Inverse Design of a Nano-Scale Surface Texture for Light Trapping

Owen D. Miller, Vidya Ganapati, and Eli Yablonovitch
Material Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720
Electrical Engineering & Comp. Sciences Dept., University of California, Berkeley 94720
Contact email: omiller@berkeley.edu

Abstract: We introduce computational inverse design to optimize nano-scale surface textures for light trapping. The approach yields a structure with a 40.8 absorption enhancement factor, the highest reported for a high-index material in the full-wave domain.
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1. Introduction

Light trapping is a concept of fundamental importance to solar cells. Light trapping by surface texturing can provide significant absorption enhancement; equally as important is the significant voltage boost that is also provided. In the ray optics regime, there is a well-known $4n^2$ absorption enhancement limit for a randomly textured surface that cannot be surpassed [1]. The limit does not apply in the wave optics regime, however, and it is an open question as to what enhancement is possible. Ref. [2] demonstrates that large enhancements are possible for periodic structures, but the proposed design utilizes specialized modal enhancement that occurs only for low-index materials. For the high-index semiconductors relevant for solar cells, a different structure will be needed.

To find a high-enhancement structure we have implemented a novel *inverse design* computational approach. Stochastic design methods, such as genetic algorithms, require far too many electromagnetic simulations to be feasible. Instead, we use "shape calculus" to compute a gradient dictating how to sculpt the surface to maximize absorption. It would seem that one would need many simulations to understand boundary sensitivity; however, through electromagnetic reciprocity and accurate dipole representations we can attain all of the necessary information with only two simulations. We optimized a 150*nm* thick weak absorber of refractive index 3.5. Within about 100 iterations, and only two simulations per iteration, we arrived at a textured structure with an enhancement factor of 40.8, averaged over all polarizations and incident angles, and a large frequency bandwidth.

2. Inverse Electromagnetic Design

We consider the absorption enhancement problem as a formal inverse problem: given a desired functionality (maximum enhancement), what structure is optimal? Shape calculus provides an efficient and effective path to an optimal structure. The relevant "merit function" for solar cell absorption enhancement measures the average absorption relative to single-pass absorption, by the ratio

$$F = \frac{\frac{1}{\omega_2 - \omega_1}\int_{\omega_1}^{\omega_2} a(\omega)d\omega}{\alpha d} \qquad (1)$$

where $a(\omega)$ is the absorptivity, α is the material absorption coefficient, and d is the cell thickness. The absorptivity in the cell is proportional to the volume integral of the electric field intensity.

Upon moving the boundary, the change in the merit function can be well approximated by the induced polarization density $\vec{P} = (\varepsilon_2 - \varepsilon_1)\vec{E}$ along the boundary, where ε_1 and ε_2 are the permittivities for the current and updated structures, respectively [3,4]. There are an infinite number of possible boundary movements, and therefore

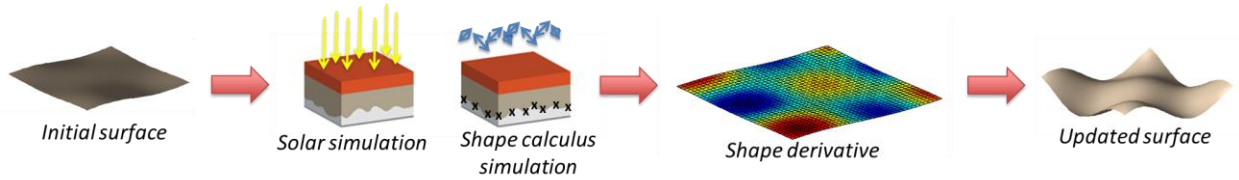

Fig. 1. Illustration of inverse design procedure. Given an initial surface (the back surface of the solar cell), two simulations are performed. The two simulations together give the "shape derivative," which is a map dictating how the surface should be updated. Red areas indicate where the height should increase, while blue indicates the opposite. The surface is updated, and the process iterates until an optimal design is reached.

an infinite number of possible polarization densities. However, through electromagnetic reciprocity, the dipole moments and measurement points can be exchanged. While the full derivation is beyond the scope of the abstract, this allows for all of the boundary sensitivity information to be obtained with only two simulations, as seen in Fig. 1.

