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*Research Paper*

# Polarization and incident angle insensitive germanium nano-pyramid array for perfect absorption in visible regime

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**Abstract:** An extraordinary light harvesting property of a periodic nano-pyramid array is reported. It is found that the nano-pyramid array can absorb light efficiently with an average absorptivity of 0.998 over the whole visible waveband. The ultra-high absorption is independent of the incoming light on polarization state and insensitive within a broad angle range. We attribute the efficient light harvesting property of the nano-pyramid array to Fabry-Perot resonance physically. This perfect absorber has advantages of easy fabrication, cost effective, and stable energy harvesting.

**Keywords:** nano-pyramid array; broadband; visible regime; absorption.

## 1. Introduction:

Solar energy is regarded as one of the most plenty harvested sources of renewable energy. Much effort has been made for the purpose of developing highly efficient photovoltaic devices. Many attentions have been paid to develop various structures such as nanowire, [1-4] nanopillar, [5-7] nanocone, [8-10] nanohole [11-14], and nanodisc [15-18] arrays. These structures have displayed unique optical and electric characteristics for the purpose of energy harvesting. Advantage of the silicon-based photovoltaic cells with short collection length for excited carriers, results in significant improvement in carrier collection efficiency. The two-dimensional periodic metamaterials-based structures designed with bulk materials of silicon and gold greatly improve optical absorptivity due to the synthesis effects of the slow light mode, localized surface plasmon resonant (LSPR) effect, and antireflection coating [7, 19, 20,21].

However, germanium and silicon belong to indirect-gap materials. Germanium has lower band gap, resulting to photons with lower energy can excite electrons from valence band to conduction band. It means the germanium material-based structures can increase optical absorptivity in broader band than silicon material. Meanwhile, with the same energy photons excitation, more heat can be produced [3, 11], and higher temperature and photoelectric conversion efficiency are obtained in germanium structures accordingly in comparison to the other materials. On the other hand, the two-dimensional (2D) periodic metamaterials-based structures are too difficult to be fabricated in industry due to the complicated nanostructures as well as material issues. The ideal fabrication technology of the photovoltaic devices should be extraordinarily absorbing light in a broad-band, incident angle-insensitive, polarization-independent, and easy production. In order to increase optical absorptivity, a nano-pyramid array is proposed here as a promising candidate for a dominant position of light scattering effort. The nano-pyramid can prolong the path of light and efficiently inhibit the reflection and transmission. And thus extraordinary optical absorption is obtained due to Fabry-Perot resonance. In this paper, we numerically analyze the influences of substrate thickness, pyramid height, and filling ratio on the optical absorption of the periodic nano-pyramid arrays. Though we focus on germanium nano-pyramid arrays only in this paper, results obtained here are also applicable and maybe interesting to other photovoltaic devices designed on the basis of the nano-pyramids array.

In nanofabrication point of view, the previously reported 18 pairs Si/Au thin films alternatively layered metamaterials [7-10, 20] with film thickness of tens nanometers is too difficult and complicated to be fabricated for mass production. In contrast, our presented structure with pure Ge film coating in total thickness of 1 μm which can be easily prepared by normal thin film coating technique such as vacuum evaporation [22]. Then the pyramid array with 0.5 μm height can be directly fabricated using focused ion beam technology. Therefore, the proposed nano-pyramid array here is capable of being fabricated using thin film coating combining with focused ion beam direct milling (FIBM) or e-beam direct lithography technique. For the prototype fabrication, FIBM is strongly recommended due to the advantages of one-step milling, less accumulated error, and no material selectivity. The cone angle can be shaped and controlled by means of tuning process parameters such as beam current and dwell time. Thus our nano-pyramid array has advantages of easy fabrication, cost effective, and functioning stable energy harvesting.

