Nano Pyramid Anti–reflective Coating Design for Improved Thin-Silicon Photovoltaics

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Abstract. Process of converting light to electrical energy in photovoltaics (PVs) depends on sequential process from photon absorption - charge separation - charge collection. The total PV's power-conversion efficiency on efficiency from each of these steps. In this study, we aim to improve photon absorption by minimizing reflection losses. For that, we design an anti–reflective coating (ARC) made by low index materials of pyramidal array geometry applied on thin-film silicon PVs. We utilize Finite Difference Time Domain (FDTD) method to determine reflection losses, optimize the design, and assess their limiting factors. We use index matching materials such as Si_3N_4 and SiO_2 as ARC where we find the reflection loss can be as low as 3.4% from the total power of incident light. With careful geometrical tuning and combined with ease processing owned by SiO_2, we believe this work open opportunities for further design and exploration for ARC for photovoltaics.

Keywords: Silicon photovoltaics, Anti–reflective coating, Si_3N_4, SiO_2, FDTD

1 Introduction

Photovoltaic or solar cells is one of several types of technology in the field of renewable energy that is reliable, environmentally friendly, and requires low costs per kWh generation when compared to the price of conventional generator fuel. In addition, photovoltaic can be said to be net zero combustion, which means that there is no combustion that can produce gas emissions.

The main obstacle that causes the use of solar cells as an energy source is still rarely used today, namely because it is still very limited, and the conversion efficiency value is still quite low. One of the factors that causes this low conversion efficiency is that not all sunlight that falls on the surface of silicon solar cells can be absorbed and converted into electrical energy. But some of them are reflected into the air. The event of reflection of light by the surface of the solar cell occurs because of the difference in refractive index between the two mediums through which the light passes is quite large [1].

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2 Photovoltaics

Solar energy is a type of electromagnetic radiation that emits light to the earth and is composed of photons or particles of solar energy that can be converted into electrical energy. This energy conversion process involves sequential process of photon absorption – electron and hole separation – and electron and hole collection (**Figure 1**) [1]. If the sunlight reaches the silicon thin film, then not all sunlight can be converted into energy. The sunlight that is not converted will be reflected (**Figure 2**) [2]. To find out how much sunlight is reflected, the total value of the reflection power from the sun can be calculated by equation (1).

$$R_{total} = \int_{300}^{800} R(\lambda)\mathrm{AM1.5}(\lambda)\mathrm{d}\lambda \tag{1}$$

After knowing how much sunlight is reflected, we can also find out how much sunlight is transmitted using the same formula as equation (1), now by replacing the R to T as Transmission. Thus, we can determine the amount of sunlight that can be absorbed by thin films of silicon (Si PVs) by using the equilibrium equation (2). Note that this equation only holds assuming the A also includes light scattering.

