Article

Simulation Study on the Effect of Doping Concentrations on the Photodetection Properties of Mg₂Si/Si Heterojunction Photodetector

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Abstract: To develop and design an environmentally friendly, low-cost shortwave infrared (SWIR) photodetector (PD) material and extend the optical response cutoff wavelengths of existing silicon photodetectors beyond 1100 nm, high-performance silicon-compatible Mg₂Si/Si PDs are required. First, the structural model of the Mg₂Si/Si heterojunction was established using the Silvaco Atlas module. Second, the effects of the doping concentrations of Mg₂Si and Si on the photoelectric properties of the Mg₂Si/Si heterojunction PD, including the energy band, breakdown voltage, dark current, forward conduction voltage, external quantum efficiency (EQE), responsivity, noise equivalent power (NEP), detectivity, on/off ratio, response time, and recovery time, were simulated. At different doping concentrations, the heterojunction energy band shifted, and a peak barrier appeared at the conduction band of the Mg₂Si/Si heterojunction interface. When the doping concentrations of Si and Mg₂Si layer were 10¹⁷, and 10¹⁶ cm⁻³, respectively, the Mg₂Si/Si heterojunction PD could obtain optimal photoelectric properties. Under these conditions, the maximum EQE was 70.68% at 800 nm, the maximum responsivity was 0.51 A/W at 1000 nm, the minimum NEP was 7.07 × 10⁻¹¹ W/Hz^{1/2} at 1000 nm, the maximum detectivity was 1.4 × 10¹⁰ Jones at 1000 nm, and the maximum on/off ratio was 141.45 at 1000 nm. The simulation and optimization result also showed that the Mg₂Si/Si heterojunction PD could be used for visible and SWIR photodetection in the wavelength range from 400 to 1500 nm. The results also provide technical support for the future preparation of eco-friendly heterojunction photodetectors.

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1. Introduction

At present, infrared photodetectors are mainly composed of HgCdTe, InSb, InGaAs, and other materials, but these materials are highly toxic and have low abundance in the Earth's crust [1]. To realize the sustainable development of shortwave infrared (SWIR) photodetectors (PDs), it is necessary to develop a material that is environmentally friendly and has no severe resource constraints, a large absorption coefficient, and a low cost. Semiconductor silicides (Mg₂Si, Ca₂Si, BaSi₂, CrSi₂, and FeSi₂) and related germanium compounds are environmentally friendly and have high absorption coefficients and narrow band gaps [2,3]. These materials may be suitable alternatives to the current SWIR sensors of toxic materials, although their current performances are low. Mg₂Si has a small lattice mismatch with Si (<2%) [4], a low cost, a narrow band gap (0.6–0.7 eV) compared with those of Mg₂Ge and Mg₂Sn (0.3–0.7 eV) [5], and a high absorption coefficient of 3 × 10⁵ cm⁻¹ near 500 nm. Furthermore, Mg and Si resources are abundant [6]. For the silicon chip industry, to further expand the optical response cutoff wavelength of the existing silicon

photodetectors to more than 1100 nm, high-performance silicon-compatible $\text{Mg}_2\text{Si}/\text{Si}$ PDs are needed. Although Mg_2Si is an attractive material for SWIR PDs, there have been few reports on Mg_2Si -based heterojunction PDs.

In this work, we established the model structure of the $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PD and studied the effects of the Mg_2Si and Si doping concentrations on the photoelectric properties of the $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PD, including the energy band, reverse breakdown voltage, dark current, forward conduction voltage, external quantum efficiency (EQE), responsivity, noise equivalent power (NEP), detectivity, on/off ratio, response time, and recovery time. The results of these photoelectric properties were analyzed and summarized, and suitable doping concentrations of Mg_2Si and Si were obtained, which were 10^{16} cm^{-3} , and 10^{17} cm^{-3} , respectively. Under these conditions, the $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PDs exhibited good photoelectric properties, such as the EQE and responsivity. The proposed simulation method could reduce the design cost and shorten the development cycle for PD devices.

