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GEOMETRIC OPTIMIZATION OF SOLAR CELLS BY CONSTRUCTAL LAW

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Abstract. *Computer modelling has become increasingly important in the design and optimization of surface textures that are used in solar cells to manipulate scattering of light. Light scattering at rough interfaces together with efficient back reflector is a standard approach to enhance absorption of light in the absorber layers of solar cells. Recently, substrates with periodic surface features have been investigated as an alternative to randomly surface-textured substrates reaching improved efficiencies. In this work, Constructal Theory is used as a framework for the geometric optimization for the surface of solar cells. The total current density is estimated through the finite-difference time domain method (FDTD) to compare different textures geometries in the overall efficiency of solar cells. Surface textures were generated using gratings of rectangular, triangular, elliptical and trapezoidal shapes, testing different aspect ratios meanwhile the total area was kept constant. Results show that the trapezoidal grating with geometrical parameters $hf= 0.286 \mu\text{m}$, $lf= 0.06 \mu\text{m}$ and $sx=0.3 \mu\text{m}$ could reach higher light absorption as estimated by the total current density. Additionally, when the texture was built from elementary blocks ($50\text{nm} \times 50\text{nm}$) using a constructal algorithm there was increased performance compared to those obtained from fixed shapes with the same spacing.*

Keywords: *Constructal Theory, solar cells, finite difference time domain, geometric optimization.*

1. INTRODUCTION

Solar energy has been utilized by humans in different forms since the distant past. However, the growing need for sustainable development and concern for environment issues has triggered society to relook at it with real interest. Sunlight photovoltaic (PV) power generation is reliable, involves no moving parts and operation and maintenance costs are very low what turned this field into a hot research trend in the last decades (Chu and Meisen, 2011). A solar PV system directly converts solar energy into electricity through a semiconductor device that captures energy from sunlight photons generating electricity. This process is affected by several factors including solar cells' reflectance, thermodynamic, charge-carrier separation, and conduction efficiency values. The efficiency of single-junction commercial solar cells is currently approaching $\approx 20\%$ and only a few laboratorial cells could reach efficiencies of $\approx 25\%$ that viabilize the harnessing of solar energy over non-renewable sources (Chu and Meisen, 2011; Zhou *et al.*, 2014; Yablonovitch *et al.*, 2012). Therefore, both absorption of light in the semiconductor and collection of photo-generated charge carriers at the electrodes need to be further optimized in solar cells to achieve greater photoconversion. Thus, light management is a key issue to improve solar cells increasing light absorption in the absorber layers (Yablonovitch *et al.*, 2012). Light management is accomplished with a number of techniques including light trapping which has been receiving substantial interest due to an excellent cost-efficiency ratio (Zeman *et al.*, 2013). Lately, nano-texturing interfaces of the absorber layers has shown exceptional capacity to couple light inside the solar cell increasing efficiency through a simple geometrical modification. This process can be attained through a number of experimental techniques such as lithography, solution coating, physical vapor deposition, etching, self-assembly and so forth (Ruby and Zaidi, 2001; Macdonald *et al.*, 2004; Chopra *et al.*, 2004; Tao *et al.*, 2008; Wang *et al.*, 2017).

Nevertheless, the geometric pattern of the grating which can harness light more effectively is still a matter of research that is now aided by the numerical methods of simulation (Zeman *et al.*, 2013). The aim of this work is to perform an optical simulation in solar cells presenting 1D gratings using the Finite Difference Time Domain (FDTD) method and calculate the increase in light absorption as a function of the geometry. The geometry was further optimized within the framework of Constructal Theory which states that the architecture form comes from a principle of maximization of flow

access, in time, and a finite size geometry that is free to morph (Bejan, 2000; Bejan and Lorente, 2008, 2010). Through the theoretical background provided by the Constructal Theory, a converging relationship in terms of geometrical parameters is reached leading to greater understanding of the underlying principles of geometrical optimization of light absorption in solar cells.