$$A + R + T = 1 \tag{2}$$

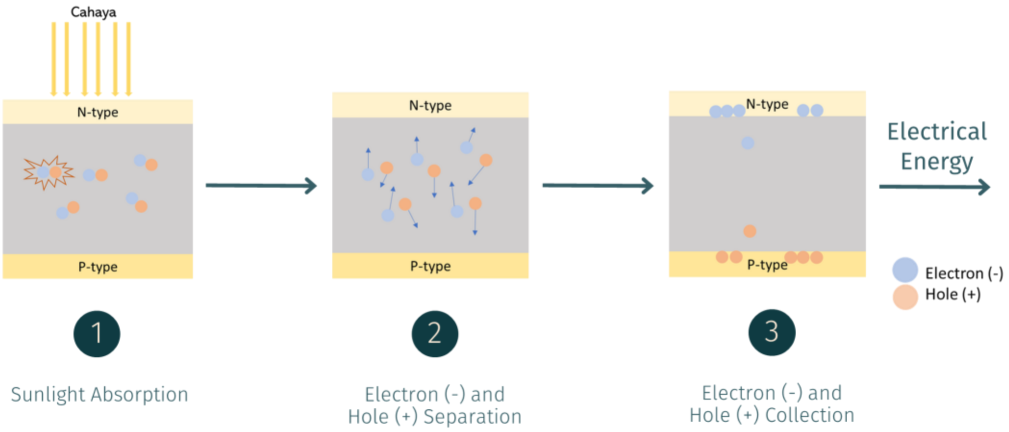

Fig. 1 The process of converting sunlight into electrical energy

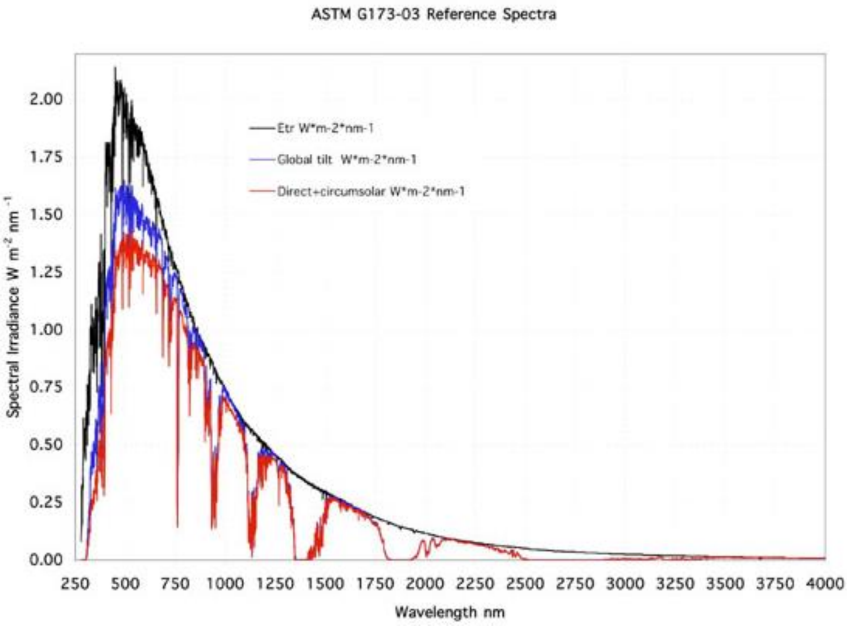

Fig. 2 Sunlight power data [2]

3 Anti–reflective Coating (ARC)

Anti–reflective Coating (ARC) is a layer that serves to reduce the reflection intensity from the photovoltaics so that the energy of sunlight that can be absorbed will be even greater.

Table 1. Comparison of previous research on anti-reflective coating.

Material	Geometry	%R total	References
Si_3N_4	pyramid	2,3 %	[3]
ZnO	sphere	2,3%	[4]
SiO_2	pyramid	3,8 %	[5]
TiO_2	flat	1,5 %	[1]

In this study, the geometric shape that will be used is in the form of a nano pyramid, as shown in **Figure 3** [6], which will be placed on the surface of silicon PVs. The reason the geometric shape used is in the form of a nano pyramid is due to this geometric shape is the most stable and the incoming light is gradual. From top to the bottom side of the pyramid, the light will experience gradual change of refractive index (from air to silicon). This contrasts with other geometrical shapes such as sphere, flat, and nanowire (Table 1). This means that the incoming photons will be converted into electrical energy slowly (starting from the tip of the nano pyramid to the surface of the nano pyramid).

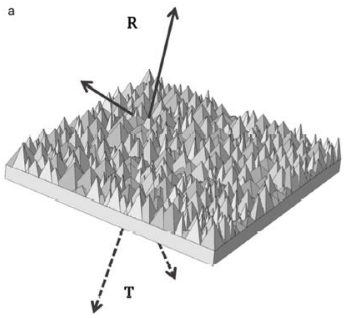

Fig. 3 The geometric structure of anti–reflective coating [6]

The anti–reflective coating used must be a transparent material so that sunlight can be transmitted to the sample. In addition, the value of the refractive index of the anti–reflective coating must be between the values of the refractive index of the air and the sample (silicon PVs). The refractive index of Si_3N_4 is between ~2.5 – 2 [7]. While the refractive index of SiO_2 is 1.461 – 1.447.

