Enhanced absorption and EQE of Si MSM photodiodes with integrated periodic arrays of holes

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Abstract. In order to enhance the absorption of thin Si film, cylindrical-shaped holes arranged in square and hexagonal lattices with different designs of hole diameter, depth and period are integrated in the surface of Si films with a thickness of 1.5 μm and 2.5 μm on either bulk Si or SOI substrate. At the wavelengths between 800 ~ 950 nm, light bending and absorption enhancement of Si film with integrated hole array is analyzed by FDTD simulation. Hole array with a period similar to the wavelength and a diameter/period ratio around 0.7 enables a higher absorption of Si film. Si film with cylindrical-shaped holes in hexagonal lattice with a Si thickness of 1.5 μm and a hole depth of 250 nm provides an absorption of 43.16 % at 850 nm wavelength on a SiO₂ substrate. Nanostructured Si MSM photodiodes are fabricated by integrating periodic arrays of holes in 1.5 μm thin absorption regions between metal fingers. The EQE is enhanced to 61 % at 850 nm, while the photodiodes without holes show only 23 %.

1. Introduction
CMOS-process-compatible silicon (Si) photodiodes could lead to a cheaper and better integrated fibre-optic communication system [1]. However, Si photodiodes are currently used predominantly in the visible wavelength regime. At near-infrared (IR) wavelengths such as 840 ~ 860 nm used for short-reach (< 300 m) data communication, traditional Si PIN photodiodes with a weak absorption coefficient of Si can hardly achieve a high external quantum efficiency (EQE, >50%) and a high data rate (20 Gb/s) simultaneously because the former needs a Si thickness of >13 μm and the latter restricts the thickness to < 2.5 μm [3]. One effective approach to enhance the absorption of a thin Si film is to integrate micro- and nanostructures in the Si film with the purpose of tailoring its optical properties and trapping the photons [3]. Such schemes include the formation of nanowires [4], nanodomes [5], nanodiscs [6], nanopencils [7], and so on. In recent studies, an all-Si PIN photodiode fabricated on a silicon-on-insulator (SOI) wafer with periodic funnel-shaped holes is presented for efficient light trapping, resulting in an enhanced EQE of 52% at 850 nm with a 2-μm-thick i-Si layer and an ultra-fast impulse response (full-width at half-maximum) of 30 ps [8]. It reveals that a beam of vertically incident light is guided laterally and confined in the nanostructured Si film until it gets absorbed [9]. Compared to typical PIN photodiodes, MSM photodiodes with a simple structure of interdigitated metal fingers on Si can provide a high response speed due to its low capacitance which leads to a low RC time. However, Si MSM photodiodes also have a low responsivity at near-IR wavelengths between 800 ~ 950 nm.

In this work, in order to increase the EQE of Si MSM photodiodes while maintaining a high-speed operation, periodic arrays of photon-trapping holes are integrated in thin absorption regions between
metal fingers. Cylindrical-shaped holes arranged in square and hexagonal lattices with different designs of hole diameter, depth and period are designed in the surface of Si films with a thickness of 1.5 μm and 2.5 μm on either bulk Si or SiO\textsubscript{2} substrate. FDTD simulation is used to investigate the absorption of nanostructured Si film at the wavelengths between 800 ~ 950 nm. The absorption of a 1.5 μm thin Si film on a SiO\textsubscript{2} substrate is enhanced to 43.16 % at 850 nm by integrating periodic cylindrical-shaped holes with a depth of 250 nm. The EQE of Si MSM photodiodes is increased to 61 % compared to photodiodes in the absence of photon-trapping hole structures which shows an EQE of 23 %.

2. Design and fabrication

The Si photodiode structure is epitaxially grown on either bulk Si wafer with a thickness of about 500 μm or SOI wafer with a thin device layer over a thick SiO\textsubscript{2} layer. Here, Si films with a thickness (t) of 1.5 μm and 2.5 μm are designed on a bulk Si substrate as shown in Fig. 1(a) and a 3-μm-thick SiO\textsubscript{2} film over a bulk Si substrate as shown in Fig. 1(b). Micro- and nanoscale periodic cylindrical-shaped holes with different designs of hole diameter (d), depth (h) and period (p) are integrated in the surface of Si films. Hole arrays are arranged in square lattice as shown in Fig. 1(c) and hexagonal lattice as shown in Fig. 1(d), respectively. FDTD simulation is used to model the nanostructured Si films with different designs of hole array and substrate, as shown in Fig. 1(e). Light reflection \( R(\lambda) \) from the top surface and transmission \( T(\lambda) \) into the substrate are simulated, and thus the absorption can be calculated by \( A(\lambda) = 1 - R(\lambda) - T(\lambda) \) at the wavelengths between 800 ~ 950 nm. Light propagation and electric field distribution in the Si film with hole array are also analyzed.