2. COMPUTATIONAL PROCEDURE

All simulations were performed in MEEP, a free FDTD simulation software package developed at MIT to model electromagnetic systems (Oskooi *et al.*, 2010). The FDTD method is a direct solution to Maxwell's time-dependent curl equations. By time-dependence inclusion, FDTD can incorporate the effects of reflection and radiation making it flexible and appropriate to study light trapping in a photovoltaic cell. The solar cell geometry was analyzed in the perspective of Constructal Theory aiming to obtain those geometries leading to improved light trapping. The Constructal Theory for geometric optimization pursues the optimal geometry that better complies with the control function (Φ) which, for the purpose of this work, was given by the total energy of the electromagnetic field. The overall improvement of the efficiency in the solar cell with the different textures geometries was compared calculating the total current density of every texture, indicated by J . The higher the value of J higher the efficiency of a given texture to harness energy from the incident light.

In this work restricted and automata geometrical optimization were performed. In the restricted optimization, variables such as lf , hf and sx were varied in different shapes for the grating while the total area of the grating was kept constant ($A=0.01 \mu\text{m}^2$). The effect on the absorption was evaluated through J . The simulation cell for this case is illustrated in Fig. 1(a-e) for the different textures. In all simulations the light was incident perpendicularly to the texture base, the frequency range simulated was that of the visible light ($0.38\mu\text{m}$ - $0.7\mu\text{m}$) and silicon absorption in this range agreed with experimentation through the implementation of the dielectric function using lorentzians for the real and imaginary parts. The FDTD was implemented with a resolution of at least $200 \text{ px}/\mu\text{m}$ corresponding to 10 pixels to every $0.05 \mu\text{m}$ that was usually the smallest feature in the simulation cell.

The automata optimization was performed in regular gratings of size $50 \text{ nm} \times 50 \text{ nm}$ which were added to the structure in the positions defined by the maximum of the control function in each optimization step. The structure was constructed layer-by-layer as illustrated in Fig. 2. The energy of the electromagnetic field was evaluated separately to determine the point where the next grating should be placed, as illustrated in Fig. 3(a-c). Meanwhile, the total current density (J) was evaluated at each optimization step and the number of blocks reaching the higher J was defined as the best for that layer. Once the optimal number of blocks is reached for a given layer, the structure starts growing in the layer above following the same algorithm.