## 2. Design of nano-pyramid array

Figure 1 shows the schematic diagram of the periodic nano-pyramid structure we proposed. The direction of the incident solar radiation is determined by the angles of $\theta$ and $\varphi$. Parameters of the structure are the period *a* of the square lattice, substrate thickness *l*, pyramid bottom length *d*, and pyramid length *h*. For the nano-pyramid structures, we need to take into account the wave effects by solving Maxwell's equations for the full wave vector. A finite-difference and time domain (FDTD) algorithm has been proven to be effective for numerically calculating such periodic structures. In our analyses, we use a fine grid (10 nm×10 nm×10 nm), which is less than 1/40 of the shortest wavelength in the whole computation domain, in order to ensure convergence of the calculation process. By energy balance, the absorptivity of the pyramid structure is given by $A(\lambda)=1-R(\lambda)-T(\lambda)$, where $\lambda$ is the wavelength of the incident wave, and *R*, *T* and *A* are the frequency dependent reflectance, transmittance, and absorptivity of the pyramid structure respectively. The wavelength is ranging from 400 nm to 700 nm, where most of the above-band-gap photons concentrate in the germanium-based substrate material.

**Figure 1** (a) Schematic diagram of the nano-pyramid array absorber; θ, φ is the angle between incident light and x-/y-axis respectively; (b) Cross-sectional view of a single nano-pyramid

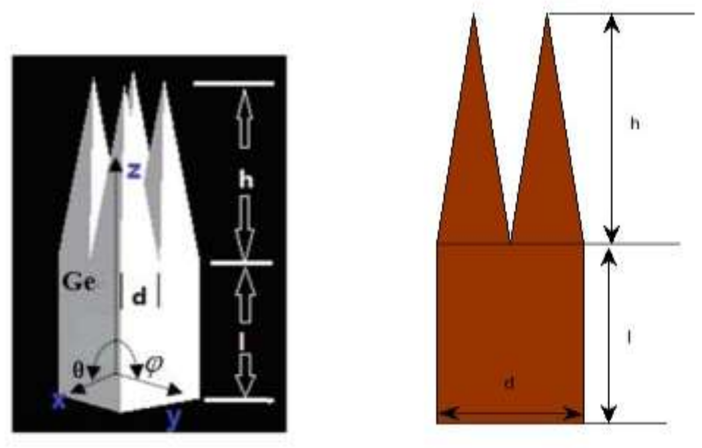


Figure 2 (a) shows the optical absorption of an array of germanium nano-pyramids. The incident wave is normal to x-y plane with the electric field polarized along the z-axis. The substrate thickness, bottom length, and filling factor are fixed to be 0.7 μm, 0.2 μm, and 1, respectively. And the optimized height varies in our calculation. For simple explanation, every pyramid is rooted on the substrate with length of 0.2 μm. As can be seen from the figure, the perfect optical absorptivity is obtained in the visible regime. And the absorptivity is superior to those solar energy absorbers reported by the literature before. For the photons with energy just above the band gap, the optical absorption is quite limited for all pyramid heights due to the fact that germanium has an indirect band gap and the optical


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absorption needs phonon assistance. With decreasing of the wavelength, absorption of the nano-pyramids increases and reaches a plateau region when height of the nano-pyramid is higher than 0.6 μm. But the optical absorptivity has a quick drop when the wavelength is larger than 630 nm. The absorptivity in the structures is more efficient in the low-energy regime in comparison to that of the high-energy regime.

## 3. Results and analyses

As large refractive index contrast between Ge and air, the electromagnetic field can be coupled efficiently into the pyramids cavity at Fabry-Perot resonances, resulting in a significant light-trapping ability boost. For the nano-pyramid array here with small filling factor, most of the incident light cannot be coupled into the nano-pyramids, but is absorbed in a single path through the array. In contrast, the nano-pyramid array with large filling factor provides efficient supported modes. Hence the absorption is greatly increased when these modes are well coupled and concentrated in the array. Figure 2 (b) shows the influence of the substrate thickness on absorption of the pyramid designed with height of 0.9 μm, and bottom length of 0.2 μm. As can be seen, optical absorptivity has the same variation tendency when the substrate thickness varies. In the case of high filling factor, the photons with energy above the band gap can be greatly absorbed by means of Fabry-Perot resonances, resulting from prolonging path of the incident light.