2. Simulation Method and Device Structure

Atlas in the Silvaco TCAD software is a device simulator that can simulate the thermal, optical, and electrical behaviors of semiconductor devices. The device simulation process included five steps: structure description, material model description, numerical calculation, solution description, and result analysis. The user can input the parameters of the material and can also customize the material, such as changing the parameter values of the physical model and editing the interface, junction, and other properties of the material.

In the simulation process, a two-dimensional mesh was first generated, and then the region, material, electrode, doping concentrations, physical model, and numerical calculation method were described in turn. Finally, the voltage, illumination, etc., were applied to obtain the device characteristics. The cross section of the p- $\text{Mg}_2\text{Si}/\text{n-Si}$ heterojunction PD model is shown in Figure 1. Figure 2 shows the structural diagram of the heterojunction PD. Among the physical models, the SRH composite model, auger composite model, conmob mobility model, fldmob electric field model, and impact self collision ionization model were selected. The optical refractive index parameters of Mg_2Si material can be imported into the file with the index file. The Newton iterative numerical calculation method was selected to solve the Poisson and continuity equations for the device and analyze its photoelectric properties. The thickness of the p- Mg_2Si was $2 \mu\text{m}$, the width was $1 \mu\text{m}$, and the doping concentrations were 10^{14} , 10^{15} , 10^{16} , 10^{17} , or 10^{18} cm^{-3} . The thickness of the n-Si was $3 \mu\text{m}$, the width was $1 \mu\text{m}$, and the doping concentrations were 10^{16} , 10^{17} , 10^{18} , 10^{19} , or 10^{20} cm^{-3} . The anode was made of Au with a thickness of $0.2 \mu\text{m}$ and a width of $0.2 \mu\text{m}$. The cathode material was Ag with a thickness of $0.2 \mu\text{m}$ and a width of $1 \mu\text{m}$. The optical and electrical parameters of Mg_2Si and Si during the simulation are shown in Table 1 [7–9].

Figure 1. The cross section of the p- $\text{Mg}_2\text{Si}/\text{n-Si}$ heterojunction PD model.

Figure 2. The structural diagram of the heterojunction PD.

Table 1. The optical and electrical parameters of Mg₂Si and Si.

Parameters and Units	Mg ₂ Si [7,8]	Si [9]
Bandgap (eV)	0.77	1.12
Affinity (eV)	4.37	4.05
Permittivity	20	11.9
Effective conduction band density (cm ⁻³)	7.8×10^{18}	2.8×10^{19}
Effective valence band density (cm ⁻³)	2.06×10^{19}	1.04×10^{19}
Electron mobility (cm ² /Vs)	550	1350
Hole mobility (cm ² /Vs)	70	500
Electron auger coefficient (cm ⁶ /s)	9×10^{-29}	2.8×10^{-31}
Hole auger coefficient (cm ⁶ /s)	9×10^{-29}	9.9×10^{-32}
SRH recombination life time, τ , h (s)	1×10^{-6}	1×10^{-7}

3. Results and Discussion

3.1. Energy Band

The energy bands of the heterojunction PDs at different doping concentrations are shown in Figure 3. When the Si substrate doping concentrations was 10^{16} and 10^{17} cm⁻³, the energy band shifted, which led to the formation of a peak barrier in the conduction band at the interface of the Mg₂Si/Si heterojunction, thus hindering the transport of some carriers. This was mainly caused by different doping concentrations on both sides of the heterojunction. Refs [10,11] reported the study of Mg₂Si/Si heterojunction in solar cells, and the band offset and peak barrier of the heterojunction were also observed. The height and width of the peak barrier decreased with the increase in the Si doping concentrations. When the doping concentrations of the Si substrate was 10^{18} cm⁻³, the band shift decreased, the height of the peak barrier at the heterojunction interface became weaker, and the peak width became narrower. When the doping concentrations of the Si substrate was 10^{19} and 10^{20} cm⁻³, the band shift further decreased, and the peak barrier at the heterojunction interface basically disappeared. A higher doping concentration was applied in the Si to reduce the effect of the bandgap space charge region, so that the height of the peak barrier became weak, and the peak width became narrow or even disappeared at the interface of the Mg₂Si/Si heterojunction [11]. The increase in the Si substrate doping concentrations could alleviate the harmful effect of the band barrier, but it would reduce the responsivity and EQE of the heterojunction device. An appropriate doping concentration is very important for the performance of the heterojunction PD. With the increase of Si doping concentration, more electrons are provided by impurities. However, the density of states that can be provided at each energy level is certain, so the impurity energy level will become an energy band and extend to the conduction band, and the energy difference between the impurity energy level and the bottom of the conduction band will be reduced. If the Si doping concentration is high enough, the impurity energy band may be connected

with the conduction band to form a whole energy band, so it seems that the width of the band gap becomes smaller.

