Designing an optimal absorbing layer for thin-film solar cells

Jeonghoon Yoo and Hyun-jun Soh

A computer-simulation-based topology optimization scheme finds optical designs that boost the efficiency of solar cells.

Solar cells are a widely applicable renewable source of electricity. Thin-film solar cells can be less expensive than ordinary bulk solar cells because they use much less active material, which is costly. In these cells, the active layer is typically only one or two microns thick, or an order of magnitude thinner than the active layer of a bulk solar cell. The cost savings of the thinner device may be offset, however, if the efficiency is much lower than the bulk version. This is particularly true for silicon (Si), which is the most commonly used active material. Thin Si films do not absorb solar energy well, especially at sunlight’s longer wavelengths in the 600–800 nm range. Improving absorption efficiency is thus a crucial part of designing efficient thin-film Si solar cells. With this goal in mind, we are developing a practical method of designing the optics in thin-film solar cells.

The basic layout of a solar cell uses an active material (which creates pairs of charge carriers) sandwiched between two electrodes. The design should maximize the light that enters the active region and then trap it to improve the chance of absorption. If the design can increase the angle of light within the cell, light can be trapped in the active layer via total internal reflection. Additional films atop the active layer may be added to trap more light. The layers are not necessarily planar: various shapes such as pyramid or wedge structures have been employed to increase solar wave transmission in specific wavelength ranges.

Many current designs for thin-film cells are the result of simple design rules or optimization methods that vary parameters to find the best result within a somewhat arbitrary set of possibilities. The design method has a strong influence on the solutions found. The final results are also strongly influenced by the starting points of these designs, which largely depend on the researchers’ theoretical knowledge and experience. In contrast to this built-in requirement for expertise, we wish to develop a method that works well for everyone.

We designed an absorbing layer structure composed of Si and a transparent conductive oxide (TCO) electrode. Unlike previous work, we applied a systematic design approach that combines topology optimization and parameter optimization methods. The former can offer the optimal material layout in the design domain and has the advantage of flexibility. We performed the numerical simulation using finite element analysis (FEA).

Figure 1 shows how topology optimization leads to an optimal structure, using an arbitrary example in which the designers wish to find the stiffest structure to support a given load. First, the design domain is divided (discretized) into multiple elements. Then the need for each element is determined according to the element density through the iteration process. Unnecessary elements are removed from the design.

For our purposes, we use a topology optimization scheme to find the optimal number and shape of thin films for our solar cell. In other words, how many layers of Si and TCO will channel the most light into the active layer and keep it there? We implemented topology optimization using a specific method called solid isotropic material with penalization. We performed the numerical simulation using finite element analysis (FEA).

Figure 2 shows a schematic of our model for numerically calculating the optimal thin-film structure using FEA: a stack of layers that make up the thin-film solar cell incorporates a periodic boundary condition along the left and right sides. This is

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our starting point for optimization. We want a design that reduces light reflection and also enhances transmission through the TCO. Therefore, we define the design objective function as the light transmittance, which is the ratio of the integrated Poynting vector values in the measuring domain and along the incident boundary during a specific time period. The Maxwell’s equation that we use as a governing equation is solved by the commercial FEA program COMSOL, with the time-dependent analysis mode selected so that we can analyze the effect of reflection. The objective function value converges to an optimal value as plotted in Figure 3. We confirm that the optimal shape also converges to a multi-layered shape during the iteration process. The layer thickness converged to the value of $\lambda/2n$ ($\lambda$: incident beam wavelength, $n$: refractive index). This thickness is well known as a value that changes neither the reflection nor the transmission of a layered medium. A benefit of this layer thickness is that it is based on a physical theory and simple structure, which eases fabrication. This may not be the optimal solution, however, because design guides such as this one tend to find the best local rather than the best global solution. Also, because the layer thickness depends on the refractive index (which changes with wavelength), the thickness of the layer will change if we design for a range of wavelengths.

Next, we consider parameter optimization. Although our method often derives multi-layered topologies, the details of optimized shapes differ slightly depending on the initial shape and the incident beam wavelength. We find that a TCO layer located at the top results in a design with high absorption, which is reasonable since the material of the top layer plays an important role in wave transmittance. Through a parameter study of

![Figure 2](image1.png)

Figure 2. Left: Unit structure of the thin-film solar cell design model before optimization. Light from 600 to 800nm enters normal to the surface. The transparent conductive oxide (TCO, black) is shaped into a wedge to increase the amount of light that enters the active layer of microcrystalline silicon (white). Adding thin layers of silicon (Si) and TCO to the area to be optimized (the design domain) can increase light absorption in the measuring domain. Right: Wave propagation pattern for 800nm light through the wedge-shaped model. ZnO: Zinc oxide.

![Figure 3](image2.png)

Figure 3. Convergence history of the objective function value, with diagrams showing the TCO and Si layers during the optimization process in the case of 800nm incident light.

![Figure 4](image3.png)

Figure 4. Left: Comparison of wave transmittance of optimized models obtained from three wavelengths. Right: Layer thickness details of the best-performing design (Model 1) across the entire waveband. $\lambda$: Incident beam wavelength. $n$: Refractive index.
varying thicknesses for this layer, we found that the best performance occurred with a top-layer thickness of $\lambda/4\eta$. This is reassuring because our design independently found the same thickness, which is typically used for single-layer antireflection coatings.

We found optimal shapes for three wavelengths (600, 700, and 800nm) starting from the wedge-shaped model, and compare them on the left side of Figure 4. The model optimized for 600nm (Model 1) gives consistently superior performance for the overall waveband from 600 to 800nm. Model 1’s detailed shape is illustrated on the right side of Figure 4, with the thickness definition of each layer related to the beam wavelength ($\lambda = 600$nm) and the material’s refractive index.

Our design method, coupling topology and parameter optimization, produces effective results when applied to designing a wave-absorbing layer for thin-film solar cells. This method should allow even non-experts to design efficient devices. Our next steps are to continue using this method to obtain the optimal shape when the entire waveband is taken into account simultaneously and to find the optimal structure of the absorbing layer for a specific waveband. We will make a prototype of the structure and verify its performance by measuring the reflection of the incident beam.

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Author Information

Jeonghoon Yoo
Yonsei University
Seoul, Republic of Korea

Jeonghoon Yoo was awarded BE and master’s degrees in mechanical design and production engineering at Seoul National University in 1989 and 1991, respectively. He received a PhD in mechanical engineering at the University of Michigan in 1999. Since 2000, he has been a professor of simulation-based design.

Hyun-jun Soh
Hyundai Motor Co.
Seoul, Republic of Korea

Hyun-yun Soh received his PhD in mechanical engineering from Yonsei University in 2012.

References