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# Simulation of the Optical Properties for Silicon Nano-pillar Array Using Finite Difference Time Domain Method

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**Abstract.** We use two-dimensional FDTD (Finite difference time domain) method to simulate light transmitting in Si nano-pillar arrays and get some results. The Si nano-pillar array, with diameters, heights, intervals respectively 50-80nm, less than 480nm, 26-44nm, is used as the testifying structure. The reflectivities of both experiment and simulation match well either for bulk silicon or for structure silicon even though small deviations are caused by the uneven size of the pillar's diameters, heights, and intervals. What's more, we find reflectivity (*ref*) increases along with diameter's (*d*) increasing for a single pillar with diameters of 20-100nm under a constant light of 600nm, and reaches 10.48% at *d*=100nm. And with a constant *d* equal to 20nm, an infinite aspect ratio (*r*) and a light 600nm, *ref* is decreasing when the intervals (*i*) of pillars are increasing. Finally, under the condition of different *i*, the relations between *ref* and *r* are investigated. The undulation of these curves shows that the reflective waves play an important role in sub-wave length optics. Analysis also reveals that there exists a best *i* for achieving the lowest *ref*, too large or too small *i* will cause high *ref*, even if *r* is great; moreover, the lager *i* is, the higher pillar is needed to achieve the lowest *ref*.

## Introduction

In recent years, the investigations of nano-structures, such as nano wires, tubes and pillars, are very hot. One of these studies is the fabrication of nano-pillar arrays on Si and its great potential application in solar cell [1,2]. For the optical properties of nano-pillar array, even though there are experiments and papers to testify and explain its light trapping effects [3,4], the fundamental principles are still remained to be fully and urgently understood. FDTD method is introduced to calculate the reflectivity of nano silicon pillars in this paper, which is a well-known and powerful electromagnetic simulation method used to calculate and optimize the performance of nano-structures in solar cells [3].

## Model

As shown in Fig. 1, it is the model of the FDTD calculation: area A absorbing boundary condition UPML (uniaxial medium perfectly matched layer), area B silicon nano-pillar array, line D the surface separating total field and scattering field, line F incident light source. One side of the square cell of FDTD is 2nm which ensures the accuracy of simulation. Light source is a spacial Gauss TE wave:

$$H_z = \exp\left(-\left(\frac{x - x_0}{\omega}\right)^2\right) * \sin\left(2\pi ft + \phi\right) \tag{1}$$

$\omega$ is the width of the Gauss wave and $f$ is frequency. Waves propagate from F and interact with B through enough time to achieve stability, and then reflective waves $E_r$ are separated from total field at D and recorded by several cells above D.

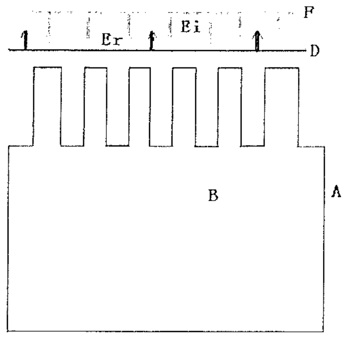


Fig 1. sketch map of simulation model

## Results

The Si nano-pillar array as shown in Fig. 2, whose diameters, heights, intervals are respectively 50-80nm, less than 480nm, 26-44nm, is used as the testifying structure. Experimental reflectivities [1] is the line of data 3 shown in Fig. 2; and reflectivities of our simulation based on above pillar array is the line of data 4 shown in Fig. 3 with incident wavelength from 400nm to 1600nm. There are 2~3% deviations between experiment and simulation results for 400-1200nm incident light, which can be explained by the uneven size of the pillar's diameters, heights, and intervals. We also calculate the reflectivities of bulk Si shown in Fig. 3, data 1 and data 2, and find that the results match very well between experiment and calculation

