Complete Optoelectronic Simulation of Patterned Silicon Solar Cells

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***Abstract*— Patterned silicon solar cells are fully modeled optically and electrically using Lumerical Solutions' optical simulation software, FDTD Solutions and electrical simulation solver, DEVICE. The optical simulation calculates the spatial distribution of photon absorption in the silicon when the cell is illuminated by unpolarized sunlight with the AM1.5 solar spectral intensity. The photon absorption data is converted into a spatial generation rate of electron-hole pairs. The electrical simulation uses this generation rate to calculate the collection efficiency of electron and hole carriers, accurately accounting for surface and bulk recombination in silicon. Two main designs are simulated, each with periodic structures: a grating structure and a square pyramid structure. The short-circuit current as well as the overall conversion efficiency for the two devices are calculated.**

I. Introduction

There has been growing interest in increasing the efficiency of solar cells by adding wavelength scale patterning or plasmonic structures to enhance the absorption of light and reduce unwanted reflections. In order to compare different designs, it is essential to calculate the maximum power conversion efficiency from sunlight to electricity. We simulate the 3D patterns optically using the finite difference time domain (FDTD) method [1] in order to calculate the full spatial distribution of absorbed photons, and therefore the spatial distribution of generated electron-hole pairs, under solar illumination. This spatial distribution is then included in an electrical simulation which solves the Poisson and drift-diffusion equations. The combined optical and electrical simulations allow us to account for both optical effects, such as unwanted reflections, as well as electrical effects, such as bulk and surface recombination, to calculate the full power conversion efficiency for the design.

II. Simulation Models

A. Optical Simulation

The FDTD Solutions software [2] is used for optical modeling of the 2D and 3D silicon solar cell designs by calculating the absorption spectrum and hence carrier generation in silicon. A planewave source is used to model the sunlight incident on the device. The incoherent average of two orthogonally polarized sources is necessary to correctly represent the incoherent unpolarized light. Two designs from [3] studied here are shown in Fig. 1. For each of the designs, one unit cell of the grating is simulated and periodic boundaries are used. Table I summarizes the design parameters for the two structures. The effective thickness of silicon is kept at 3um for both cases. In the rectangular groove design, silicon is etched to achieve the grating. In the square pyramid design, the grating is made of TiO_2.

The absorption per unit volume is calculated by

$$L(r,\lambda) = -\tfrac{1}{2}\omega|E(r,\lambda)|^2 Im[\varepsilon(r,\lambda)] \qquad (1)$$

where L is absorbed power per unit volume at wavelength λ, E is the electric field, ω is the angular frequency and ε is the permittivity of the material. Absorbed power, electric field and the permittivity are functions of position r and wavelength λ. Absorption data is post processed to reflect the AM1.5G illumination over the wavelength range 0.4-1.1μm.

The generation rate is calculated assuming every photon absorbed yields one electron-hole pair.

$$G(r)\alpha \int L(r,\lambda)\left(\frac{\lambda}{hc}\right)d\lambda \qquad (2)$$

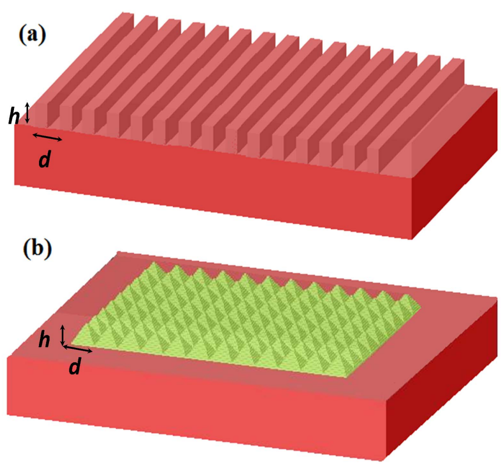

Fig. 1. Schematic of **(a)** rectangular groove and **(b)** square pyramid solar cell

TABLE I. Design Parameters

Name of Design	Grating parameters		
	Duty cycle(%)	h(nm)	d(nm)
Rectangular groove	50	1000	600
Square pyramid	100	900	750

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where G is the generation rate per unit volume, h is Planck's constant and c is the speed of light in vacuum. The generation rate is then used in the electrical simulation to study the distribution of charge and current collection at the contacts.

B. Electrical Simulation

The solar cells are electrically characterized using DEVICE software [2]. The Poisson and drift-diffusion equations are solved on a finite element mesh. The dopant concentration in silicon is introduced in the Poisson equation and the optical stimulus imported from the FDTD simulation is accounted for by the continuity equation. Aluminum and silver are used for the base and emitter contacts respectively. In both designs, the substrate is assumed to have a background p-type doping concentration of $2\times10^{16} cm^{-3}$. The front and back contact regions are n- and p-type diffusion doped respectively with a surface concentration of $10^{19}\ cm^{-3}$ falling off with an error function to a reference concentration of $10^{10} cm^{-3}$.

