Spontaneous Symmetry Breaking in the Optimization of Subwavelength Solar Cell Textures for Light Trapping

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ABSTRACT — **Light trapping in solar cells allows for increased efficiency and reduced materials cost. It is well known that a $4n^2$ factor of enhancement in absorption can be achieved by randomly texturing the surface of the solar cell, where n is the refractive index of the material. However, this limit only holds when the thickness of the solar cell is much greater than the wavelength of light. In the subwavelength regime, the fundamental question remains unanswered: what surface texture realizes the optimal absorption enhancement? We turn to computational inverse electromagnetic design in order to find this optimal nanoscale texture for light trapping, and observe spontaneous symmetry breaking in the final design. We achieve a factor of 40 in enhancement at normal incidence and above 20 for angle-averaged incidence (averaged over an energy bandwidth of 1/8) for n = 3.5.**

Index Terms **— light trapping, photovoltaics, solar cells, subwavelength, surface texture, absorptivity**

I. Introduction

Texturing of solar cell surfaces allows for absorption enhancement, due to the ability of incident light rays to couple to modes that are totally internally reflected within the cell (see Fig. 1). It is well known that in the ray-optics regime (where the thickness of the solar cell is much greater than the wavelength of light), that the maximum enhancement of optical path length in a medium is $4n^2$ times the single pass absorption of αd, where n is the refractive index of the material, α is the absorption coefficient, and d the thickness [1]. This maximum enhancement occurs when the light rays are ergodic in the medium, and can occur when there is a random surface texture on the solar cell.

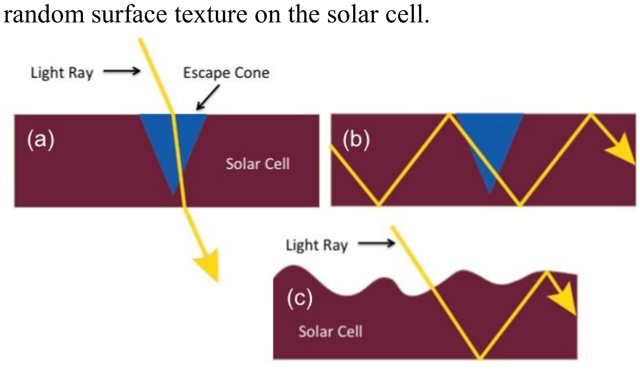

Fig. 1. (a) An external light mode, (b) an internal mode, and (c) coupling from an external to an internal mode with the aid of a randomly textured surface.

However, in recent years, light trapping has seen renewed interest due to the problem of light trapping in the subwavelength regime (see Fig. 2). Currently, this is an important question as increasingly thin materials are being utilized for increased efficiency and lower cost. In this regime, traditional ray optics does not hold, and two fundamental questions are of great importance: (1) What is the maximum absorption enhancement available in this regime, and (2) what surface texture allows us to realize this maximum? We show how to find the optimal surface texture in the subwavelength regime through inverse electromagnetic design. Though Stuart and Hall [2] calculate the absorption enhancement available in thin films, they make assumptions about the modal structure and do not specify the surface texture. Textures in the subwavelength regime that exceeds $4n^2$ light trapping are described [3-4], however, they utilize low-index materials for the absorber layer. In our work, we find the optimal texture for a typical semiconductor with refractive index of n = 3.5.

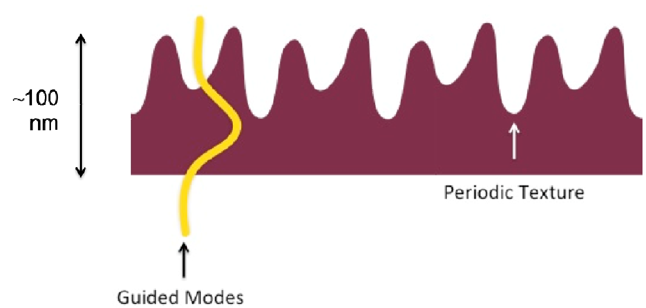

Fig. 2. In the subwavelength regime, we aim to design a periodic texture to couple incident light into guided modes.