Figure 3. The energy bands of the heterojunction PDs at different doping concentrations. (a) Si- 10^{16} cm^{-3} . (b) Si- 10^{17} cm^{-3} . (c) Si- 10^{18} cm^{-3} . (d) Si- 10^{19} cm^{-3} . (e) Si- 10^{20} cm^{-3} . (f) The effect of doping concentrations on dark current.

3.2. Current–Voltage (*I*–*V*) Curves

In the absence of light, when the voltage of the heterojunction PD was reverse-biased to -90 V. Figure 4 shows the reverse current–voltage (*I*–*V*) curves of the heterojunction PD with different Mg_2Si doping concentrations under the conditions of Si doping concentrations of 10^{16} , 10^{17} , 10^{18} , 10^{19} , and 10^{20} cm^{-3} , respectively. The doping concentrations of Si and Mg_2Si had a significant influence on the reverse breakdown voltage of the heterojunction PD. The reverse breakdown voltages of the heterojunction PD were calculated to be in the range from 5 to 90 V at different doping concentrations. The formula of the reverse breakdown voltage under the avalanche effect of the PN junction is shown as follows [12]:

$$V_B = \frac{\epsilon_s E_{\text{crit}}^2}{2eN_B} \quad (1)$$

where e , ϵ_s , E_{crit}^2 , and N_B are the elementary charge, material dielectric constant, the critical field, and the doping concentrations of the low-doped side of the single-side junction, respectively. Figure 4 shows that when the doping concentrations of Si was constant, the reverse breakdown voltage of the heterojunction PD decreased with the increase in the doping concentrations of Mg_2Si . This is consistent with the conclusion of Equation (1). As shown in Figure 4f, the reverse breakdown voltage also decreased with the increase in the Si substrate doping concentrations. However, a high doping concentration of Si had little influence on the reverse breakdown voltage of the heterojunction PD. This was because the doping concentrations of the Mg_2Si layer was lower when Si was at a high doping concentration. Equation (1) shows that the doping concentrations of the low-doped side of the single-side junction had a significant influence on the reverse breakdown voltage. Figure 3f shows the dark current versus doping concentrations curve of the heterojunction PD without illumination and with a bias voltage of -3 V. When the Si doping concentrations was constant, the dark current decreased with the increase in the Mg_2Si layer doping concentrations. The dark current was reduced from 10^{-10} to 10^{-14} A. The Si substrate doping concentrations had little effect on the dark current of the heterojunction PD. The widths of the pn, p^+n , and n^+p junction space charge regions are shown, respectively, as follows [12]:

$$W = \sqrt{\frac{2\epsilon_r\epsilon_0(N_A + N_D)(V_{bi} + V)}{eN_A N_D}} \quad (2)$$

$$W \approx x_n = \sqrt{\frac{2\epsilon_r\epsilon_0(V_{bi} + V)}{eN_D}} \quad (3)$$

$$W \approx x_p = \sqrt{\frac{2\epsilon_r\epsilon_0(V_{bi} + V)}{eN_A}} \quad (4)$$

where e , ϵ_r , ϵ_0 , N_A , N_D , V_{bi} , and V are the elementary charge, material dielectric constant, vacuum dielectric constant, acceptor doping concentrations, donor doping concentrations, contact potential difference, and applied bias voltage, respectively. The formula for the maximum electric field in the pn junction is as follows [12]:

$$E_{\text{max}} = \frac{-2(V_{bi} + V)}{W}. \quad (5)$$

As shown by Equation (4), an increase in the Mg_2Si doping concentrations would result in a decrease in the width of the space charge region. Equation (5) shows that a decrease in the width of the space charge region would cause an increase in the electric field strength, and then the barrier height would also increase and the carrier transport ability would decrease. Thus, the dark current would decrease with an increase in the doping concentrations of the Mg_2Si layer.