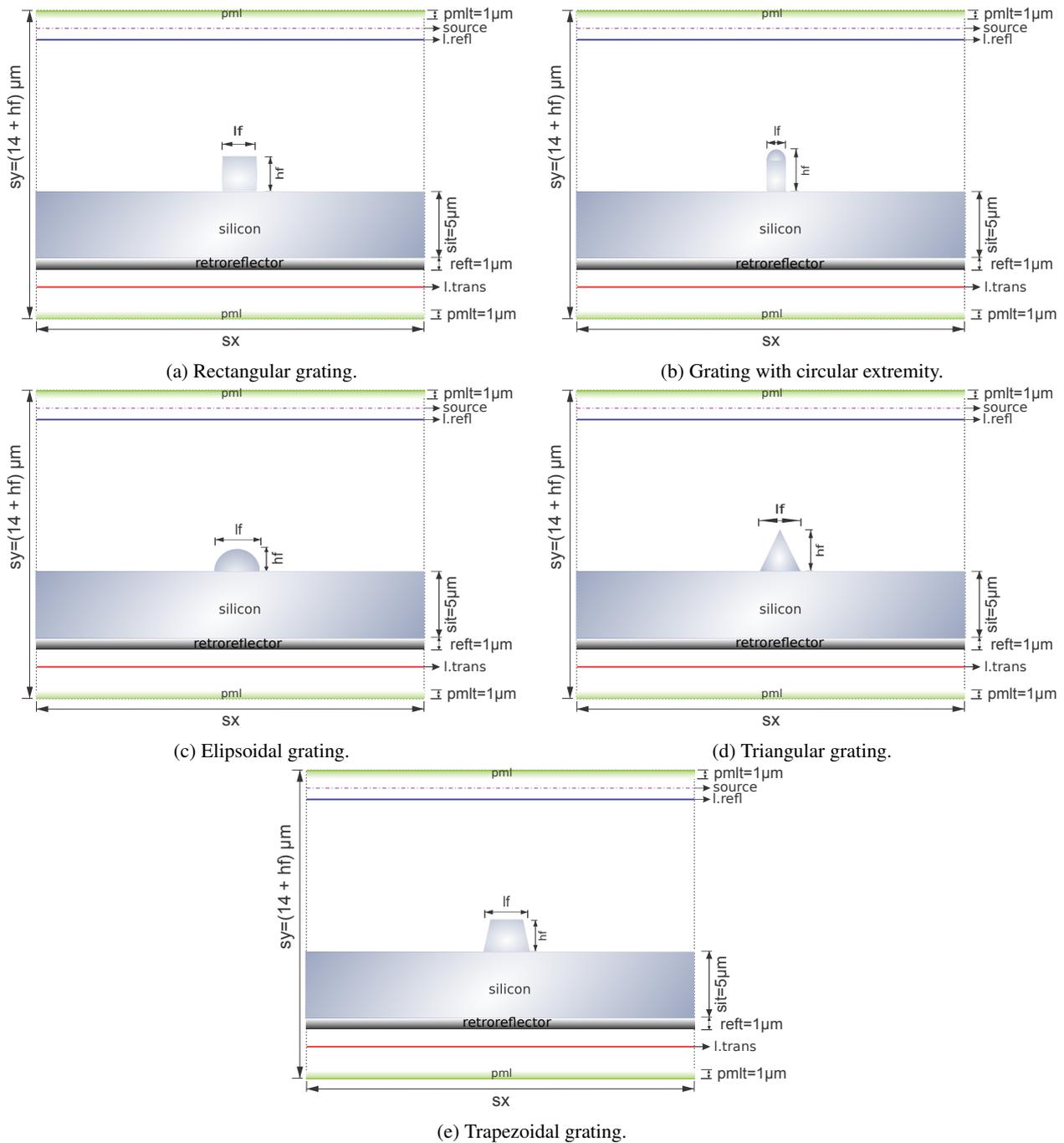


Figure 1: Different grating geometries tested with different values of hf and lf while the area of the grating was maintained equal to $0.01\mu\text{m}^2$

3. RESULTS AND DISCUSSION

The aim of the restricted optimization was to find the optimal geometrical ratios that would improve light absorption on the solar cell. Graphs in Fig. 4 show the effect of the parameters hf and lf in the J of the resulting textures. Since the grating area was constant, hf and lf are interdependent and their corresponding values are presented.

Table 1 shows the best hf and lf for every geometry tested for the grating. The best result was attributed to the triangular grating that produces better penetration of light in the solar cell due to the angle light does with the texture. Figure 5 shows the accumulated energy of the incident light in the optimal triangular tested shape ($lf=0.05\mu\text{m}$ $hf=0.4\mu\text{m}$). Field distribution into the cell indicates an increase in the average path length that light travels and therefore increases the overall light absorption. Solar cell texture also works as an intermediate of the dielectric constant of air to the dielectric constant of bulk silicon, improving light absorption through a smooth transition between both media.

