Minimizing surface reflectance of crystalline silicon: A simulation based study

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Abstract. Silicon has been a popular choice for optoelectronic devices and solar cells since its discovery mainly due to its abundance in nature. However, methods to improve light trapping and hence increase the efficiency of these devices has always been a subject of great interest. The objective of this study has been to minimize the surface reflectance of thin film silicon through use of anti-reflection coating and surface patterning. In this study, the most effective anti-reflectance coating (ARC) is determined amongst three well known materials namely, Silicon Nitride(Si₃N₄), Titanium Dioxide(TiO₂) and Magnesium Fluoride (MgF₂) by simulation through S4 software by implementing Rigorous Coupled Wave Analysis Algorithm (RCWA). The best possible combination of the substrate and ARC is determined for a working wavelength range of 300 nm to 900 nm by varying the thickness of ARC. The best possible combination of substrate and ARC has been subjected to further investigation by imparting patterns and minimum average reflectance of 0.135986 was obtained experimentally.

1. Introduction
Since the mid twentieth century, the use of silicon has taken a big leap. Nowadays, Silicon is practically used everywhere from wristwatches to international space stations. Silicon has played a major role in converting solar energy to electrical energy.
The very first solar cell was developed in 1954 at Bells Labs, which in theory could give a 23% efficiency provided the physical parameters were ideal [1]. Although, the energy conversion efficiency obtained was about 4% which at the least was a proof of a new concept. Apart from overcoming the band gap, there were mainly two hurdles faced by the leading physicists- one that it was very difficult to make a proper electrical contact with the silicon due to the poor adhesion with metals and secondly the high reflectance by the silicon wafers itself.
Since, bare Crystalline Silicon shows a very low efficiency in the absorption of light, i.e most of the energy of the incident light is lost due to reflection, depending on various physical factors such as surface texture, refractive indices of the mediums to the Silicon, thermodynamic parameters, etc. In order to decrease the reflectance usually mainly two widely used approaches are taken in combination

• Introduction of patterns or surface textures.
• Application of an antirefection coating(ARCs) on the top bare Silicon surface.

In the former approach regular patterns are introduced using techniques such as wet etching, dry etching, photolithography, etc[2]. These patterns help in entrapment of the incident light predominantly by increasing the net internal reflection [3].
In the later approach a coating of suitable material is applied on the top layer of the bare Silicon which can transmit light as much as possible and reduce the reflectance of the incident light. The entrapped light waves scattering in the bulk of the ARC then undergo coupling and quantum interference effect helps in absorption in the bulk [4]. Ideally, an ARC should be able to minimize the reflectance for a range of wavelengths [5]. By using ARCs the overall efficiency can be increased by up to 40% [6]. Since reflectance of an ARC depends on its thickness and its refractive index (with respect to Silicon). So, it is in our best interest to study variation of reflectance with respect to the variation of the thickness and the material. Optimization of the above said parameters can reduce the loss in overall reflectance and in turn increase the efficiency of the solar cell. In addition to adding an ARC, patterns can be introduced on the topmost layer to decrease the reflectance further, as per Fresnel Theory. Although, introducing patterns or textures on the ARC itself opens the possibility of many configurations that can occur in practice which may not necessarily increase the overall efficiency of the cell. So this makes it crucial to study the variation of reflectance in respect to these configurations as well [7][8]. This paper presents the investigation of various anti reflective coatings for minimization of the reflectance with polychromatic sources in respect to two physical factors – surface textures (patterns) and thickness of the antireflection coatings. Also, it presents the study of the introduction of patterns on ARCs with different configurations.

2. Methodology
A significant and well proven method to promote light absorption and reduce surface reflectance has been the use of effective anti-reflection coatings and creation of patterns on layer. In this study, a comparative analysis is performed to determine the most suitable configuration of substrate and coating which produces the least mean surface reflectance and hence provides the most efficient combination for use in devices. The analytic work carried out in this study is performed on the data obtained by a series of simulations carried out in the S4 software. The detailed procedure is enlisted below in sections for easier understanding.

2.1. Comparative Analysis of Anti Reflection Coatings(ARCs)
A comparative study is performed to determine the most effective anti-reflection coating on the bare silicon amongst three well known materials for the role, namely, Magnesium Fluoride (MgF2), Titanium Dioxide (TiO2) and Silicon Nitride (Si3N4). A 1000nm Silicon substrate along with a single layer of one of the three ARCs is considered (with an initial thickness of 50nm). Surface reflectance values for a wavelength range of 300nm to 900 nm with steps of 3nm for this configuration is obtained. After this, keeping the thickness of the Si substrate constant, reflectance values using thickness of the ARC layer as 60nm, 70nm, 90nm, 110nm, 130nm and 150 nm was obtained to identify the best working thickness for the given substrate thickness. After this, reflectance values for each of the above mentioned ARC layer thickness is calculated by changing Si substrate thickness to 10,000nm, 25,000nm and 50,000nm. This same process is repeated for each of the materials as the ARC and the average reflectance value for all the combinations of each material is calculated. The material, substrate and ARC thickness combination which provides the least average reflectance is selected to further investigate the effect of patterns on the surface reflectance.