Figure 4. Reverse breakdown voltage curves of the heterojunction PDs with different doping concentrations. (a) Si- 10^{16} cm^{-3} . (b) Si- 10^{17} cm^{-3} . (c) Si- 10^{18} cm^{-3} . (d) Si- 10^{19} cm^{-3} . (e) Si- 10^{20} cm^{-3} . (f) The effect of doping concentrations on reverse breakdown voltage.

Under illumination conditions, the calculation results of the forward I-V curves of the heterojunction PD with different Mg_2Si doping concentrations under the Si doping concentrations of 10^{16} , 10^{17} , 10^{18} , 10^{19} , and 10^{20} cm^{-3} are shown in Figure 5. Figure 5f shows that when the doping concentrations of the Mg_2Si layer was low, the forward conduction voltage was around 0.5 V. When the doping concentrations of the Mg_2Si layer was high, the forward conduction voltage was around 0.27 V. When the Si doping concentrations was constant, the forward conduction voltage of the heterojunction PD tended to decrease with the increase in the Mg_2Si layer doping concentrations. The specific on-resistance of the $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PD decreased with the increase in the doping concentrations of the Mg_2Si layer. Consequently, the forward conduction current of the PD increased, the I-V curve underwent a certain degree of upward shifting, and the forward conduction voltage of the x -axis decreased.

Figure 5. Forward I-V curves of the heterojunction PDs with different doping concentrations. (a) Si- 10^{16} cm^{-3} . (b) Si- 10^{17} cm^{-3} . (c) Si- 10^{18} cm^{-3} . (d) Si- 10^{19} cm^{-3} . (e) Si- 10^{20} cm^{-3} . (f) The effect of doping concentrations on forward conduction voltage.

3.3. Responsivity

The spectral responsivity is a figure of merit representing the sensitivity of a PD to photon irradiation, which can be defined as [13,14],

$$\text{Responsivity} = \frac{I_{\text{photo}}}{P_{\text{incident}}} \quad (6)$$

where I_{photo} is the photocurrent, and P_{incident} represents the incident light power. The responsivity values of the heterojunction PD with different Mg_2Si doping concentrations under the Si doping concentrations of 10^{16} , 10^{17} , 10^{18} , 10^{19} , and 10^{20} cm^{-3} were calculated, and the results are shown in Figure 6. Different Mg_2Si and Si doping concentrations had a certain influence on the responsivity of the heterojunction PD. The responsivity increased first and then decreased when the incident wavelength increased from 400 to 1500 nm. The responsivity reached the maximum value when the incident light was around 1000 nm. The results also showed that the responsivity was higher when the doping concentrations of the Mg_2Si layer was lower, and the responsivity was lower when the doping concentrations of the Mg_2Si layer was higher. When the doping concentrations of the Mg_2Si layer and the Si layer were 10^{16} and 10^{17} cm^{-3} , respectively, the heterojunction photodetector obtained the maximum responsivity, and its value was 0.51 A/W. For shorter light wavelengths, the greater the photon energy, the more energy the photons would lose when they hit the surface of the device. The absorption by the front surface of the device would be greatly reduced, resulting in low responsiveness [15]. When the wavelength was greater than 1000 nm, the responsivity decreased because the absorption of long-wavelength light by the Mg_2Si absorption layer would slowly decrease. According to Figure 6f, the peak responsivity of the heterojunction PD ranged from 0.23 to 0.51 A/W at different doping concentrations. The responsivity of the Gr/Si heterojunction PD reported previously [16] was 0.73 A/W, and the responsivity of the ZnO/Si heterojunction PD reported previously was 0.36 A/W [17].

Figure 6. Cont.

Figure 6. Responsivity curves of the heterojunction PDs with different doping concentrations. (a) Si- 10^{16} cm⁻³. (b) Si- 10^{17} cm⁻³. (c) Si- 10^{18} cm⁻³. (d) Si- 10^{19} cm⁻³. (e) Si- 10^{20} cm⁻³. (f) The effect of doping concentrations on responsivity.