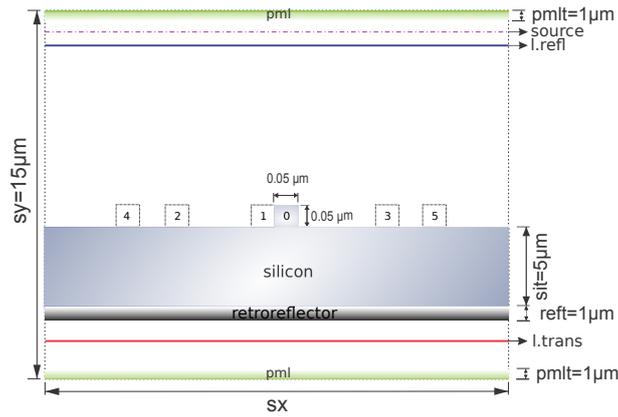


Figure 2: Illustration of constructal optimization using elementary blocks of dimensions 50 nm x 50 nm, shows the start of optimization for first layer up to optimal number of blocks in this layer (e.g. 5 blocks)

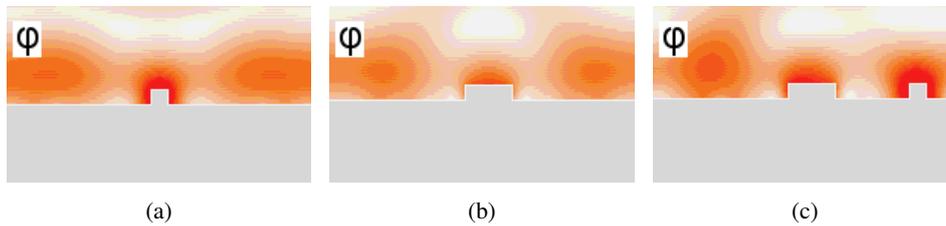


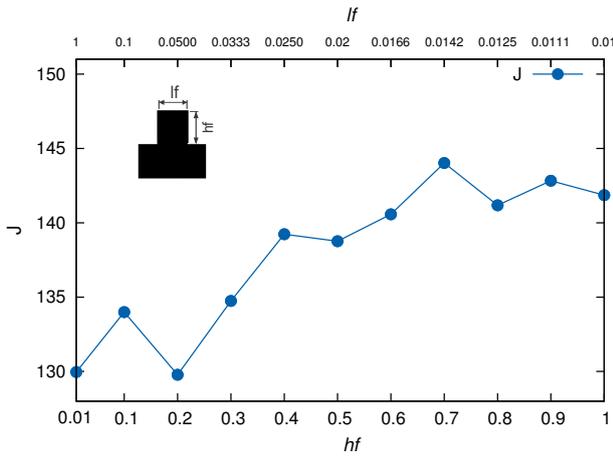
Figure 3: Field of control function (Φ) for the textures. (a), (b) and (c) show subsequent steps of constructal optimization where the region of higher contrast indicates the position where the next block will be added.

Table 1: Results of the best geometries of gratings found through restricted optimization.

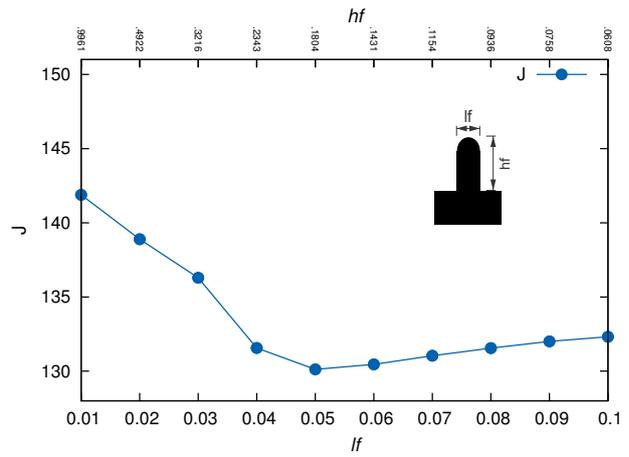
Geometry of grating	hf	lf	J
Rectangular	0.7 μm	0.0142 μm	144.01942 W/m^2
Rectangular with circular extremity	0.9961 μm	0.01 μm	141.88467 W/m^2
Elipsoidal	0.1592 μm	0.04 μm	143.30563 W/m^2
Triangular	0.4000 μm	0.05 μm	148.25016 W/m^2
Trapezoidal	0.2857 μm	0.06 μm	144.38871 W/m^2