II. Inverse Design Algorithm

We call our approach “inverse” design, because instead of “forward solving” by using intuition to create surface textures and then using an electromagnetic solver to determine performance, we start with some arbitrary initial surface, and optimize iteratively towards a Figure of Merit. Many papers have taken a “forward solving” approach towards tackling this problem [5-7], however, this approach may miss solutions that are non-intuitive. There are examples of “inverse” design in the literature [8], but so far, they describe two-dimensional solutions with absorber thicknesses greater than 1 um.

A. Optimization Setup

We optimized a surface texture function composed of a truncated series of Fourier coefficients of a certain periodicity for a weakly absorbing solar cell material of 100 nm average thickness. We applied this texture to the back surface of the absorbing material. Our setup is shown in Fig. 3; we also included a back dielectric layer, an antireflection coating, and a perfect back reflector.

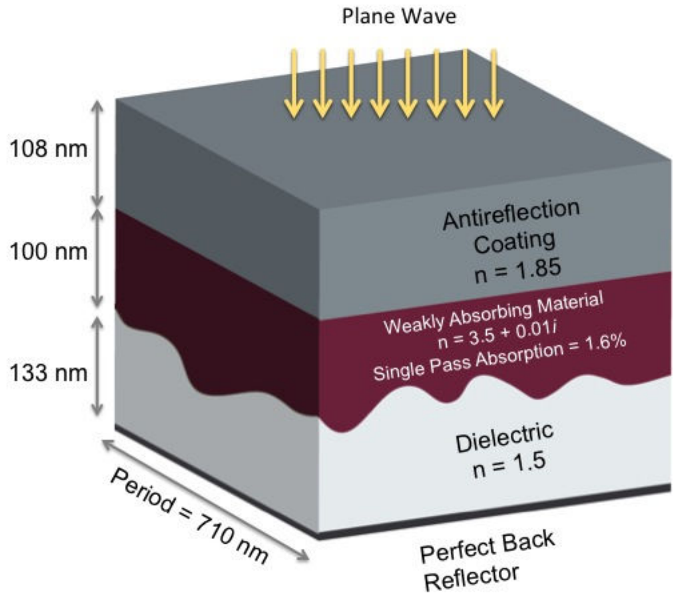

Fig. 3. A schematic of the solar cell structure.

B. Figure of Merit

The absorption enhancement is given by *a*, the absorptivity (a function of frequency, incident angle and polarization), divided by αd, the single pass absorption. We chose a minimax Figure of Merit [9]. Our Figure of Merit is the absorption enhancement at the frequency with the lowest absorption, averaged over the two perpendicular polarizations of normally incident light.

$$\text{Figure of Merit} = \frac{1}{2} \sum_{\substack{\text{x and y polarizations,} \\ \text{normal incidence}}} \min\left[\frac{a(f)}{\alpha d}\right] \quad (1)$$

With this Figure of Merit, we will show that we can achieve broadband absorption, which is useful for a solar cell.

B. Shape Calculus Algorithm

In our algorithm, we start with some arbitrary initial conditions, calculate the “shape derivative” of our texture with two adjoint simulations per polarization, and iterate to the optimal final shape (see Fig. 4). Our optimization uses an adjoint gradient method to search for a local optima [10].

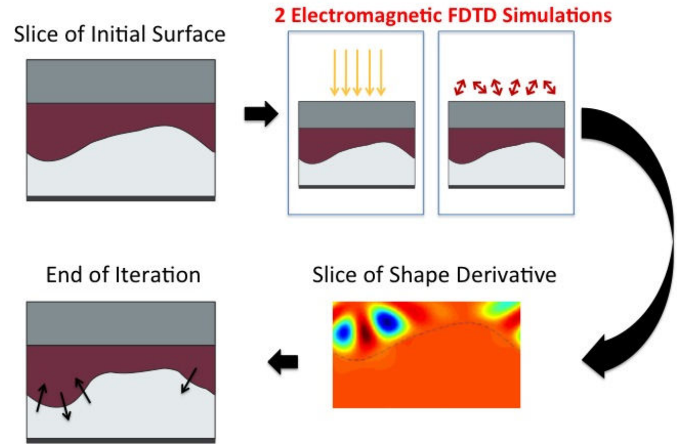

Fig. 4. An iteration of our inverse design algorithm.