Si MSM photodiodes were fabricated on a SOI substrate that has 1.5 μm device layer (p-Si) and 3 μm BOX layer. 100 nm thick interdigitated aluminum (Al) fingers were fabricated on Si by sputtering and lift-off processes. Afterwards, periodic holes with different diameters and periods were patterned and etched by electron beam lithography and reactive ion etching to form 0.25 μm deep cylindrical holes in Si. A device without holes was also fabricated in the same process as a comparison. Five different designs of diameter (d), period (p), and arrangement of holes are shown in Table 1. The width (w) and spacing (s) of Al fingers are also shown in the table. Fig. 1 (e) shows the scanning electron microscopy (SEM) image of a fabricated device with holes with a diameter/period (d/p) of 700/1000 nm.

![Figure 1](image_url)

**Figure 1.** Design of nanostructured Si film and fabricated MSM photodiode with integrated hole array. (a and b) Si film with hole array on a bulk Si wafer (a) and a SOI wafer with a 3-μm-thick SiO\textsubscript{2} film (b), showing cylindrical-shaped holes integrated in the surface of Si film. (c and d) Holes arranged in square lattice (c) and hexagonal lattice (d). (e) FDTD model of the holes integrated Si film on a SOI
substrate illuminated by a vertical incident light. (f) SEM image of a fabricated device with holes with a diameter/period ($d/p$) of $700/1000$ nm.

Table 1. Si MSM photodiodes with different designs of holes and fingers

| d/p (nm) | arrangement | w (nm) | s (nm) |
|---------|-------------|--------|--------|
| 1#      | -           | 150    | 740    |
| 2#      | 700/1000    | square lattice | 150    | 740    |
| 3#      | 630/900     | hexagonal lattice | 130    | 670    |
| 4#      | 700/1000    | hexagonal lattice | 150    | 740    |
| 5#      | 1400/2000   | hexagonal lattice | 300    | 1440   |

3. Results and discussion

3.1. Optimized absorption of Si film with integrated photon-trapping holes

In order to figure out the relationship between optical absorption and photodiode structure with integrated holes, we have done a series of comparative simulation based on FDTD. Fig. 2(a) shows the absorption of a 1.5-μm-thick flat Si film and Si films integrated with hole arrays on bulk Si and SiO$_2$ substrates at the wavelengths between 800 ~ 950 nm. Hole arrays are integrated in the surface of Si films in square and hexagonal lattices with a diameter/period ($d/p$) of $700/1000$ nm and a depth of 250 nm. Fig. 2(a) reveals that the flat Si film has a very low absorption (< 10%) on either bulk Si or SiO$_2$ substrate at 800 ~ 950 nm wavelengths. The absorption of the flat Si film on a SiO$_2$ substrate is a little higher than that of the Si film on a bulk Si substrate due to the back reflection of SiO$_2$ layer. The absorption of Si film is enhanced by integrating periodic holes in the surface. For Si film on a bulk Si substrate, the absorption is improved to 10% ~ 20% at the wavelengths between 800 ~ 950 nm and the absorption of Si films with different hole arrangements has little difference. For Si film on a SiO$_2$ substrate, the absorption is significantly enhanced by integrating hole array. Taking the data communication wavelength of 850 nm for an example, the absorption of the flat Si film with a thickness of 1.5 μm on bulk Si and SiO$_2$ substrates are 3.66% and 6.9%, respectively. Si film with hole array on a bulk Si substrate has an absorption of 11.5%, whereas the absorption of Si film with the same thickness on a SiO$_2$ substrate is enhanced to 35.43% for square hole lattice and 43.16% for hexagonal hole lattice. This represents over 1100% improvement compared to Si film on a bulk Si substrate without integrated nanoholes. Generally, Si film with holes in hexagonal lattice has a higher absorption than its counterpart with holes in square lattice due to a higher porosity and lower surface reflection with the same diameter and period of holes. At the wavelengths between 800 ~ 950 nm, Si film with hole array in hexagonal lattice provides a high absorption of 30.45% ~ 47.53%.