Effect of sx , the period or spacing between gratings, on the overall absorption was also evaluated and is shown in Tab. 2. Values of sx close to 0.3 μm provided the best results for most geometries. Constancy of this value can be associated with the smallest wavelength simulated being 0.390 μm corresponding to the beginning of the visible range. Values of sx smaller than this would hinder absorption of larger wavelengths and for a larger spacing small wavelengths would not perceive the texture. Therefore, after optimizing the spacing between gratings, the best value of J found in restricted optimization was that of the trapezoidal grating with $hf=0.2857 \mu\text{m}$, $lf=0.06 \mu\text{m}$ and $sx=0.3 \mu\text{m}$ reaching a $J=198.65388 \text{ W}/\text{m}^2$. Energy field of this grating is shown in Fig. 6 along with the energy field of a lower J texture. Figure 6 shows how the penetration and distribution of light energy fields into the cell is much better in trapezoidal grating.

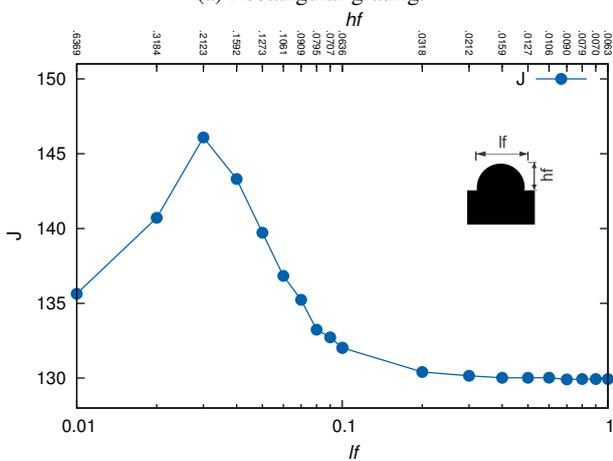
It's important to highlight that obtaining some of these textures (e.g. trapezoidal or rectangular gratings) experimentally with enough precision may require advanced texturing techniques such as photolithography or self-assembly. Meanwhile, triangular or elipsoidal geometries can be obtained through relatively simpler methods such as etching, solution coating or physical vapor deposition.



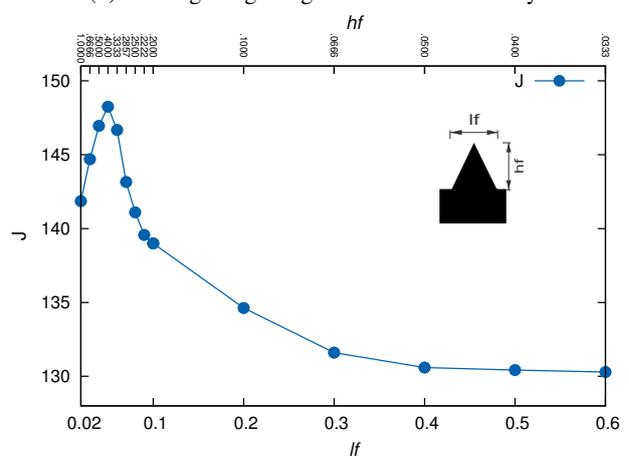
(a) Rectangular grating.