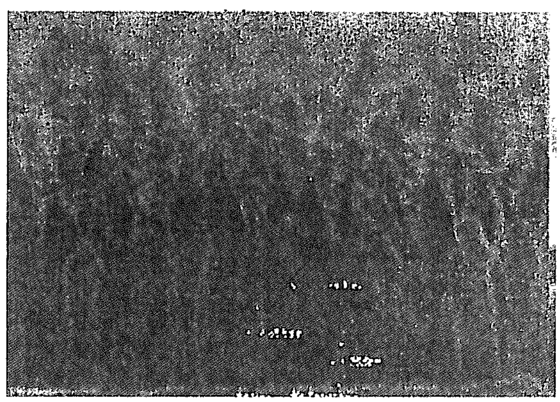

*Fig 2. (quoted from[1]) Si nanopillar arrays with diameters 50-80nm, height <=480nm, intervals 26-44nm*

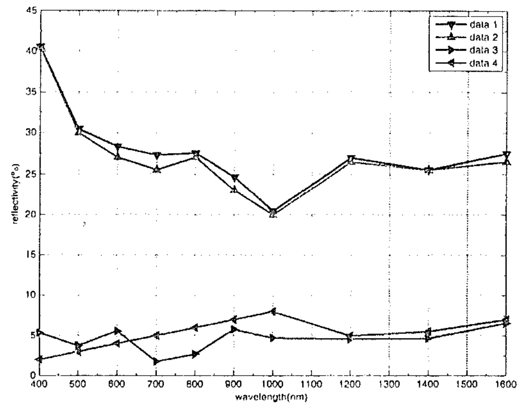


*Fig 3. reflectivities of different wavelengths λ(nm) data1,3 are simulated reflectivities and data2,4 are experimental reflectivities; data1,2 are reflectivities of bulk Si and data3,4 are reflectivities of Si nano-pillar array*

The reflective performance of pillar array under constant incident light is decided by the pillar's parameters: diameter *(d)*, aspect ratio(*r* ) and intervals *(i)*.

In Fig. 4, the reflectivity(*ref*) increases along with *d* 's increasing for a single pillar with diameters from 20nm to 100nm under a constant incident light of 600nm, and reaches 10.48% at *d*=100nm.

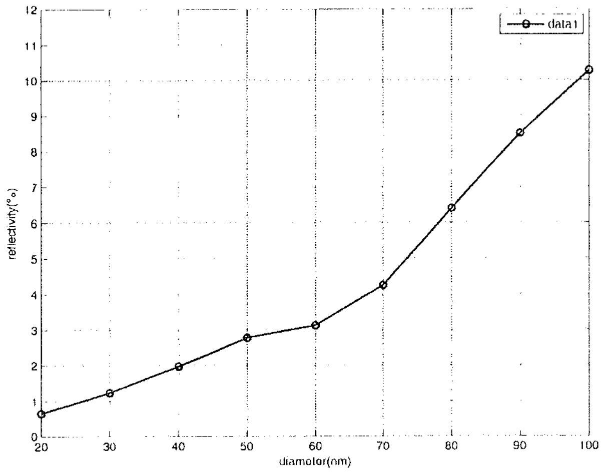


*Fig 4. reflectivities of a single Si nano-pillar with different diameters(nm)*

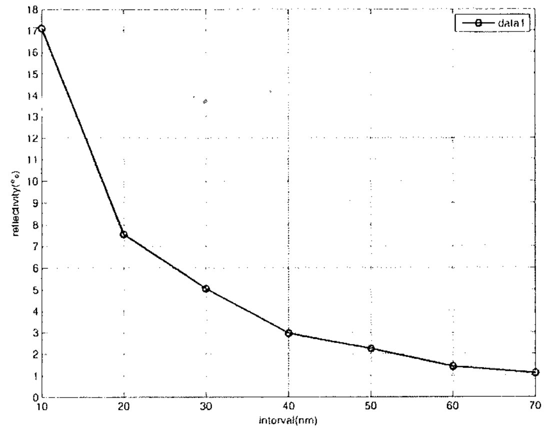


*Fig 5. reflectivities of Si nano-array with different intervals(nm), while diameter of nano-pillar is constant 20nm*

In Fig. 5, with a constant *d* equal to 20nm, an infinite *r* (which means that there are no effect of reflective waves from bottom) and a light 600nm, *ref* is decreasing with *i*'s increasing, which can be explained by the fact that the smaller *i* will cause more scattering light to be reflected by side pillars.