The Fresnel equation can be used to design an anti–reflective coating with a flat geometric shape.

$$n_{ARC} = \sqrt{n_1 n_2} \quad (3)$$

$$d = \lambda / 4 n_{ARC} \quad (4)$$

The value of the refractive index of the anti–reflective coating in theory according to equation 3 and equation 4 will be used to calculate the index matching value. To determine the material that can be used as an anti–reflective coating for Si PVs, it is necessary to calculate the index matching value first. The index matching value should be close to 0, so that the error obtained will be even smaller. In this work, two type of materials, Si_3N_4 and SiO_2, are compared. The Si_3N_4 is commonly used in industry, while SiO_2 is a material that is easy to fabricate (see Table 2).

Table 2. Comparison Si_3N_4 and SiO_2 anti-reflective coating.

Si_3N_4	SiO_2
1) Semiconductor and transparent material	1) Semiconductor and transparent material
2) Has index matching value <0.6	2) Has index matching value between 0,04 – 0,092
3) Commonly used in industry (feasible)	3) Easy to form into a pyramid
4) Difficult to form into a pyramid	4) Fabrication process using sol gel method [8]
5) Fabrication process using PECVD [3]	5) Requires a low cost
6) Requires an expensive cost	

4 Finite Difference Time Domain (FDTD)

Finite Difference Time Domain or FDTD solutions are electromagnetic wave simulation based on Maxwell's equations which can be solved by a numerical method in the time domain basis.

In this study, the silicon sample structure that will be used is flat with boundary conditions on the x and y axes, which is a periodic structure, and on the z axis is a perfectly match layer (PML). The periodic boundary condition is to repeat the simulation along the walls of the structure (x and y axes) as shown in **Figure 4**. Meanwhile, the PML boundary condition can be interpreted as a wall that absorbs reflection and transmittance values.

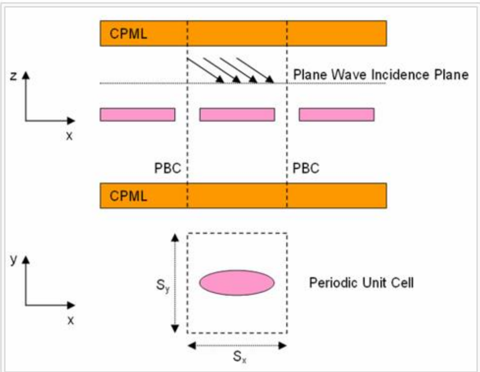

Fig. 4 Mechanism of periodic boundary condition [9]

As shown in **Figure 5**, the experimental procedure is started with simulation. The simulation is carried out by building a simulation model for silicon photovoltaics, which starts by creating a simulation room, filling in the geometry size and providing boundary conditions, then adding a sun for the source, creating a sample structure, adding sample material, and adding reflection and transmittance monitor. After that, the development of the simulation model was carried out by adding a new structure for anti–reflective coating with variations in the thickness of the structure.

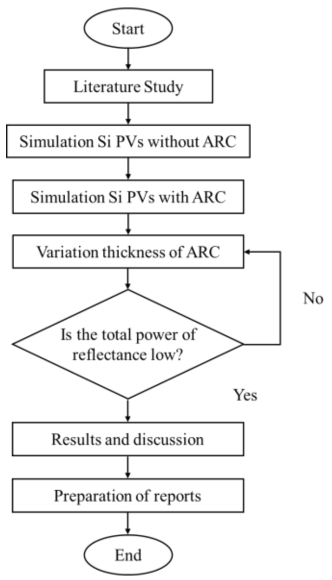

Fig. 5 Research flow chart

The research variable in this paper consists of independent variables, dependent variables, and fixed variables. The independent variable is a variable that is made independent and varies, such as the type of anti–reflective coating and variations in the thickness of the anti–reflective coating from 50 nm to 300 nm with 50 nm intervals. The dependent variable is the variable that changed because of the independent variables, such as the reflectance and transmittance values of sunlight. The fixed variable is a variable that is not influenced by other variables, namely the thickness of the silicon PVs.