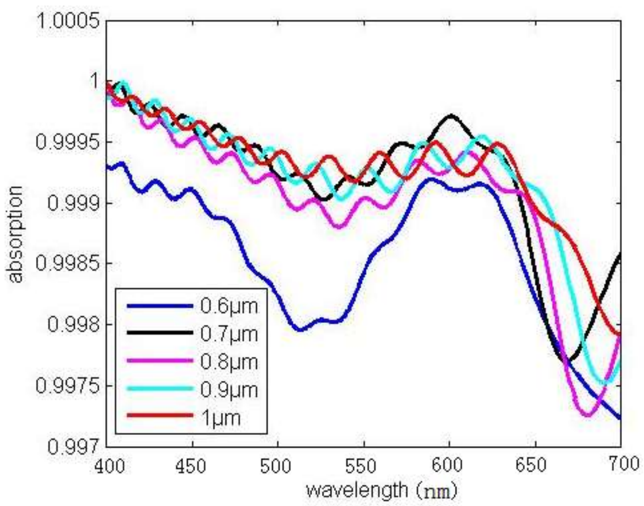
Figure 2 (c) shows the influence of the filling factor on absorption of the pyramid designed with height of 0.9 μm and the thickness of 0.7 μm. However, as can be seen, with increasing of the filling factor, the optical absorptivity increases as well. Large filling ratios give rise to high absorption in the whole visible regime. Moreover, in the long-wavelength regime, nano-pyramid array with small filling ratios absorb the same light energy. To evaluate the overall absorption performance of the nano-pyramid array, we calculated the ultimate efficiency $\eta$, which is defined as the efficiency of a pyramid as the temperature approaches 0 and each photon with energy greater than that of the band gap produces one electron hole pair [23]

$$\eta = \frac{\int_0^{\lambda_g} I(\lambda) A(\lambda) \frac{\lambda}{\lambda_g} d\lambda}{\int_0^{\infty} I(\lambda) d\lambda} \tag{1}$$

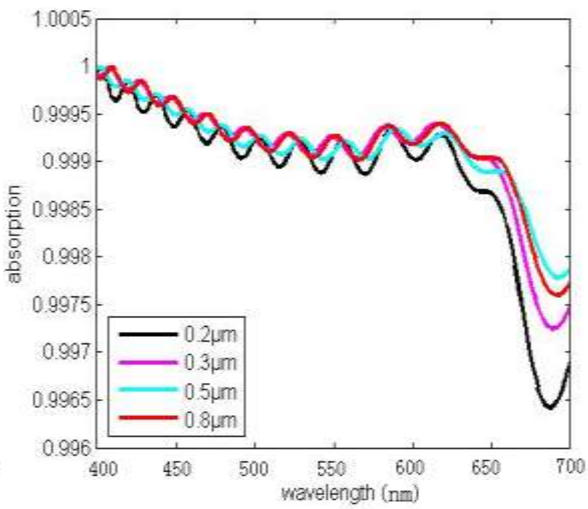
where $I$ is the solar intensity per wavelength interval, $A$ is the absorptivity, $\lambda$ is the wavelength, and $\lambda_g$ is the wavelength corresponding to the band gap. For the solar intensity, we use the testing standard of Air Mass 1.5 as basis of our spectrum.[24] Equation (1) shows that for a given absorption and solar radiation spectrum, $\lambda/\lambda_g$ can be regarded as a weighting factor for integration. As the wavelength decreases from the band gap, the contribution of the absorbed solar energy to the ultimate efficiency decreases because the excess energy of photons above the band gap is wasted and converted into heat.[3,11] Furthermore, the long wavelength absorption in the nano-pyramid structures can be improved by means of employing light trapping so as to increase the optical path.

Moreover, current practical optical absorption structures tend to exhibit a strong angle-dependent optical response and the corresponding solar cells require bulky solar tracking systems to trace the position variation of sun at different periods of time in order to maximize their daily energy output. Figures 2 (d) and (e) show the absorptive spectrum at various incident angles for TE and TM wave respectively. As can be seen, the absorptivity keeps nearly unchanged in the visible regime when incident angle changes from 30° to 90°. The most important issue is that the absorptivity can still keep a high level: >0.7 in a broad angle range, *i.e.*, influence of the absorptivity is insensitive on incident angle in the broad visible regime. Figure 2 (f) displays the absorptivity of the nano-pyramid absorber under different polarization states of the incident light with wavelength fixed to be 700 nm. We adopted the framework of leaky-mode resonances (LMRs) that was originally developed for micrometer-scale resonators to explain the mechanism. [3] As small size of the nano-pyramid, the resonant modes in the nano-pyramids array become leaky and interact more effectively than the outside world, and thus carrying out a valuable antenna effects. The nature of the antenna effects in nano-pyramids naturally provides for a desirable weak angle-dependence and polarization-independence of the optical response. To our knowledge, this is the unique features of our presented nano-pyramid array at present.