For bulk silicon, trap-assisted recombination, Auger recombination and radiative recombination processes are taken into account. Also, surface recombination at the interface of silicon with SiO_2 is modeled assuming a carrier recombination velocity of 10 cm/s. For the square pyramid design, the carrier recombination velocity at the interface of silicon with TiO_2 is 1000 cm/s. The simulation for the rectangular groove design is carried out in 2D. The simulation for the square pyramid design can be done in both 2D and 3D. For the 2D simulation, the 3D generation rate data calculated in the optical simulation is averaged in one dimension for use in the 2D electrical simulation.

III. Results and Discussion

The spatial distribution of the generation rate under incoherent illumination for the two designs is shown in Fig. 2. The generation rate pattern closely follows the absorption pattern in silicon.

Fig. 3 shows the *I-V* and power curves from the three simulations. The bias across the contacts is varied from 0 to 0.7 volts. The short circuit current and the overall conversion efficiency can be extracted from these plots. Table II lists the short circuit current values for each design. The short circuit current is a direct function of the optical generation rate. Absorption and hence generation is higher in the square pyramid design. The 2D and 3D short circuit current values for the square pyramid design are in close agreement implying that for this particular symmetry, computation time and resources can be saved by running only the optical simulation in 3D and the electrical simulation in 2D.

Assuming an input power of 100 mW/cm, the overall conversion efficiency of the solar cells is calculated and shown in Table II. The gratings in both designs minimize reflections from the surface; however, for the same effective thickness of silicon, the rectangular groove grating has increased silicon-oxide surface area which leads to more surface recombination at this interface. Regardless, the conversion efficiency of the rectangular grating design is higher than that of the square pyramid design by about 6%. For complex designs such as the ones studied here, this proves the importance of carrying out simulations to characterize and further optimize the behavior of the device.

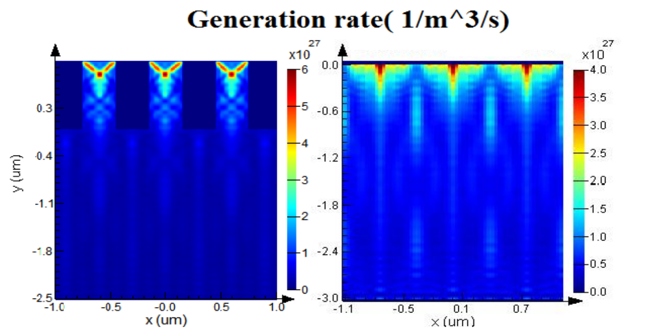

Fig. 2. Generation rate of electron-hole pairs for the rectangular groove (left) and square pyramid (right) solar cells

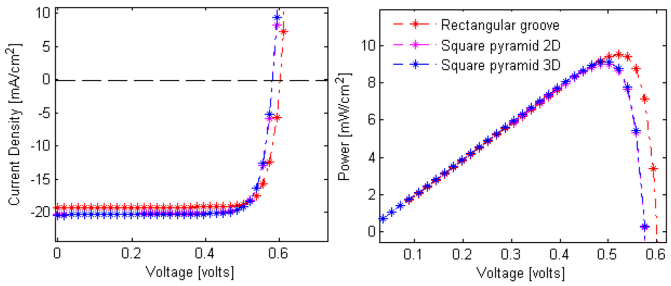

Fig. 3. Current desity and power versus voltage for solar cell designs

TABLE II. Solar Cell Short Circuit Current and Efficiency

Name of Design	*Jsc (mA/cm^{-2})*	*η (%)*
Rectangular groove	19.3	9.53
Square pyramid 2D	21.4	9
Square pyramid 3D	21.5	9.1

IV. CONCLUSION

Patterned silicon solar cells have been fully simulated optically and electrically using the FDTD method and a drift-diffusion solver. The optical simulation accounts for the incoherent nature of sunlight and the 1.5AM solar spectrum. The electrical simulation accounts for the optical stimulus, doping concentrations, bulk and surface recombination processes. Such complete characterization of these devices allows for the calculation of full optical-to-electrical figures of merit which is essential to optimize the power conversion efficiency of new solar cell designs.

References

[1] A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, 3rd ed. Boston, MA: Artech House, 2005.

[2] Lumerical Solutions Inc., Canada (http:// www. Lumerical.com).

[3] T. K. Chong, J. Wilson, S. Mokkapati, K. R. Catchpole, Optimal wavelength scale diffraction gratings for light trapping in solar cells, J. Opt. A 14, p. 024012, 2012.

[4] E. D. Palik, Handbook of Optical Constants of Solids. San Diego, CA:Academic, 1998.