III. Surface Texture Optimization

A. Starting from Noise

We started the algorithm from initial starting conditions of noise. It took 143 iterations to reach the optimal texture (our algorithm takes approximately 25 min/iteration with our 80 core computing setup), in which we achieve a figure of merit of minimum enhancement of 33 times single pass absorption for a 100 nm thick absorber layer at normal incidence. The progression of the surface texture and absorption enhancement as a function of frequency from the first iteration to the last is shown in Fig. 5 and Fig. 6. The reciprocal space representation of the surface is shown in Fig. 7. The effect of our Figure of Merit in optimizing for the lowest absorbing frequency can be seen in this progression, as resonant peaks flatten out, and both the minimum and average absorption enhancement improve.

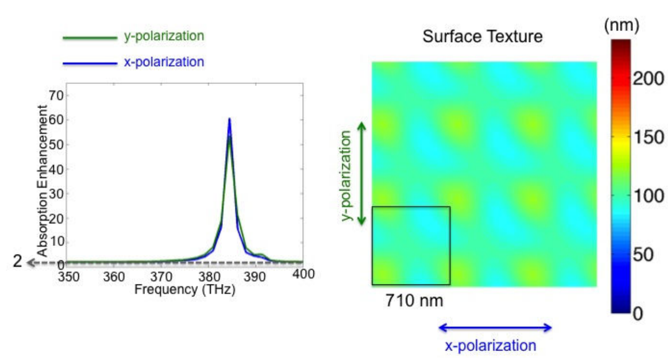

Fig. 5. The initial absorption enhancement as a function of frequency and a top-down view of the surface texture.

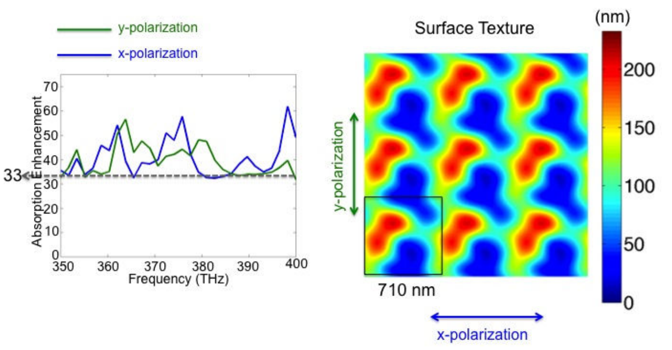

Fig. 6. The final absorption enhancement as a function of frequency and a top-down view of the surface texture.

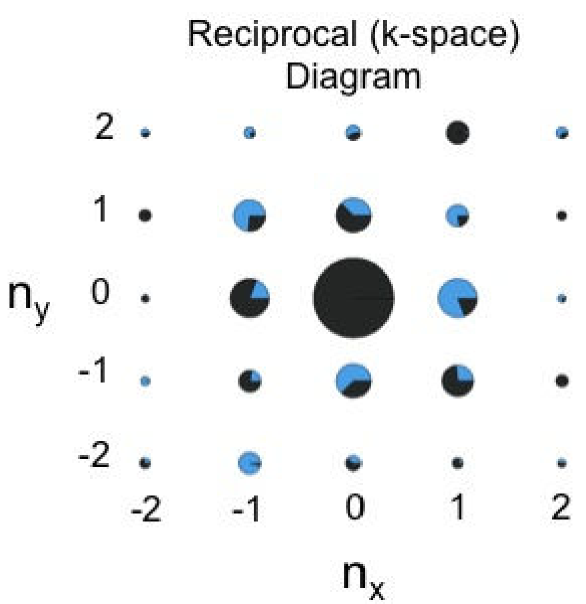

Fig. 7. The reciprocal space representation for the final texture. The blue pie slices represent the phase of the complex exponential Fourier coefficients.