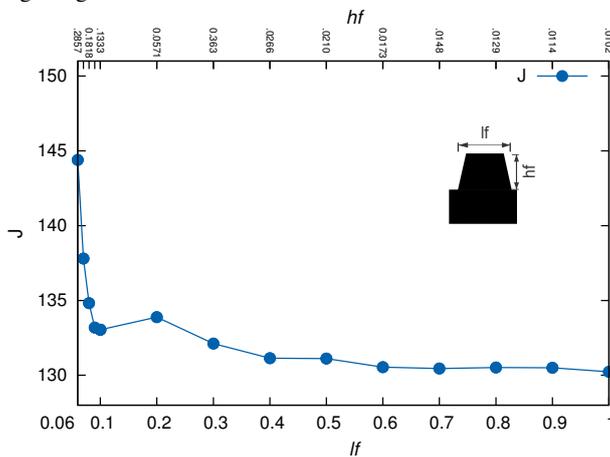
(b) Rectangular grating with circular extremity.



(c) Elipsoidal grating.



(d) Triangular grating.



(e) Trapezoidal grating.

Figure 4: Total current density for the different grating geometries.

In the constructal automata optimization, the elementary block was added progressively in each optimization step in the same layer. Once the peak J was found for a number of elementary blocks growth would continue in the layer above until a total of 30 blocks were added. Results shown in the graph of Fig. 7 indicate that the arbitrary shape built through the constructal algorithm has potential for improved light trapping in the solar cell. Figure 7 also shows that the increase of total current density is not linear and the result is highly dependent on the position of the blocks instead of total grating area.

A few considerations can be outlined on the result of the constructal optimization. Firstly, the spacing between the gratings formed by the algorithm were similar and close to $0.3 \mu\text{m}$ what can be linked to the optimal sx found in restricted optimization. Moreover, shape of the gratings resemble that of the trapezoidal or triangular grating. This structure can be

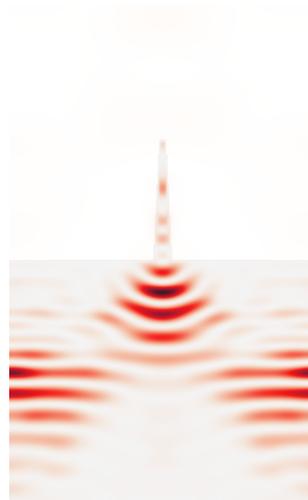


Figure 5: Light energy field for a triangular grating ($lf=0.05\mu\text{m}$ $hf=0.4\mu\text{m}$ $sx=1\mu\text{m}$). Silicon is represented in gray, air is represented in white, the energy field is shown in shades of red.

Table 2: Results of the optimal sx for the best geometries found through restricted optimization.

Geometry of grating	sx	J
Rectangular	$0.14\ \mu\text{m}$	$175.33977\ \text{W/m}^2$
Rectangular with circular extremity	$0.3\ \mu\text{m}$	$177.83553\ \text{W/m}^2$
Elipsoidal	$0.3\ \mu\text{m}$	$184.66418\ \text{W/m}^2$
Triangular	$0.3\ \mu\text{m}$	$197.17562\ \text{W/m}^2$
Trapezoidal	$0.3\ \mu\text{m}$	$198.65388\ \text{W/m}^2$

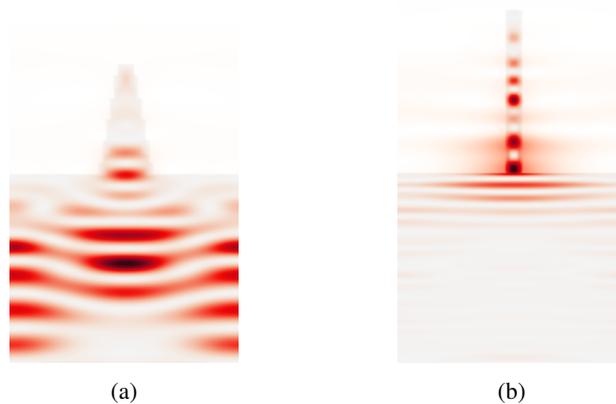


Figure 6: Light energy field for (a) trapezoidal grating ($lf=0.06\mu\text{m}$, $sx=0.3\mu\text{m}$) and (b) rectangular grating with round extremity ($lf=0.01\mu\text{m}$, $sx=0.3\mu\text{m}$). Silicon is represented in gray, air is represented in white, the energy field is shown in shades of red.