Figure 2. Absorption of 1.5-μm-thick holes integrated Si films with different designs of hole arrangement, substrate and period of holes. (a) Absorption of a 1.5-μm-thick flat Si film and Si films with hole arrays on bulk Si and SiO$_2$ substrates at the wavelengths between 800 ~ 950 nm. Hole arrays are integrated in the surface of Si films in square and hexagonal lattices with a diameter/period ($d/p$)
of 700/1000 nm and a depth of 250 nm. (b) absorption of 1.5-μm-thick Si films with hole arrays in hexagonal lattice with different periods of holes on bulk Si and SiO$_2$ substrates at the wavelengths between 800 ~ 950 nm. Hole arrays have a hole diameter of 700 nm and a depth of 250 nm.

Fig. 2(b) shows the absorption of 1.5-μm-thick Si films with integrated hole arrays in hexagonal lattice with different periods of holes on bulk Si and SiO$_2$ substrates at the wavelengths between 800 ~ 950 nm. Hole arrays have a hole diameter of 700 nm and a depth of 250 nm. It shows that the absorption of Si films with hole arrays on a SiO$_2$ substrate outperform their counterparts with the same hole structures on a bulk Si substrate. When the period of holes increases from 900 nm to 1500 nm, higher absorption is achieved for the Si film with smaller periods of holes ($p = 900$ nm and $p = 1000$ nm, $d/p = 0.78$ and $d/p = 0.7$) on either bulk Si or SiO$_2$ substrate. The absorption decreases with increasing period of holes. Holes integrated Si film with a period of 1000 nm has a lower absorption at the wavelengths of 800 ~ 850 nm and higher absorption at the wavelengths of 850 ~ 900 nm compared to holes integrated Si film with a period of 900 nm.

Fig. 3(a) and Fig. 3(b) shows the absorption of 1.5-μm-thick and 2.5-μm-thick Si films with hole arrays in hexagonal lattice with different hole depths on a SiO$_2$ substrate at the wavelengths between 800 ~ 950 nm, respectively. Hole arrays are integrated with a diameter/period ($d/p$) of 700/1000 nm. Absorption of the flat Si film without holes with the same thickness is also presented. Fig. 3(a) reveals that when the holes span the whole Si film ($h = 1.5$ μm), although the absorption is higher than that of the flat Si film, the nanostructured Si film has the lowest absorption compared to Si films with hole arrays of other depths ($h < 1.5$ μm). The highest absorption is obtained with a hole depth of 250 nm. Fig. 3(b) shows that for the 2.5-μm-thick Si film, the absorption of holes integrated Si film with a hole depth of 2.5 μm is also the lowest compared to other hole depths, and 250 nm is still a hole depth that can provide a high absorption especially for the longer wavelengths between 840 ~ 950 nm. A high absorption can also be obtained by the Si film with hole array with a hole depth of 2 μm which provides a higher absorption at the wavelengths of 800 ~ 840 nm. It can be concluded that it is advantageous for light absorption to keep a layer of flat Si film without holes with a certain thickness between SiO$_2$ substrate and the hole array, which is helpful to guide the light in laterally propagating modes in the Si film.

![Figure 3](image.png)
μm (d) with six different designs of diameter (d) and period (p) at the wavelengths between 800 ~ 950 nm

Hole arrays with similar diameter/period (d/p) around 0.7 and different designs of hole diameter and period are integrated in Si films on a SiO$_2$ substrate. Absorption of 1.5-μm-thick Si films with a hole depth of 250 nm and 2.5-μm-thick Si films with a hole depth of 2 μm at the wavelengths between 800 ~ 950 nm are shown in Fig. 3(c) and Fig. 3(d), respectively. The holes have six different designs of diameter (d) and period (p): (I) $d = 630$ nm, $p = 900$ nm ($d/p = 0.7$), (II) $d = 700$ nm, $p = 1000$ nm ($d/p = 0.7$), (III) $d = 1050$ nm, $p = 1500$ nm ($d/p = 0.7$), (IV) $d = 1300$ nm, $p = 2000$ nm ($d/p = 0.65$), (V) $d = 1400$ nm, $p = 2000$ nm ($d/p = 0.7$), (VI) $d = 1500$ nm, $p = 2000$ nm ($d/p = 0.75$). It shows that smaller periods of holes ($p = 900$ nm and $p = 1000$ nm) lead to a higher absorption of Si film regardless of Si film thickness and hole depth. The absorption decreases as the period of holes increases, which is consistent with the results shown in Fig. 2 (b). Si film with hole array with a period of 900 nm has a higher absorption at the lower wavelengths while Si film with hole array with a period of 1000 nm has a higher absorption at the higher wavelengths. It can be concluded that a higher absorption of the holes integrated Si film can be obtained with a diameter/period (d/p) around 0.7 and a smaller period of holes similar to the wavelength.