5 Novelty of this work

In this work, we leverage the use of nanopyramid SiO_2 anti-reflective coating previously employed in reference [5] and [6] and study their optical characteristics based on simulated transmission, reflection, scattering and absorption. Using these chatacteristics, we optimized the geometrical factor of the nanopyramid which is thickness and aspect ratio. Then, we tried to understand their limiting performance under simulated 1 sun illumination and silicon flat slab representing the actual experimental condition for silicon photovoltaics test. Parameter test and setup from this simulation are guding principle and should benefit researchers working on fabrication of nanopyramid SiO_2 anti-reflective coating for photovoltaic applications.

6 Results and Discussion

The monitor test is carried out to find out how much sunlight is reflected. In this study, the total energy of incoming sunlight at a wavelength of 351 nm to 800 nm is 57.6 mW/cm^2.

Figure 6 shows that the total value of reflected sunlight power from silicon PVs without using an anti–reflective coating is 24.7 mW/cm^2, which is calculated using equation (1), or about 42.9%.

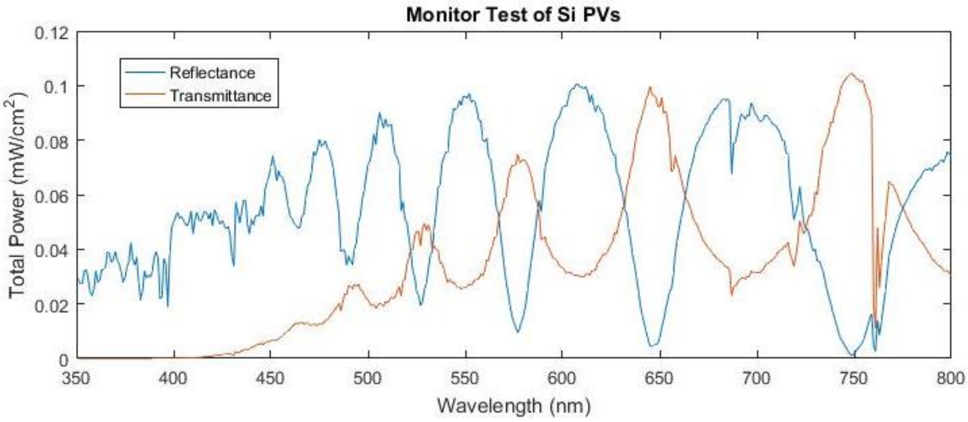

Fig. 6 Monitor test of silicon PVs

To find out if the anti-reflective used has decreased the reflection value of sunlight, it is necessary to add the reflection power value of Si PVs in the graph without using anti–reflective coating and make it as a baseline. In addition, the total R value of Si PVs that have used anti–reflective coatings in the form of Si_3N_4 and SiO_2 needs to be compared with Si PVs that use Si material as anti–reflective coating.

For flat geometry structure, the Si_3N_4 and SiO_2 material can decrease the spectrum of Si PVs as shown in **Figure 7**.