clearly defined when the elementary block dimensions are reduced. Finally, although the coarse size of the elementary block there is a significant improvement in J value reaching $J = 161.76322\ \text{W/m}^2$, this value is higher than achieved by restricted optimization using the same sx ($< 150\ \text{W/m}^2$) as can be seen on the graphs of Fig. 4. This result is in agreement to the principle of distribution of imperfections, stated by Constructal law, that maximizes the global flow access (Bejan and Lorente, 2008, 2010), in this case, the penetration of light in the solar cell to be further converted in electricity.

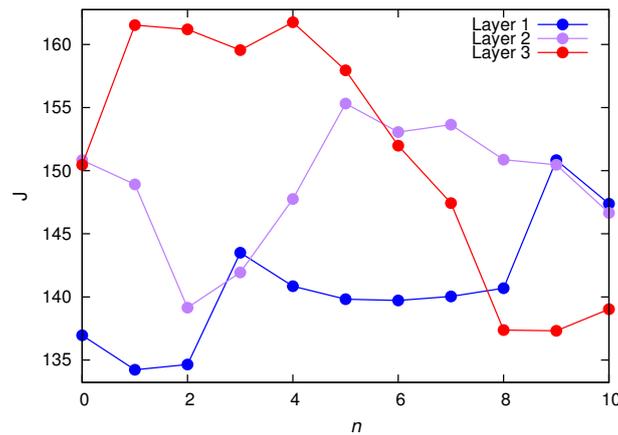


Figure 7: Total current density versus number of blocks and layer number, elementary block had dimensions $50\text{nm} \times 50\text{nm}$ and $sx=1\mu\text{m}$.

4. CONCLUSION

This work performed two modes of constructal optimization to study textures to improve light absorption in solar cells leading to increased efficiency. All simulations were performed with incident light perpendicular to the texture base and frequency range corresponding to visible light ($0.38\mu\text{m}$ - $0.7\mu\text{m}$). Silicon dielectric function was modelled in this frequency range using Lorentzians for the real and imaginary part leading to absorptions accurate to what is expected experimentally.

The first method was called restricted optimization and the grating shape was fixed. The study concentrated on the effect of each geometrical parameter while the area of the grating was kept constant, optimizing both the shape of the grating (defined by lf and hf) and the spacing between them (defined by sx). Optimal grating had trapezoidal shape with parameters $lf=0.06\mu\text{m}$, $hf=0.2857\mu\text{m}$, $sx=0.3\mu\text{m}$ with $J=198.65388\text{ W/m}^2$. Trapezoidal and triangular shapes presented better penetration of the light in the solar cell working as intermediate between the two distinct dielectric media. It's also important consider that obtaining textures such as trapezoidal or rectangular gratings can be more challenging experimentally while triangular or ellipsoidal geometries can be obtained through relatively simpler methods.

The second method named automata optimization applied the constructal algorithm to build textures from elementary blocks with fixed dimensions. In every loop of the algorithm, position for the next block was defined from a predefined control function (Φ) and texture was grown layer-by-layer until a total number of blocks was reached. In this method, the final texture had gratings that resemble the triangular and trapezoidal shapes found in the first method and a $J=161.76322\text{ W/m}^2$ that was superior to the J obtained with restricted optimization using the same $sx=1\mu\text{m}$.

Finally, this work evidences the applicability of the framework provided by the Constructal Theory to the problem of solar cell optimization. There was a general improvement in the efficiency as measured by the total current density that could be found by both optimization methods applied here. Results are therefore coherent to the principle of facilitation of flow access (which in this case is the penetration of light in the solar cell) through the optimal distribution of the imperfections (the gratings generating the texture).

5. ACKNOWLEDGEMENTS

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