B. Starting from Symmetric Conditions

To demonstrate the fundamental nature of the symmetry breaking in our final texture, we started another optimization from initial symmetrized conditions, with a slight perturbation along the diagonal, as shown in Fig. 8. The results of the algorithm are shown 15 iterations later in Fig. 9, demonstrating spontaneous symmetry breaking. We see growth of the asymmetric component in Fig. 9, evidence that broken mirror symmetry is beneficial for subwavelength light trapping.

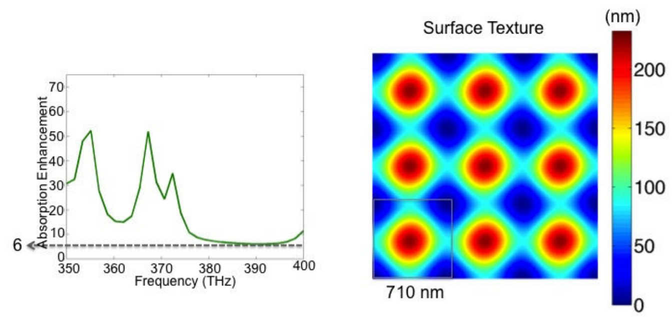

Fig. 8. The initial absorption enhancement as a function of frequency and a top-down view of the surface texture, for a symmetric texture with a slight perturbation along the diagonal.

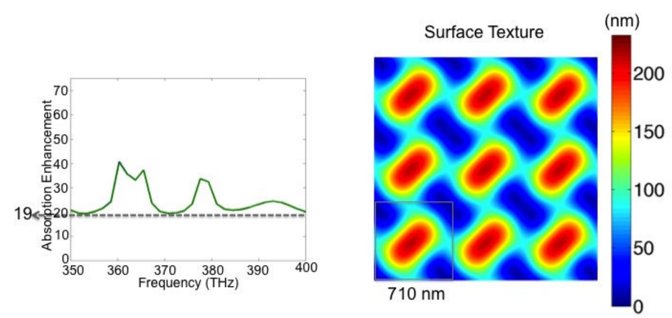

Fig. 9. The initial absorption enhancement as a function of frequency and a top-down view of the surface texture, showing broken mirror symmetry, at 15 iterations from the starting almost symmetric condition.

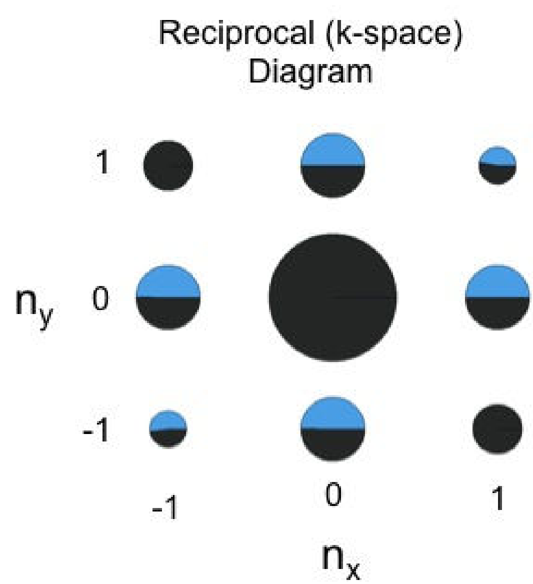

Fig. 10. The reciprocal space representation for the texture with broken mirror symmetry. The blue pie slices represent the phase of the complex exponential Fourier coefficients.

IV. Comparison to Random Texture

The periodic surface texture function generated by our optimization, shown in Fig. 6, was compared to a surface texture function of the same periodicity, but composed of randomly generated Fourier coefficients (see Fig. 11).