When the Si layer doping concentrations was constant, the responsivity of the heterojunction PD increased first and then decreased with the increase in the Mg₂Si layer doping concentrations. When the low-doping concentrations Mg₂Si layer and the low-doping concentrations Si layer formed a heterojunction, the space charge region was almost equally divided on both sides of the junction, and the photogenerated carriers were generated less in the Si layer, such that the space charge region extended in the Si layer had less ability to collect photocurrent. When a low-doping concentrations Mg₂Si layer and a high-doping concentrations Si layer formed a heterojunction, the space charge region was mainly distributed in the Mg₂Si layer. A space charge region extended in the absorption layer contributes greatly to the collection of photocurrents and can effectively improve the responsivity [18]. The Mg₂Si layer was the main region for absorbing light to generate carriers, and the space charge region on the Mg₂Si layer could play a role in the photocurrent to a greater extent, which was beneficial for the improvement of the responsivity. With the increase in the Mg₂Si absorption layer doping concentrations, the Mg₂Si layer had more holes, the carriers generated by absorbing light increased, the photocurrent was improved to a certain extent, and the responsivity increased. However, with the further increase in the doping concentrations of the Mg₂Si absorption layer, the space charge region would be distributed to the Si layer side, the photocurrent collection ability of the space charge region would become weak, and the responsivity would decrease.

3.4. External Quantum Efficiency (EQE)

The EQE is defined as the number of electron–hole pairs generated per incident photon at a certain wavelength, which can be calculated as follows [19,20]:

$$\text{EQE} = \frac{hc}{e\lambda} R \times 100\% \quad (7)$$

where h , c , e , λ , and R are Planck's constant, speed of light, elementary charge, wavelength, and responsivity, respectively. The EQE curves of the heterojunction PD with different Mg_2Si doping concentrations under the Si doping concentrations of 10^{16} , 10^{17} , 10^{18} , 10^{19} , and 10^{20} cm^{-3} are shown in Figure 7. When the wavelength of the incident light increased from 400 to 1500 nm, the EQE first increased and then decreased. The EQE reached the peak value in the range of 750–950 nm. When the doping concentrations of the Mg_2Si and Si layers were 10^{16} and 10^{17} cm^{-3} , respectively, the heterojunction photodetector obtained the maximum EQE of 70.68%. As shown in Table 2, Ref. [17] reported that the EQE of the ZnO/Si heterojunction PD was 93%. Ref. [21] reported that the EQE of the InSb/Si heterojunction PD was 25%. Ref. [22] reported that the EQE of the $\text{Bi}_2\text{Te}_3/\text{Si}$ heterojunction PD was 120%. The maximum EQE value of the heterojunction PD designed in this work is at the middle level, and further research is needed to improve the EQE. According to Equation (7), when the wavelength of the incident light is constant, the EQE is proportional to the responsivity, and both the EQE and the responsivity increase first and then decrease with the increase in the wavelength. When the doping concentrations of Si was constant, the wavelength corresponding to the peak EQE shifted to longer wavelengths with the increase in the doping concentrations of the Mg_2Si layer. The wavelength was red-shifted from 750 to 950 nm. This was due to a shift in the heterojunction band with increasing doping concentrations, resulting in a red shift in the peak wavelength due to band narrowing [23–25], as shown in Figure 3.

Table 2. Key performance parameters of $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PDs and several other reported heterojunction PDs.

Device	Responsivity (A/W)	EQE (%)	NEP ($\text{WHz}^{-1/2}$)	Detectivity (Jones)	On-off Ratio	Spectral Range (nm)	References
$\text{Mg}_2\text{Si}/\text{Si}$	0.51	70.68	7.07×10^{-11}	1.4×10^{10}	1.4×10^2	400–1500	This work
Gr/Si	0.73		7.5×10^{-14}	4.2×10^{12}		300–1100	[16]
ZnO/Si	0.36	93	10^{-11}	7.2×10^{10}		200–1000	[17]
InSb/Si	0.312	25	1.15×10^{-12}	6.7×10^{10}	2.9×10^3	635–2700	[21]
$\text{Bi}_2\text{Te}_3/\text{Si}$	1	120		2.5×10^{11}			[22]
SnSe/Si	0.566			4.4×10^{12}	4.9×10^5	300–1100	[25]
WS_2/Si	0.224			1.5×10^{12}	10^6	200–3043	[26]
Gr/HgCdTe	7.33	85.8	4.72×10^{-20}	4.4×10^{10}		2000–12,000	[27,28]
Gr/ $\text{Al}_2\text{O}_3/\text{In-GaAs}$	0.52						