For a given surface, two simulations are completed. The first determines the performance of the structure, while the second simulates merit function-dependent dipoles to provide boundary sensitivity information. A shape derivative arises, dictating how the boundary should move in order to increase the merit function.

3. Surface Texture Optimization

We considered the solar cell structure seen in Fig. 2(a). The solar material is taken to be a weak absorber with refractive index $n = 3.5 + 0.001i$. It has a thickness of only $150nm$, well into the wave domain. To ensure smoothness, the surface is decomposed into thirty-two Fourier sine/cosine basis functions. For comparison, a genetic algorithm optimizing such a surface would likely require at least 100 "chromosomes" and 100 generations, resulting in at least 10,000 simulations. A simple one-layer anti-reflection coating is used to reduce reflection. For the purposes of understanding how high the absorption enhancement can go, we use a perfectly reflecting mirror below the absorber, and air between the absorber and the mirror. It should be emphasized that the inverse design approach we are describing can seamlessly accommodate any choice of materials, dispersive or otherwise, and any structural constraint or representation.

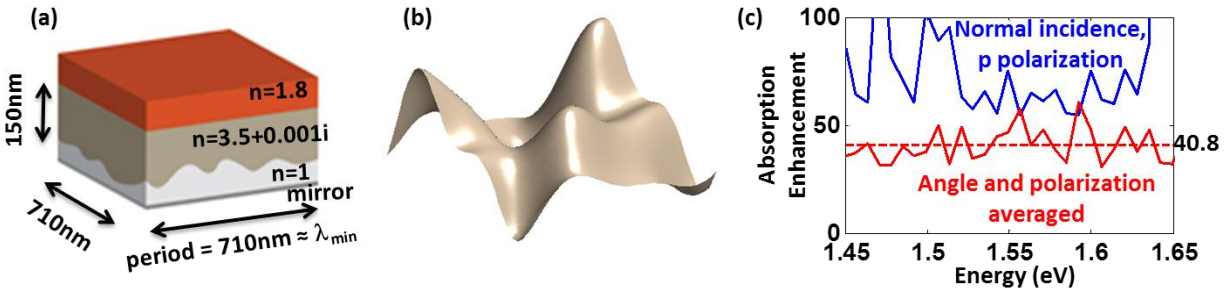

Fig. 2. (a) Solar cell structure, which consists of a 108-nm anti-reflection coating, a weak absorber with average thickness of 150nm, then air and a backside mirror. (b) Optimal surface texture, consisting of thirty-two Fourier sine/cosine basis functions. (c) Optimization results. Even though the optimization is only performed at normal incidence and for a single polarization, the structure maintains an average absorption enhancement of 40.8 over all incident angles and both orthogonal polarizations.

To minimize the number of simulations required, we only designed for a single polarization and incidence angle (normal incidence). Consequently, we opted to optimize a slightly different merit function than the average absorption of Eqn. (1). Instead, we optimized the *minimum* absorption enhancement over the energy range considered. This ensured good performance over the entire bandwidth. The resulting performance in Fig. 2(c) proves the robustness of our structure, validating our choice of merit function. The minimum absorption enhancement at the optimized incidence angle and polarization is 54. After averaging the optimal structure's response to all incidence angles and both polarizations, the average absorption enhancement was 40.8.

While it is important to attain a large enhancement factor for the weakly absorbed photons, it is equally important to fully absorb the strongly absorbed photons at the higher energies of the solar spectrum. The optimal structure, designed in the weakly absorbing regime, also achieves full absorption in the strongly absorbing regime. For $\alpha d = 0.5$, 99% of the incident photons are absorbed. This is an essential requirement of any future solar cell.

We have demonstrated a nano-scale surface texture capable of angle- and polarization-averaged absorption enhancement of 40.8 times the single-pass absorption αd. This surpasses the planar thin film limit calculated in [5], and to our knowledge is the largest absorption enhancement demonstrated for a high-index thin-film structure. The non-intuitive, non-random surface structure was only possible because of the novel inverse design method introduced. Further work towards thin-film light trapping structures, potentially including manufacturing and material constraints, will almost certainly use such a design method. Such structures will enable thinner, cheaper solar cells with superior performance to those currently in production.

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