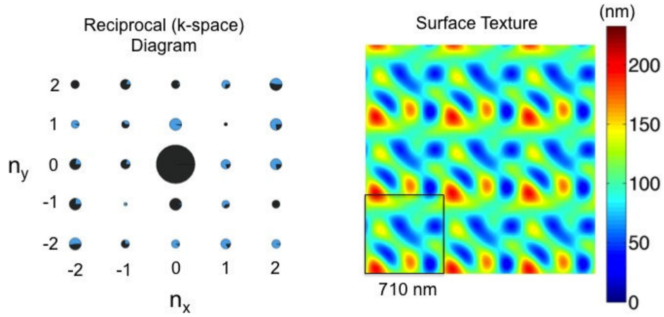

Fig. 11. Reciprocal and real space representations of a periodic structure with randomly chosen Fourier coefficients.

At normal incidence, averaged over perpendicular polarizations, the randomly generated texture had an absorption enhancement of a minimum of 6 and an average of 24. The optimized surface texture had an absorption enhancement of a minimum of 33 and an average of 40 (see Fig. 12).

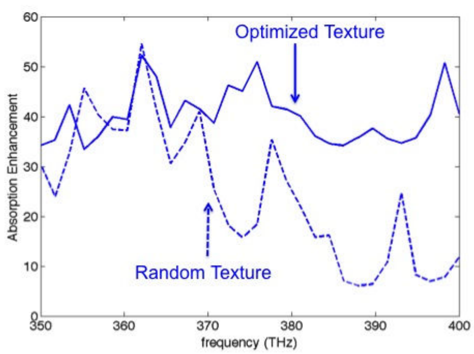

Fig. 12. Comparisons of the "random" texture and the optimized texture from Fig. 6. Absorption enhancement is given as a function of frequency for normally incident light, averaged over two perpendicular polarizations.

For Lambertian angle-averaged incident light, the randomly generated texture had an absorption enhancement of a minimum of 9 and an average of 21. The optimized surface texture had an absorption enhancement of a minimum of 17 and an average of 23 (see Fig. 13).

Though we only applied normally incident light at two polarizations while optimizing the structure, we were still able to improve upon the angle-averaged result. This angular robustness possibly arises because in every iteration of our algorithm, we modify the surface in order to enhance the worst absorbing frequency, ignoring the behavior of the other frequencies. Thus, we eliminate resonances that are very sensitive to changes in incident angle and frequency.

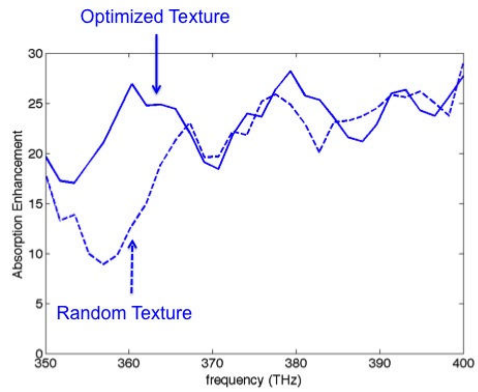

Fig. 13. Comparisons of the "random" texture and the optimized texture from Fig. 6. Absorption enhancement is given as a function of frequency, Lambertian-averaged over all incident angles.

VI. Conclusions

We demonstrate an optimization procedure to design periodic surface textures for subwavelength solar cells for improved absorption. At both normal incidence and averaged over all incident angles, the optimized surface texture function has improved average and minimum enhancement over the randomly generated surface. We observe spontaneous symmetry breaking in the generation of the optimal surface texture.

Though our optimization algorithm takes into account only absorption for normally incident light, this framework can be used to optimize for multiple angles of incident light in the future.

Gallium arsenide (GaAs), a material that can create high efficiency single junction solar cells, is typically on the order of a few microns thick. With these surface textures to enhance light trapping on a subwavelength scale, it may be possible to achieve material cost savings by reducing thickness to 100 nm and. We can potentially also see an increase in efficiency for other subwavelength thick materials of lower quality, because the material can be optically thick to get high absorption, but thin in order for good carrier extraction, resulting in a high external quantum efficiency.

Acknowledgement

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