficiency reduction by the rejection of a certain percentage of incoming solar photons [7].

III. CONCLUSION

Thus, the proposed design strategies provide a way to realize more efficient thin-film solar cells for the ubiquitous harnessing of solar energy at low-wattage levels, thereby promoting widespread adoption of thin-film solar cells as local energy sources [1]. Also, cheap, small-scale off-grid generation of electricity will provide access to energy for populations living without electricity far from central grids in less-developed and developing regions of our planet, thus equalizing opportunity and decreasing income and gender gaps.

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References

- [1] R. Singh, G. F. Alapatt, and A. Lakhtakia, 'Making solar cells a reality in every home: opportunities and challenges for photovoltaic device design,' *IEEE J. Electron Dev. Soc.*, 2013, vol. 1, pp. 129–144.
- [2] F. Ahmad, T. H. Anderson, P. B. Monk, and A. Lakhtakia, 'Efficiency enhancement of ultrathin CIGS solar cells by optimal bandgap grading,' Appl. Opt., 2019, vol. 58, pp. 6067– 6078; errata: 2019, vol. 59, p. 2615.
- [3] F. Ahmad, A. Lakhtakia, T. H. Anderson, and P. B. Monk, 'Towards highly efficient thin-film solar cells with a graded bandgap CZTSSe layer,' J. Phys.: Energy, 2020, vol. 2, art. no. 025004; errata: 2020, vol. 2, art. no. 039501.
- [4] F. Ahmad, P. B. Monk, and A. Lakhtakia, 'Optoelectronic optimization of graded-bandgap thin-film AlGaAs solar cells,' Appl. Opt., 2020, vol. 59, pp. 1018–1027.
- [5] T. H. Anderson, B. J. Civiletti, P. B. Monk, and A. Lakhtakia, 'Coupled optoelectronic simulation and optimization of thin-film photovoltaic solar cells,' *J. Comput. Phys.*, 2020, vol. 407, art. no. 109242; errata: 2020, vol. 418, art. no. 109561.
- [6] R. Storn and K. Price, 'Differential evolution—a simple and efficient heuristic for global optimization over continuous spaces,' J. Global Optim., 1997, vol. 11, pp. 341–359.
 [7] F. Ahmad, T. H. Anderson, T. Lenau, and A. Lakhtakia,
- [7] F. Ahmad, T. H. Anderson, T. Lenau, and A. Lakhtakia, 'Optoelectronically optimized colored thin-film CZTSSe solar cells,' *Proc. SPIE*, 2019, vol. 11371, art. no. 1137107.
- [8] F. Ahmad, A. Lakhtakia, and P. B. Monk, 'Double-absorber thin-film solar cell with 34% efficiency,' Appl. Phys. Lett., 2020, vol. 117, art. no. 033901.