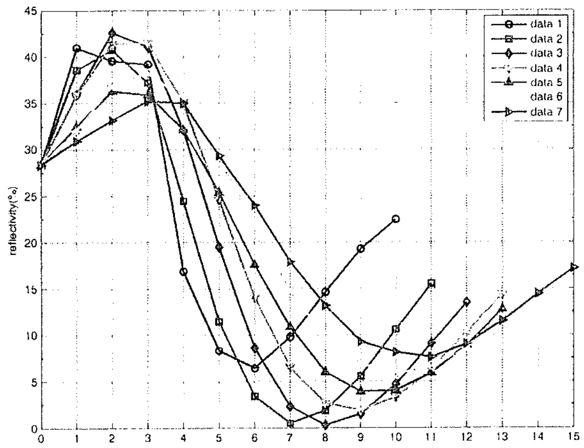


*Fig 6. reflectivities v.s different aspect ratios of Si nano-pillar with different intervals; intervals of data1,2,3,4,5,6,7 are respectively 10,20, 30,40,50,60,70nm; diameter is constant 20nm*

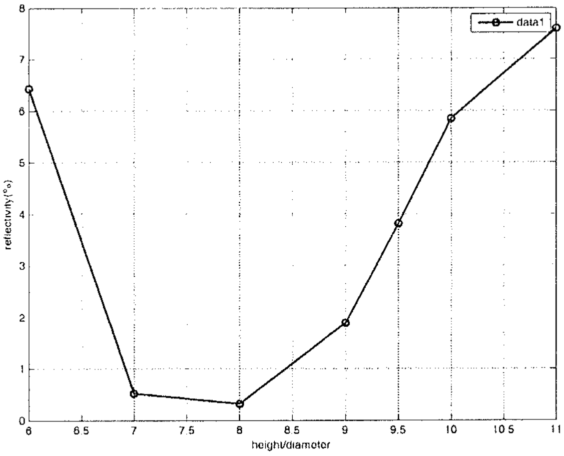


*Fig 7. lowest reflectivities v.s aspect ratioes where they appear; a,b,c,d,e,f,g respectively indicates different intervals 10,20,30,40,50,60,70nm of nano-pillar*

Fig. 6, shows the relations between *ref* and *r*, at the conditions of incident light 600nm, *d* 20nm, and different *i*. The trending of these curves firstly increases, then falls and finally increases again. It shows that *ref* does not always reduce with the increasing of pillar height as normal thought, otherwise increases when pillar height is above some value.

Fig. 7 shows the relation between the lowest *ref* and the corresponding *r* at different *i* selected from Fig. 6. It reveals that there exists a best *i* for achieving the lowest *ref*, too large or too small *i* will cause high *ref*, even if *r* is great; moreover, the lager *i* is, the higher pillar is needed to achieve the lowest *ref*.

**Summary**

From Fig. 3 we can see that FDTD is a reliable method in such a nano-scale simulation; however, if we want to get more precise results, more details of the pillar's shape should be considered.

Fig. 4 shows that the shorter $d$ is, the less reflectivity is, which accords with Rayleigh scattering law $ref \propto \frac{1}{\lambda^4}$. Not considering the bottom reflective wave, we prove that too small $i$ will cause more wave reflected by the side pillar, which is easy to be understood by the fact that infinitesimal $i$ will lead to solid Si.

For a certain $d$ and $i$, reflection are not always reducing along with increasing of $r$, which is revealed in Fig. 6. This phenomenon indicates that reflective wave combine with incident wave can reduce the total field intensity for the phase difference. However, the reflective waves come from both bottom and sides of pillar so that the total field intensity is effected not only by $r$ but also by $i$ and $d$, which can be supported by the fact in Fig. 7 that certain $d$ and different $i$ require different $r$ to achieve the lowest *ref*. The accurate theory of this phenomenon requires careful study of near field optics which is not contained in this paper.

Finally, the fact in Fig. 7 that the lager $i$ is, the higher pillar is needed to achieve the lowest *ref*, can attribute to that smaller $i$ will cause more reflections between the pillars than larger $i$ do for a certain $r$.

**References**

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