3.2. Laterally propagating modes of light in Si film with holes

In order to verify the light bending effect of hole array, electric field distribution in nanostructured Si films with $d/p = 700/1000$ nm and $d/p = 1500/2000$ nm are simulated and shown in Fig. 4 at the wavelength of 850 nm. The holes arranged in square lattice with a depth of 1 μm are integrated in the surface of Si films with a thickness of 1.5 μm on a SiO$_2$ substrate. Light is vertically illuminated at one point on the Si surface between two holes with a coordinate value of 0 at the time of $t = 0$ fs. Electric field distribution in nanostructured Si films at $t = 5$ fs, $t = 7$ fs, $t = 9$ fs, $t = 11$ fs and $t = 20$ fs shows light propagation over time in the Si films with different designs of hole array. It can be seen that the vertically incident light undergoes a bending and propagates laterally for each nanostructured Si film due to the diffraction of hole array. It shows a strong electric field distribution in the holes, and the effective optical path of light in Si film is also increased with an enhanced absorption. In the Si film with hole array with $d/p = 700/1000$ nm, a strong electric field distribution can be observed in the holes 2 μm away from the incident point at $t = 5$ fs. For the Si film with hole array with $d/p = 1500/2000$ nm, more than 11 fs is needed to form a strong electric field in the holes at the same distance of 2 μm. Light has a higher laterally propagating speed in the nanostructured Si film with a smaller period of holes.

![Figure 4](image-url)

**Figure 4.** Electric field distribution over time in nanostructured Si films with $d/p = 700/1000$ nm (a) and $d/p = 1500/2000$ nm (b) at the wavelength of 850 nm. The holes arranged in square lattice with a depth of 1 μm are integrated in the surface of Si films with a thickness of 1.5 μm on a SiO$_2$ substrate.
Light is vertically illuminated at one point on the Si surface between two holes with a coordinate value of 0 at the time of $t = 0$ fs.

### 3.3. Enhanced EQE of Si MSM photodiodes with photon-trapping holes

The electrical and optical characterization of fabricated Si MSM photodiodes as shown in Table 1 were measured at the wavelength of 850 nm. Fig. 5(a) shows the IV curves of the photodiodes without holes and with holes with $d/p = 700/1000$ nm under dark and under illumination. The dark current of the photodiodes is lower than 1 μA. An increase in photocurrent can be observed in photodiodes with holes. Fig. 5(b) shows the simulated absorption and measured EQE of the five fabricated photodiodes. The photodiode without holes exhibits an EQE of 23%. By integrating photon-trapping holes, the EQE is significantly increased. The EQE of photodiodes with holes in hexagonal lattice outperform their counterparts with holes in square lattice. When the period of holes in hexagonal lattice decreases from 2000 nm to 900 nm, higher EQE is achieved for the photodiodes with smaller periods of holes ($p = 900$ nm and $p = 1000$ nm). This is consistent with the simulation results. The maximum EQE is 61% measured from a photodiode with holes with $d/p = 630/900$ nm.

![Figure 5.](image)

*Figure 5.* Electrical and optical characterization of fabricated Si MSM photodiodes. (a) IV curves of the photodiodes without holes and with holes with $d/p = 700/1000$ nm under dark and under illumination. (b) Simulated absorption and measured EQE of the five fabricated photodiodes with different designs of holes and fingers.

### 4. Conclusions

In this paper, we have presented a theoretical and experimental study on enhanced absorption and EQE of Si MSM photodiodes with periodic cylindrical-shaped holes at the wavelengths between 800 ~ 950 nm. Hole arrays, designed with different diameter, depth and period, are arranged in square and hexagonal lattices in Si films with a thickness of 1.5 μm and 2.5 μm on bulk Si and SiO$_2$ substrates. Absorption and electric field distribution in nanostructured Si films are simulated to analyze the light bending effect of hole arrays. Si film with hole array with a diameter/period ($d/p$) around 0.7 and a smaller period comparable to the wavelength provides a higher absorption due to more bending of light. For the holes integrated Si film on a SiO$_2$ substrate, light is more trapped and absorbed due to multiple reflections and diffractions, resulting in an enhanced absorption of 30.45% ~ 47.53% at 800 ~ 950 nm wavelengths with a Si thickness of 1.5 μm and a hole depth of 250 nm. EQE of Si MSM photodiodes with photon-trapping holes is enhanced to 61% at 850 nm which represents 262% improvement over the photodiodes without holes.

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