According to Figure 7f, the peak EQE of the heterojunction PD ranged from 29.14% to 70.68% at different doping concentrations. When the doping concentrations of the Si layer was constant, the EQE of the heterojunction PD increased first and then decreased with the increase in the doping concentrations of the Mg_2Si absorption layer. Initially, as the doping concentrations of the Mg_2Si absorption layer increased, the Mg_2Si layer could absorb more lights and provide more photogenerated carriers, which was conducive to the improvement of the EQE.

However, as the doping concentrations of the Mg_2Si absorption layer further increased, the space charge region was distributed to the side of the Si layer, and the number of photogenerated carriers collected by the space charge region was reduced, which reduced the EQE of the device. The Si layer had a significant influence on the EQE at low doping concentrations, but it had little influence on the EQE at high doping concentrations. This was because the space charge region was mainly distributed on the Mg_2Si absorption layer side when the Si layer had a high doping concentration. Even with the increase in the doping concentrations of the Mg_2Si absorption layer, there were still some space charge

regions distributed on the side of the Mg_2Si absorption layer, and the ability to collect photogenerated carriers was not greatly reduced. When the doping concentrations of the Si layer was low, as the doping concentrations of the Mg_2Si absorption layer increased or even exceeded the doping concentrations of Si, the space charge was partially or completely distributed on the Si side. At this time, the capacity of the space charge region to collect photogenerated carriers was significantly weakened.

Figure 7. EQE curves of the heterojunction PDs with different doping concentrations. (a) Si- 10^{16} cm^{-3} . (b) Si- 10^{17} cm^{-3} . (c) Si- 10^{18} cm^{-3} . (d) Si- 10^{19} cm^{-3} . (e) Si- 10^{20} cm^{-3} . (f) The effect of doping concentrations on EQE.

3.5. Noise Equivalent Power (NEP)

The NEP is defined as follows [29,30]:

$$\text{NEP} = \frac{\sqrt{2eI_{\text{dark}}}}{R} \quad (8)$$

where e , I_{dark} , and R are the elementary charge, dark current, and responsivity, respectively. The smaller the NEP, the smaller the incident light power effectively detected by the device, and the better the detection performance of the device. Figure 8 shows the calculated NEP values of the heterojunction PDs with different Mg_2Si doping concentrations under the Si doping concentrations of 10^{16} , 10^{17} , 10^{18} , 10^{19} , and 10^{20} cm^{-3} . The Mg_2Si and Si doping concentrations had a significant impact on the NEP of the heterojunction PDs. The peak NEP ranged from 3.68×10^{-13} to $7.15 \times 10^{-9} \text{ WHz}^{-1/2}$. The minimum value of the NEP was $3.68 \times 10^{-13} \text{ WHz}^{-1/2}$. The NEPs of the PDs reported in Refs. [14,19] were 7.5×10^{-14} and $1.15 \times 10^{-12} \text{ WHz}^{-1/2}$, respectively (see Table 2 for details). When the wavelength of the incident light increased from 400 to 1500 nm, the NEP decreased first and then increased with the increase in the wavelength of the incident light. The NEP reached the minimum at the wavelength of 1000 nm. The NEP decreased with the increase in the Mg_2Si absorption layer doping concentrations. According to Figure 3f, the dark current decreased significantly with the increase in the Mg_2Si layer doping concentrations, and the dark current decreased by one order of magnitude with an increase of one order of magnitude of the Mg_2Si layer doping concentrations. The dark current had a greater influence on the NEP than on the responsivity. According to Equation (8), as the doping concentrations of the Mg_2Si absorption layer increased, the dark current decreased significantly, leading to a gradual decrease in the NEP. Figure 3f shows that the doping concentrations of the Si layer had little influence on the dark current, and thus, it had little influence on the NEP.