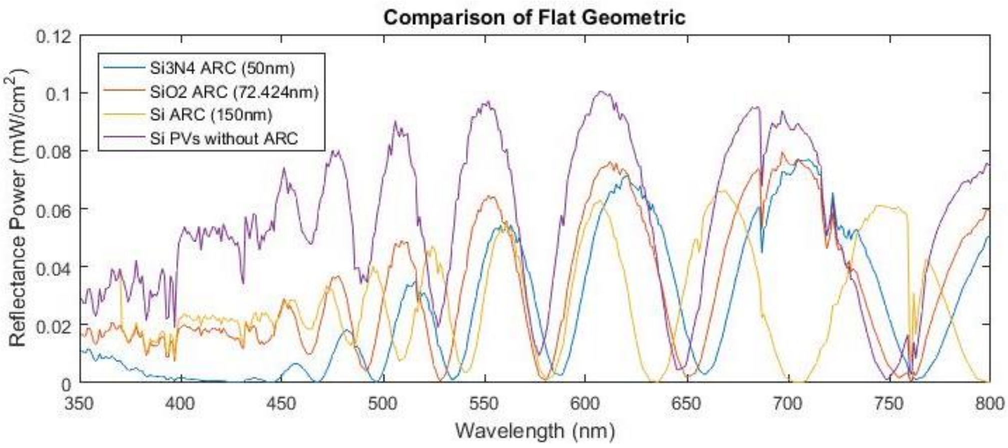

Fig. 7 Comparison of flat geometric at optimum thickness

Table 3. Percentage comparison of flat anti-reflective coating.

ARC Material	Thickness (nm)						
	50	72.424	100	150	200	250	300
Si_3N_4	20.1%	20.9%	31.8%	33.2%	30.3 %	28.5 %	30.5 %
SiO_2	32.0%	25.7%	25.8%	35.8%	36.4 %	33.6 %	32.7 %
Si	44.0%	44.8%	42.8%	21.7%	42.5 %	41.5 %	42.4 %

The flat geometry structure has decreased the value of sunlight. However, in this study, the desired structure is a nano pyramid with a low price. Thus, it is necessary to re–simulate it using a nano pyramid geometry structure.

For the nano pyramid geometry structure, the reduction of the value of sunlight reflection by using Si_3N_4 and SiO_2 materials has succeeded in reducing the spectrum of Si PVs as shown in **Figure 8**.

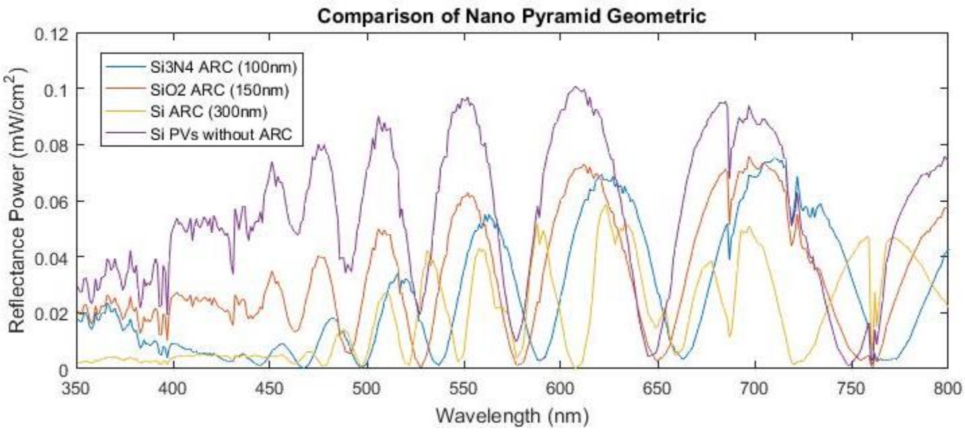

Fig. 8 Comparison of nano pyramid geometric at optimum thickness

These results are in accordance with the concept of nano pyramid anti–reflective coating where the incoming photons will enter slowly so that it is better and more stable. However, the total reflection power of the nano pyramid is still slightly larger than the flat ones. This is because the sunlight that enters directly touches the gap between the nano pyramids. The power of reflected sunlight is already under silicon PVs without anti–reflective coating. Thus, it can be interpreted that Si_3N_4 and SiO_2 can be used as anti-reflective coatings for Si PVs with nano pyramid geometry.

Table 4. Percentage comparison of nano-pyramid anti-reflective coating.

