A Stochastic Gradient Descent Method for Computational Design of Random Rough Surfaces in Solar Cells

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Abstract. In this work, we develop a stochastic gradient descent method for the computational optimal design of random rough surfaces in thin-film solar cells. We formulate the design problems as random PDE-constrained optimization problems and seek the optimal statistical parameters for the random surfaces. The optimizations at fixed frequency as well as at multiple frequencies and multiple incident angles are investigated. To evaluate the gradient of the objective function, we derive the shape derivatives for the interfaces and apply the adjoint state method to perform the computation. The stochastic gradient descent method evaluates the gradient of the objective function only at a few samples for each iteration, which reduces the computational cost significantly. Various numerical experiments are conducted to illustrate the efficiency of the method and significant increases of the absorptance for the optimal random structures. We also examine the convergence of the stochastic gradient descent algorithm theoretically and prove that the numerical method is convergent under certain assumptions for the random interfaces.

AMS subject classifications: 35J05, 35Q60, 49M41, 49Q10, 65C05, 65C30, 60H35 **Key words**: Optimal design, random rough surface, solar cell, Helmholtz equation, stochastic gradient descent method.

1 Introduction

Thin-film silicon solar cell is an attractive photovoltaic device because it attains a small thickness, which results in significant savings of material and energy during the fabrication. The cell consists of hydrogenated amorphous silicon (a-Si:H) as the absorbing layer,

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Figure 1: A schematic plot of thin-film solar cells.

sandwiched between the transparent conductive oxide (TCO) layers for conducting the electric current. Fig. 1 shows the structure of a typical thin-film solar cell, wherein the glass substrate on the top allows the incoming light to enter the cell and the highly reflective aluminum contact layer at the bottom enhances the absorption of light within the cell.

The a-Si:H layer in the thin-film solar cell is sufficiently absorptive at smaller optical wavelengths but poorly absorptive at larger wavelengths (typically > 600 nm), which is responsible for the low overall efficiency of the cell. One way to increase the absorption within the solar cell and enhance its performance is to engineer the structure by texturing the interfaces between the different layers in a random manner [1, 10, 11, 13, 18, 22]. The randomly textured surfaces lower the reflection losses at the entrance facet and scatter the light, thereby increasing the optical path of each photon in the solar cell. In realistic fabrication, the surfaces of the TCO layers in Fig. 1 are textured randomly, which is achieved at low cost by controlling the deposition parameter of TCO films sputtered on substrates [16]. We would also like to point out several other ways to increase the absorption efficiency of solar cells, such as anti-reflection coating, dielectric gratings, and plasmonic nanoparticles [3, 6, 9, 12, 19], although these techniques may be costly in fabrication.

The design and optimization of random surfaces in thin-film solar cells are mostly performed by the ad hoc procedures, where one computes the absorptance of the cell for chosen statistical parameters and obtains the optimal parameters from the comparison of the computed absorptance values [10, 11, 13, 18]. Such ad hoc schemes are computationally inefficient and the optimal solutions heavily depend on the set of statistical parameters being chosen. To provide a systematic computational framework, in [4] we formulate the optimal design of random surface textures as a random PDE-constrained problem and apply the gradient-based algorithm to solve the optimization problem. The optimization problem seeks to maximize the mean absorptance function for the solar