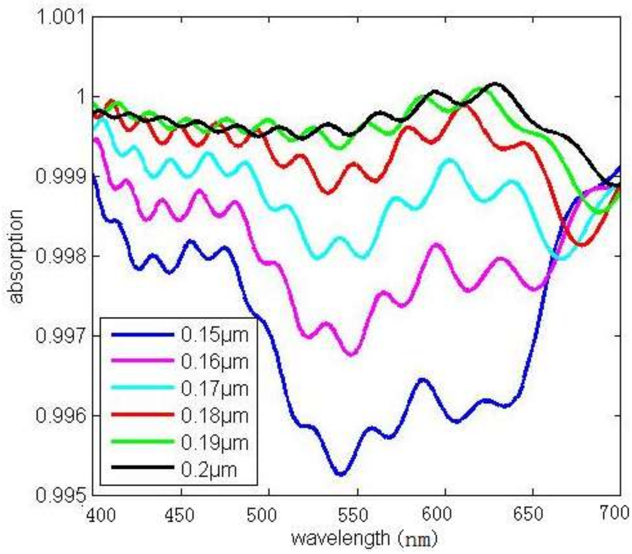
**Figure 2** (a) different heights *h* and fixed parameters of *l*=0.7 μm, *d*=0.2 μm; (b) different thicknesses *l* when *h*=0.9 μm, *d*=0.2 μm; (c) different bottom lengths *d* when *h*=0.9 μm, *l*=0.7 μm; (d) different incident angles of 30°, 45°, 60° and 90° for TE wave; (e) different incident angles of 30°, 45°, 60° and 90° for TM wave; (f) different polarization state for λ=700 nm under illumination at the normal incident angle.



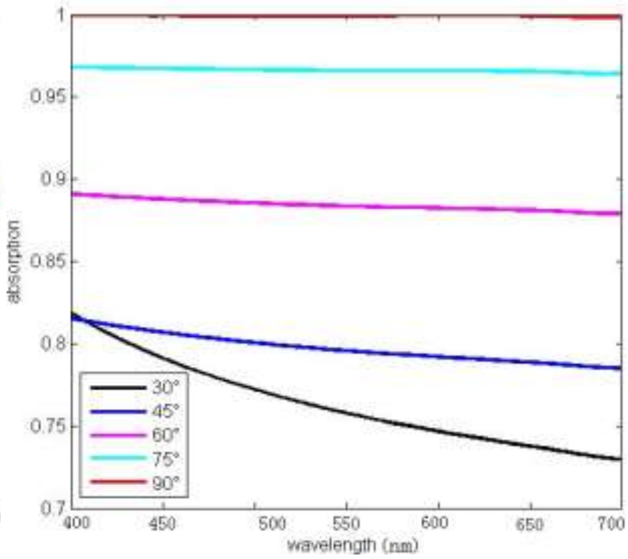

(a)



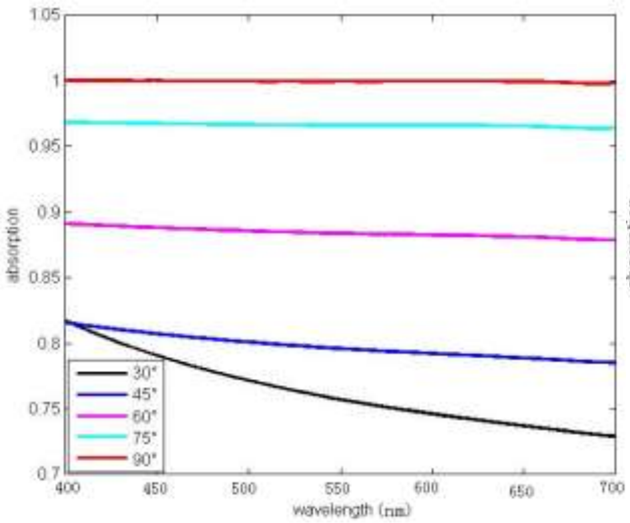

(b)