2.2. Comparative analysis of different configurations for the selected Substrate ARC combination
The substrate and ARC thickness combination that provides the least mean surface reflectance is chosen for further investigation. Five different configurations for the selected pair is simulated and the mean reflectance values are compared to obtain the best possible configuration for reduced reflectance. These five configurations are explained in details below along with their cross sectional views.
2.2.1. Case 1
This configuration (fig 1) is simulated first. It is simply the combination of the substrate and ARC that produces the minimum mean reflectance without any patterns.

![Case 1 Configuration](image)

**FIGURE 1:** Case 1 Configuration

2.2.2. Case 2
In this configuration (fig 2), circular holes are made on the structure with a diameter of 100 nm, pitch of 350 nm and thickness being the same as the ARC thickness. This is accomplished by creating a circular pattern in the center of the 350 nm*350 nm space lattice in the layer 1 which is the ARC layer and filling it with vacuum.

![Case 2 Configuration](image)

**FIGURE 2.** Case 2 Configuration

2.2.3. Case 3
In this configuration (fig 3), circular holes are made in the structure with the same diameter of 100 nm and pitch 350 nm but with a thickness of an additional 200 nm into the substrate apart from the entire ARC thickness. The results are obtained by simulating a three layered structure with a circular pattern in the center of 350 nm*350 nm space lattice with the material as vacuum running through layers 1 and 2 which are the ARC layer and 200 nm of substrate respectively. The remaining thickness of the substrate forms the third layer. This case is a representation of an ideal configuration which is not possible to produce in real life.
2.2.4. **Case 4**

This configuration is feasible in reality and hence is referred to as the practical case. In this configuration (fig 4), circular holes are made in the structure with the same diameter of 100 nm and pitch 350 nm. A thickness of an additional 200 nm is made into the substrate (apart from the entire ARC thickness) and the removed ARC thickness settles within the created void in the substrate. The results are obtained by simulating a four layered structure with a circular pattern in the center of 350 nm*350 nm space lattice with the material as vacuum running through layers 1 and 2 which are the ARC layer (let, thickness= b nm) and (200- b) nm thickness of substrate respectively. The third layer consists of substrate with thickness same as the ARC thickness (=b nm) with a circular pattern in the center of the lattice filled with material as the ARC. The remaining portion of the substrate constitutes the fourth layer.
2.2.5. Case 5
This configuration is the extension of the prior configuration wherein the top layer of residual ARC after creating the holes is removed, known as ‘top cleaning’. This configuration (fig 5) can be simulated by disabling the first layer only and defining the other parameters same as the preceding case.

![Case 5 Configuration](image)

On obtaining the data for all these cases with the specifications as mentioned for a wavelength range of 300 nm to 900 nm with a step of 3 nm, compute the mean surface reflectance values for all the cases and compare them to find the best suitable configuration for reduced reflectance of the combination of the silicon substrate and best performing anti-reflection coating.

3. Simulation of optical properties
Minimization of surface reflectance has always been a critical challenge to resolve the issue of optical losses in solar cells where crystalline silicon is used mainly. In this method, we have attempted to minimize the surface reflectance for silicon substrate by running simulations using an open source software available on Nanohub, ‘Stanford Stratified Structure Solver’ which is more commonly known as S4.

4. Results and Discussions
As mentioned earlier, three materials are taken as Anti-reflection Coating (ARC) – Silicon Nitride(SiN4), Magnesium Fluoride(MgF2) and Titanium Dioxide(TiO2). Simulations were run for bare ARC with no pattern, taking the substrate as c-Si. A comparative study was done to check the reflectance capability for all the above three ARCs individually at different thicknesses. An average reflectance is calculated at every thickness of the ARC for a constant substrate thickness. This is done to find the material which has the least reflectance value. The following table (Table 1) depicts the best combination of Substrate ARC thickness for achieving minimum surface reflectance value.
Comparing all the mean reflectance values for different materials at different thicknesses and different substrate thicknesses we have found out the least values for all the three materials. The ideal results for all the above materials are mentioned in bold in the table itself. This is represented graphically in Figure 6.

From the plot, we can see that Silicon Nitride (Si$_3$N$_4$) gives the least reflectance. The cost of patterning is very high. So for the subsequent cases with patterns, Silicon Nitride is selected as the most appropriate material as an anti-reflection coating.

FIGURE 6. Average surface reflectance plot for MgF$_2$, TiO$_2$ and Si$_3$N$_4$

After selecting the best anti-reflection coating as Silicon Nitride, we move on to the several cases that have been discussed in Section 2.2. These configurations are considered for study to find out the influence of patterns in the surface reflectance result. The first case is the most basic configuration and hence its surface reflectance value is taken as the comparison yardstick for the other cases involving patterns. In keeping with our objective, we perform a comparative analysis of all the configurations.
This is done to select the best possible patterned configuration for Silicon. Simulations are run in the S4 tool and the results which are obtained are depicted below in the result table 2.