Figure 8. Cont.

Figure 8. NEP curves of the heterojunction PDs with different doping concentrations. (a) Si-10¹⁶ cm⁻³. (b) Si-10¹⁷ cm⁻³. (c) Si-10¹⁸ cm⁻³. (d) Si-10¹⁹ cm⁻³. (e) Si-10²⁰ cm⁻³. (f) The effect of doping concentrations on NEP.

3.6. Detectivity

The detectivity and NEP are inversely proportional, and the higher the detectivity, the better the detection performance of a device. Considering the differences of the effective detection area of the device, the definition of the detectivity is as follows [31,32]:

$$\text{Detectivity} = \frac{\sqrt{S}}{\sqrt{2eI_{\text{dark}}}}R = \frac{\sqrt{S}}{\text{NEP}} \quad (9)$$

where S , e , I_{dark} , and R are the effective working area, elementary charge, dark current, and responsivity of the heterojunction PD, respectively. Figure 9 shows the calculated detectivity values of the heterojunction PD with different Mg₂Si doping concentrations under the Si doping concentrations of 10¹⁶, 10¹⁷, 10¹⁸, 10¹⁹, and 10²⁰ cm⁻³. The Mg₂Si and Si doping concentrations had a significant influence on the detectivity of heterojunction PD. Figure 9f shows the peak detectivity ranged from 1.4×10^8 to 2.7×10^{12} Jones. The maximum detectivity of the heterojunction PD was 2.7×10^{12} Jones. It was comparable to that reported in Refs. [26,27]. When the wavelength of the incident light increased from 400 to 1500 nm, the detectivity increased first and then decreased with the increase in the wavelength of the incident light. The detectivity reached the maximum value when

the incident light was around 1000 nm. The detectivity increased with the increase in the doping concentrations of the Mg_2Si absorption layer. As shown by Equation (9), the detectivity and the NEP are inversely proportional, and the NEP would gradually decrease with the increase in the doping concentrations of the Mg_2Si absorption layer. Thus, the detectivity gradually increased with the increase in the doping concentrations of the Mg_2Si absorption layer.

Figure 9. Detectivity curves of the heterojunction PDs with different doping concentrations. (a) $\text{Si}-10^{16} \text{ cm}^{-3}$. (b) $\text{Si}-10^{17} \text{ cm}^{-3}$. (c) $\text{Si}-10^{18} \text{ cm}^{-3}$. (d) $\text{Si}-10^{19} \text{ cm}^{-3}$. (e) $\text{Si}-10^{20} \text{ cm}^{-3}$. (f) The effect of doping concentrations on detectivity.

3.7. On/Off Ratio

The formula for the on/off ratio is as follows [33]:

$$\text{on/off ratio} = \frac{I_{\text{light}}}{I_{\text{dark}}} \quad (10)$$

where I_{light} is the output current with light, and I_{dark} is the output current without light. Figure 10 shows the calculated on/off ratios of the heterojunction PDs with different Mg_2Si doping concentrations under the Si doping concentrations of 10^{16} , 10^{17} , 10^{18} , 10^{19} , and 10^{20} cm^{-3} , respectively. The Mg_2Si and Si doping concentrations had a significant influence on the on/off ratios of the heterojunction PDs. As shown in Figure 10f, the peak on/off ratio ranged from 1.39 to 2.72×10^4 . The on/off ratio of the PD reported in Refs. [19,34] were 2.9×10^3 and 4.9×10^5 , respectively. When the incident light wavelength increased from 400 to 1500 nm, the on/off ratio increased first and then decreased with the increase in the incident light wavelength. The on/off ratio reached the maximum near the incident light wavelength of 1000 nm. The on/off ratio increased with the increase in the doping concentrations of the Mg_2Si absorption layer. As shown in Figure 5, when the doping concentrations of the Mg_2Si layer was low, the photocurrent was on the order of 10^{-5} A , and when the doping concentrations of the Mg_2Si layer was high, the photocurrent was on the order of 10^{-4} A . The dark current decreased from 10^{-10} to 10^{-14} A as the Mg_2Si layer doping concentrations increased. The dark current had a significant influence on the on/off ratio, and the dark current decreased significantly with the increase in the Mg_2Si layer doping concentrations, which led to an increase in the on/off ratio with the increase in the Mg_2Si layer doping concentrations.