ARC Material	Thickness (nm)						
	50	72.424	100	150	200	250	300
Si_3N_4	37.0%	24.9%	20.6%	21.6%	26.0	27.0	27.4

ARC Material	Thickness (nm)						
	50	72.424	100	150	200	250	300
					%	%	%
SiO_2	40.5%	35.4%	30.6%	26.0%	27.4 %	30.4 %	32.4 %
Si	40.6%	39.3%	37.5%	30.8%	22.8 %	18.0 %	15.1 %

Table 4 shows that the anti–reflective coating with Si_3N_4 and SiO_2 materials has a total reflectance value that is quite close to Si material. Thus, the optimization of the nano pyramid geometry structure has been successful. However, the only anti–reflective coating that will be used is SiO_2. This is because the fabrication process for Si_3N_4 is too complicated and requires an expensive cost. Whereas, if using SiO_2, the fabrication process will be easier because it is used in the form of sol–gel (easy to form into a pyramid) and the cost is relatively cheap. Therefore, it is necessary to re–optimize the pyramid nanostructure using SiO_2 to get even lower reflectance.

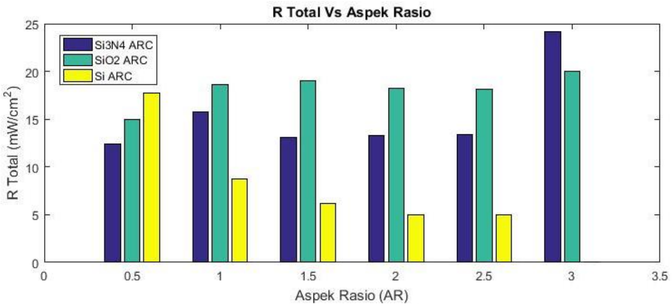

Fig. 9 R total versus aspect ratio graph

In this aspect ratio comparison, when the material is in the form of Si_3N_4 or SiO_2, if it is used as an anti-reflective coating, the total reflectance value is still greater than Si (**Figure 9**). This is because Si has a high refractive index value, which is around 3.4 to 4, which indicates that Si has a high light absorption ability, so that sunlight will be reflected more slowly. In contrast to Si_3N_4 and SiO_2, which have refractive index values of around 2 and 1.4, which indicates that Si_3N_4 and SiO_2 have a low ability to absorb sunlight. In addition, in the aspect ratio 3 (thickness at 900 nm), only certain material is calculated because silicon has a high refractive index so that a Brewster angle can occur where reflected light that is not polarized can turn to be polarized.

The nano pyramid anti-reflective coating needs to be optimized by changing the thickness of the nano pyramid to 95 nm with a base size of 83.79 nm x 83.79 nm.

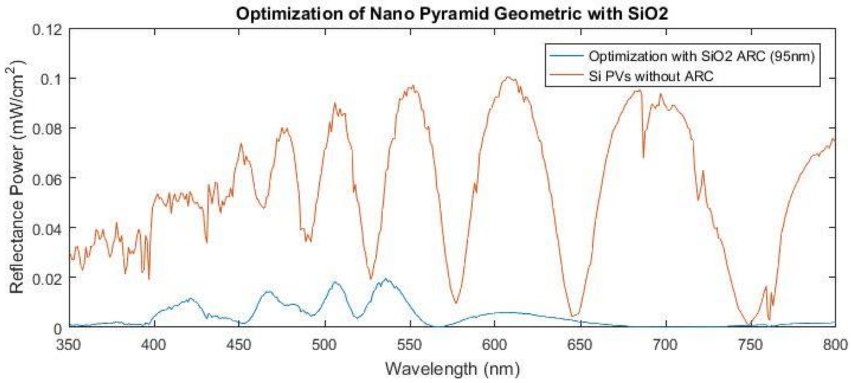

Fig. 10 Optimization of nano pyramid anti–reflective coating witn SiO_2

The optimization carried out on the pyramidal nanostructure with SiO_2 material has been successful. As shown in **Figure 10**, where the value of the reflected sunlight power is very good and has a total reflection power value of 1.94 mW/cm^2 or has a total reflectance of 3.38%. This a total reflectance value is smaller than total reflectance of Si ARC at a thickness of 600 nm, which is 8.6%. In addition, based on equation (2), the sunlight absorbed by Si PVs is quite large, which is around 29.22%, although the transmitted sunlight is still quite large, which is around 67.4%, it is reasonable because we only used a very thin Si wafer in our simulation.