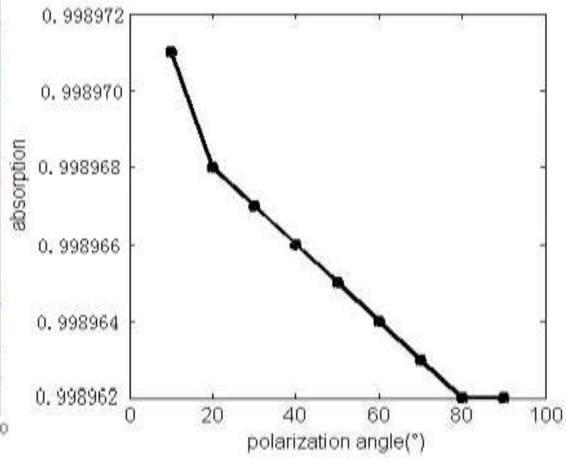

(c)




(d)



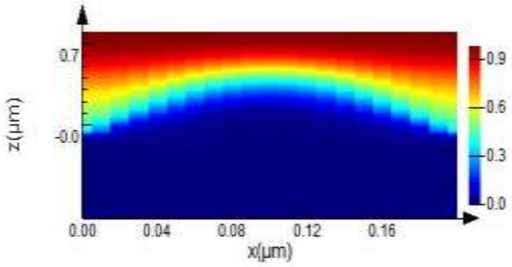

(e)



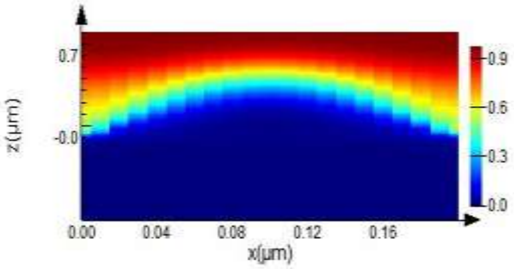

(f)

To further understand the physical mechanism of the ultra-broad waveband of the nanopyramid array, the electric field distribution for different incident wavelengths is investigated, as shown in Fig. 3. In our case, light is mainly absorbed on the top or edge of the nanopyramids. A nano-pyramid can actually absorb not only the portion of an incident wave directly but also the surrounding wave. It is well-known that a small single particle can have larger absorption cross section than its geometrical cross section. [4] What we mentioned in above paragraphs is confirmed this point in Fig. 3. The photons with energy above the band gap are extraordinary absorbed at Fabry-Perot resonances on the top or edge of the nanopyramids. With high filling factor, most of the incident light cannot be absorbed in the substrate, but is coupled into the nano-pyramids.

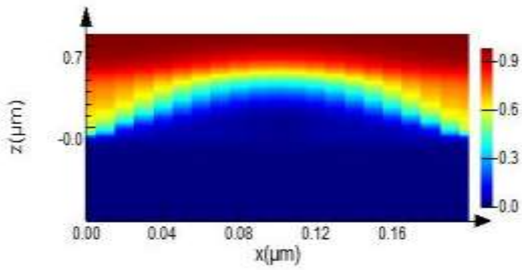
**Figure 3** Electric field distribution at y=0 plane for different wavelengths. (a) λ=400 nm; (b) λ=500 nm$\lambda = 450$nm; (c) λ=600 nm; and $\lambda = 506$nm(d) λ=700 nm.




(a)




(b)

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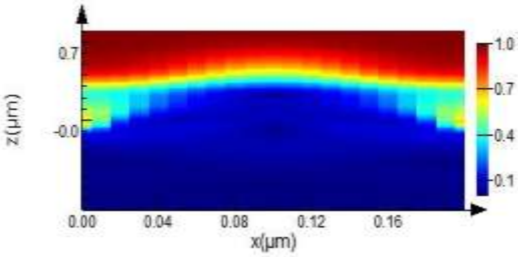


(d)

## 4. Conclusions

In conclusion, we have proposed a nano-pyramid array which is capable of achieving an average absorptivity of 0.998 in the whole visible waveband. The absorber is shown to be insensitive to the light polarization state, and able to retain very high absorptivity in a broad incident angle range. We analyzed the phenomena in physical mechanism point of view by means of regarding germanium as a bulk material according to the corresponding band gap theory. The high absorptivity of the nano-pyramid array was investigated with the efforts of the Fabry-Perot resonances. With the vast demand of the sustainable and green energy nowadays, it is reasonable to believe that the proposed absorber will find its potential applications in those light harvesting related areas.

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