### Table 2: Compact result table for all the cases.

| CASE | FRONT VIEW | MEAN SURFACE REFLECTANCE VALUE | COMPARATIVE ANALYSIS |
|------|------------|-------------------------------|----------------------|
| 1    |            | 0.13997                       | Taken as the initial value and is compared with other cases |
| 2    |            | 0.1405032                     | Increases by 0.38%   |
| 3    |            | 0.136691                      | Decreases by 2.34%   |
| 4    |            | 0.1359801                     | Decreases by 2.85%   |
| 5    |            | 0.3828156                     | Increases by 173.5%  |

From Table 2, we can see that the mean reflectance value decreases in Cases 3 and 4. Case 2 shows a slight increase in surface reflectance. In Case 5, reflectance increases rapidly. This is due to the fact that the top part i.e, the Silicon nitride layer is top cleaned. As there is no definite anti-reflection coating layer, so the light doesn’t get trapped. So the amount of light reflected back increases swiftly. Comparing the surface reflectance values for all the cases we can say that Case 4 exhibits the best result amongst others with the least surface reflectance. Here the light gets trapped inside the hole causing a very small portion of it to be reflected back. It is the closest depiction of the real case. In actual practice during etching, small amounts of the ARC gets trapped in the cylindrical structures formed on Silicon.
A combined plot for all the different cases is shown in Figure 7. From the plot, we notice that almost all the cases (except for Case 5) show the same nature, while Case 5 shows a completely different curve nature as there is rapid increase in reflectance at all wavelength values due to the absence of a definite ARC layer as compared to the other cases.

The surface reflectance is almost zero in the wavelength range of ~470-520nm which basically means that the patterned and the coated substrate will absorb all the incident light in this range. In addition to photovoltaic, such a substrate can have applications for absorbing incident green laser light, which can create problems in aviation industry [9].

5. Conclusion
This study was done as an attempt to reduce the surface reflectance of crystalline silicon through use of anti-reflective coatings (ARCs) and hence determining the most effective configuration. The method was successful as the average surface reflectance was reduced by determining the best performing ARC and the suitable configuration. The fourth configuration where the ARC gets trapped inside the hole gives the best result with a total 2.85% reduction in surface reflectance.

6. References
[1] D. M. Chapin; C. S. Fuller & G. L. Pearson (May 1954). "A New Silicon p-n Junction Photocell for Converting Solar Radiation into Electrical Power". *Journal of Applied Physics*. 25 (5): 676–677.
[2] Mehul C. Raval and Sukumar Madugula Reddy (May 15th 2019). *Industrial Silicon Solar Cells*, Solar Cells, Majid Nayeripour, Mahdi Mansouri and Eberhard Waffenschmidt, IntechOpen, DOI: 10.5772/intechopen.84817.
[3] Moona, Girija & Kapruwan, Pankaj & Sharma, Rina. (2017). Silicon Wafer Surface Reflectance Investigations by Using Different Surface Texturing Parameters. *Proceedings of the National Academy of Sciences, India Section A: Physical Sciences*. 88, 10.1007/s40010-017-0384-3.
[4] Raut, Hemant & Venkatesan, Anand Ganesh & Nair, Sreekumaran & Ramakrishna, Seeram. (2011). Anti-Reflective Coatings: A Critical, In-Depth Review. *Energy & Environmental Science*. 4, 3779-3804. 10.1039/C1EE01297E.
[5] Hashmi, Galib & Rashid, Mohammad & Mahmood, Zahid & Hoq, Mahbubul & Rahman, Md. (2018). Investigation of the impact of different ARC layers using PC1Dsimulation:
application to crystalline silicon solar cells. *Journal of Theoretical and Applied Physics.* 12. 10.1007/s40094-018-0313-0.

[6] "From 40.7 to 42.8 % Solar Cell Efficiency". *University of Delaware.* July 30, 2007. Retrieved 2008-01-16.

[7] S. C. Baker-Finch, K. R. McIntosh and M. L. Terry, "Isotextured Silicon Solar Cell Analysis and Modeling 1: Optics," in *IEEE Journal of Photovoltaics,* vol. 2, no. 4, pp. 457-464, Oct. 2012, doi: 10.1109/JPHOTOV.2012.2206569.

[8] A. Goswami, S. Aravindan and P.V.Rao (December 2016) “Optimization of nanohole array parameters for improving the ultimate efficiency of nanohole structured c-Si solar cells” in *Proceedings of the Institution of Mechanical Engineers, Part N: Journal of Nanomaterials, Nanoengineering and Nanosystems,* 230, 4, 231-240.

[9] “https://www.boeing.com/commercial/aeromagazine/articles/qtr_01_10/3/” retrieved on 9 February 2021.