Figure 10. Cont.

Figure 10. On/off ratio curves of the heterojunction PDs with different doping concentrations. (a) Si- 10^{16} cm^{-3} . (b) Si- 10^{17} cm^{-3} . (c) Si- 10^{18} cm^{-3} . (d) Si- 10^{19} cm^{-3} . (e) Si- 10^{20} cm^{-3} . (f) The effect of doping concentrations on on/off ratio.

3.8. Response Time and Recovery Time

The response time and the recovery time are parameters used to express the transient characteristics of heterojunction PDs. It is generally specified that the response time of a heterojunction PD is from 10% to 90% of the peak value, and the recovery time of PD is from 90% to 10% of the peak value [35,36]. Figure 11 shows the calculation results of the response time and recovery time curves of the heterojunction PDs with different Mg₂Si doping concentrations under the Si doping concentrations of 10^{16} , 10^{17} , 10^{18} , 10^{19} , and 10^{20} cm^{-3} , respectively. The response and recovery times increased with the increase in the doping concentrations of the Mg₂Si layer. The response time mainly included the carrier transit time in the depletion region, the carrier diffusion time in the non-depletion region, and the RC time constant. The recovery time mainly included the RC time constant and the carrier lifetime. The RC time constant, which characterizes the time required to charge and discharge the junction capacitor through the series and load resistances of the PD, was most important. The width of space charge region decreased with the increase in the Mg₂Si layer doping concentrations. The decreased space charge region formed a larger junction capacitance, which caused the charge and discharge times of the capacitor to increase, and

the RC time constant increased. The response and recovery times increased as the RC time constant increased. As shown in Figure 11f,g, the response time ranged from 0.79 to 2.59 ns and the recovery time ranged from 5.78 to 7.89 ns for different doping concentrations of the Mg_2Si layer.

Figure 11. Cont.

Figure 11. Response time and the recovery time curves of the heterojunction PDs with different doping concentrations. (a) Si- 10^{16} cm^{-3} . (b) Si- 10^{17} cm^{-3} . (c) Si- 10^{18} cm^{-3} . (d) Si- 10^{19} cm^{-3} . (e) Si- 10^{20} cm^{-3} . (f) The effect of doping concentrations on response time. (g) The effect of doping concentrations on recovery time.

4. Conclusions

In this work, a model of the $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PD was established, and the effects of different doping concentrations of Mg_2Si and Si on the photoelectric properties of the heterojunction PD were studied. The simulation results were obtained using Silvaco Atlas. The results showed that different doping concentrations of Mg_2Si and Si affected the performance of the heterojunction PDs. The energy band of the heterojunction exhibited a certain shift at different doping concentrations. When the doping concentrations of Si and Mg_2Si were low, a peak barrier appeared in the conduction band of the heterojunction interface. When the doping concentrations of Si and Mg_2Si were high, the height and width of the peak barrier decreased and narrowed, and in some cases, the peak barrier even disappeared. When the Si layer doping concentrations was 10^{17} cm^{-3} and the Mg_2Si layer doping concentrations was 10^{-16} cm^{-3} , the $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PD had better optical and electrical properties, including the EQE and responsivity. Under these conditions, the reverse breakdown voltage was 59.87 V, the dark current was $7.26 \times 10^{-12} \text{ A}$, the forward conduction voltage was 0.28 V, the NEP was 70.68%, the responsivity was 0.51 A/W, the NEP was $7.07 \times 10^{-12} \text{ WHz}^{-1/2}$, the detectivity was 1.4×10^{10} Jones, the on/off ratio was 141.45, the response time was 0.79 ns, and the recovery time was 5.79 ns. The simulation results also showed that the $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PD could detect visible and SWIR light in the range of 400–1500 nm. Thus, it has great potential as an alternative to other toxic and harmful heterojunction PDs with higher costs. This simulation method can reduce the design cost and shorten the development cycle of the device. The simulation results can be used to guide the preparation of environmentally friendly $\text{Mg}_2\text{Si}/\text{Si}$ heterojunction PDs.

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