The optimum condition described in here is achieved through (1) material selection based on index matching condition, (2) base size of the nano pyramid, and (3) thickness of the nano pyramid (represented as aspect ratio). While the use of SiO_2 materials as anti-reflective coating might not as great as in Si_3N_4 or Si in term of low reflectance, the SiO_2 can be fabricated by replica moulding which is low cost and opens a very rich playground for light management through geometrical modification of anti-reflective coatings. Consideration for the geometrical factors are not very stright forward and can not be analytically described. This is the reason of why numerical simulation as shown in this work is veyr important. The performance of sub-micron size anti-reflective coating are not quite intuitive compared to traditional ray optics. Therefore, the optimum condition should be thourghly assessed using simulation (as shown here) before fabrication started. The condition is sensitive to how the light intensity and angle take place on the actual photovoltaics. At 1 sun standard illumination and 0 deg angle, the optimum condition for SiO_2 anti-reflective coating is having a base size of 83.79 nm x 83.79 nm and 0.5 aspect ratio.

7 Conclusion

FDTD simulation suggests that Si_3N_4 and SiO_2 are anti–reflective coating materials feasible to reduce the value of reflected sunlight because they have index mis-matching values that are close to ideal. The design of the anti–reflective coating has been successful using the nano pyramid geometry applied on thin-film Si photovoltaics. We discuss the effect of geometrical thickness, aspect-ratio, and material selectivity for designing nano-pyramid anti-reflective coating. The total power reflectance value of sunlight after optimizing the SiO_2 nano pyramid anti–reflective coating is 1.95 mW/cm^2 or about 3.38% at a thickness of 95 nm. This is very significant improvement compared to 25 % reflectance losses in flat silicon slab without anti-reflective coating.

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References

[1] G. S. Vicente, A. Morales, and M. T. Gutirrez, "Preparation and Characterization of Sol-gel TiO_2 Antireflective Coatings for Silicon," *Elsevier Ltd*, pp. 133–137, 2001.

[2] C. A. Gueymard, D. Myers, and K. Emery, "Proposed Reference Irradiance Spectra for Solar Energy Systems Testing," *Elsevier Ltd*, vol. 73, no. 6, pp. 443–467, 2002.

[3] S. Duttagupta, F. Ma, B. Hoex, T. Mueller, and A. G. Aberle, "Optimised Antireflection Coatings using Silicon Nitride on Textured Silicon Surfaces based on Measurements and Multidimensional Modelling," *Elsevier Ltd*, vol. 15, pp. 78–83, 2012.

[4] Y. F. Makableh, H. Alzubi, and G. Tashtoush, "Design and Optimization of the Antireflective Coating Properties of Silicon Solar Cells by Using Response Surface Methodology," *MDPI*, vol. 11, no. 721, pp. 1–13, 2021.

[5] H. Cao, Y. Bai, and L. Qiao, "Antireflection Effect of SiO_2 Thin Film on the Pyramidal Textured Surface of Monocrystalline Silicon," *Elsevier Ltd*, 2015.

[6] N. R. Thangavel *et al.*, "Disorderes Polymer Antireflective Coating for Improved Perovskite Photovoltaics," *ACS Publ.*, vol. 7, pp. 1971–1977, 2020.

[7] H. R. Philipp, "Optical Properties of Silicon Nitride," *IOP Publ. Ltd*, vol. 120, no. 2, pp. 295–300, 1973.

[8] W. Zhang, J. Tu, W. Long, W. Lai, Y. Sheng, and T. Guo, "Preparation of SiO2 Anti-reflective Coatings by Sol-gel Method," *Elsevier Ltd*, vol. 130, pp. 72–76, 2017.

[9] "A Review of Maxwell's Equations & Computational Elegtromagnetics (CEM)," *Basic Principles of The Finite Difference Time Domain Method*, 2018. http://www.emagtech.com/wiki/index.php/Basic_Principles_of_The_Finite_Difference_Time_Domain_Method#Time_Domain_Simulation_of_Periodic_Structures (accessed Feb. 20, 2022).