Design and optimization of diamond mid-infrared phase shifter

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Abstract

Herein, the mid-infrared (7.7–13.7 μm) diamond-based phase shifter was designed and optimized by finite-element analysis. The ridge-shaped diamond waveguide is designed and doped to form the internal p–n structure, and the internal carrier distribution is changed by applying forward and reverse voltages to change the effective refractive index to achieve the effect of π-phase shift. The results show that when p-doping concentration is 4 × 10¹⁷ cm⁻³ and n-doping concentration is 1 × 10¹⁸ cm⁻³, upon the reverse voltage (8 V) is applied, the change of the real part of effective refractive index (ΔR) is 1.6 × 10⁻⁵, and the length of the phase shifter (L) required to realize the π-phase shift is 241 mm; upon the forward voltage (–8 V) is applied, ΔR increases to 3.2 × 10⁻⁴, and the length of the phase shifter required is shortened to 12.03 mm. Such a short length is relatively easy in industrial production. In order to make the refractive index distribution more uniform, the carrier concentration has been optimized as 1 × 10¹⁷ cm⁻³ for p-type and 4 × 10¹⁷ cm⁻³ for n-type, respectively.

1. Introduction

As the basic unit of optical communication [1], the optical phase shifter plays an important role in phase dimension adjustment [2, 3]. Especially in the structural design of optical devices, the deviation of the processing size accuracy will cause the optical signal to deviate during the propagation process, particularly for some devices that strictly require the interference of the optical signal, the phase shifter is extremely important. There are two major types of phase shifters based on the free carrier dispersion effect [4]: one is carrier injection [5] and the other is carrier depletion [6]. The carrier injection phase shifter mainly injects carriers into the waveguide through the diffusion of carriers. Although it offers a higher efficiency, its diffusion rate limits the carrier rate and thus consumes decent amount of energy. The carrier-depleted phase shifter mainly extracts carriers to change the carrier concentration in the waveguide area so the rate is not limited by the carrier diffusion rate and can match the electron moving rate. As a result, this kind of shifter can achieve rapid phase change [7–9].

At present, the phase shifter is based on the waveguide structure, and its phase is changed by changing the effective refractive index of the waveguide to realize the adjustable phase shift function. Generally speaking, phase shifters based on free carrier dispersion effect can achieve high-speed phase shifting. The most commonly used semiconductor phase shifters are mainly focused on silicon/germanium-based material [10–12]. Although mature technology and relatively low cost are its advantage, its disadvantages are also obvious. The silicon/germanium-based materials are easy to corrode [13, 14] and weak [15, 16], which makes the devices fabricated have a short service life and thus requires good protection during application. Moreover, its low transparency also limits its application in the mid-infrared band. The mid-infrared band is sensitive to thermal infrared remote sensing, fire [17, 18], active volcano [19, 20], and other high-temperature target recognition, making it capable of capturing high-temperature information. It also has a wide range of applications in substance detection [21]. Therefore, under many extreme environmental conditions, silicon/germanium-based waveguide phase shifters cannot meet their performance requirements.

Diamond has many excellent physical and chemical properties and is an ideal material in many fields. In addition to high hardness, diamond has excellent thermostability and optical property in the 1–100 μm waveband except for the optical opacity caused by two-photon self-absorption at 4.5–5.6 μm [22, 23], a very narrow waveband. Thus, it has excellent optical transparency, and the attenuation in the mid-infrared range is less than 1 dB/cm [24]. Therefore, it is an ideal waveguide material in the infrared waveband. In general, optical
equipment needs to be used under some extreme conditions, so diamond is undoubtedly the most suitable material. However, because of its high hardness, it requires a huge cost to precisely fabricate the waveguide devices. As far as our knowledge, the application of diamond on phase shifter has not yet been reported. In our previous work, we have studied the size of the diamond waveguide and what substrate material can well constrain the light field when the light wavelength is 7.7–13.7 μm [25]. According to the research of the previous work, we chose AlN material in the choice of base material, which can have greater stability. Therefore, it is timely to simulate and design the diamond phase shifter to obtain a feasible scheme, providing theoretical support for actual processing and reducing the required processing cost. Hence, the design and optimization of diamond phase shifter based on carrier-depleted dispersion effect is carried out by using COMSOL MULTIPHYSICS simulation in this paper, which provides theoretical support for the actual preparation of phase shifters.

In this work, we first constructed the diamond ridge waveguide phase shifter and designed its relevant parameters. Then, we observed the changes of carriers and refractive index after applying voltage through simulation and test the phase shift effect of the diamond phase shifter. In addition, we simulated and analyzed the different doping concentrations of the phase shifter to determine the most suitable doping concentration to achieve the best phase shift effect.

2. Structure design and theory

2.1 Structure design of phase shifter

All analysis and model construction are performed using COMSOL MULTIPHYSICS. The structure of the waveguide phase shifter designed in this paper is shown in Figure 1. In Figure 1, the left end is the p-type doped area, and the right end is the n-type doped area, in which the dark part is a heavily doped region and the light part is a normal doped region. Because high-concentration doping will produce high absorption for the propagation of infrared signals inside the waveguide, the waveguide structure adopts a ridge waveguide structure. The ridge structure can set the heavily doped carrier area on the slab layer on both sides, which greatly reduces the influence of the heavily doped area on the optical signal propagation area. And we set the carrier normal doped area on the center waveguide. The part of the geometric structure size is shown in Figure 1(b). The waveguide height (Hwg) is 17 μm, the width of the slab layer (Wslab) is 31 μm, and the width of the common doped area is Sdop = 21 μm. For the ridge waveguide structure, the geometric conditions of the waveguide design need to be met [26],

\[ \frac{a}{b} \geq \frac{1}{\sqrt{r}}, \quad r < \frac{1}{2} \]

where \( a/b \) is the ratio of the width to the height of the ridge and \( r \) is the ratio of the slab layer on both sides to the height of the waveguide.

As for the applied concentration of carriers, the p-type doping concentration in the heavily doped region is \( 1 \times 10^{20} \text{ cm}^{-3} \), the doping concentration in the n-type region is \( 1 \times 10^{20} \text{ cm}^{-3} \), and the boundary conditions at both ends of the heavily doped region are set as metal contact; in the normal doping area, in order to achieve better performance of the phase shifter, this article sets up multiple sets of doping concentrations for comparative analysis. Based on the doping concentration of the silicon-based phase shifter in some literatures, we refer to the doping concentration of the silicon-based phase shifter on this basis. And at the same time, we compare it with the concentration that can be doped on diamond experimentally, so we choose the doping concentration distribution is shown in Table 1.

In order to improve the working efficiency of the phase shifter, it is necessary to enlarge the width of the depletion layer so that the optical field and the refractive

![Figure 1. a) Structure design of phase shifter and (b) dimensional drawing of cross-section geometry of simulation model.](image-url)
index change region (the depletion layer) have a larger overlapping area. Therefore, we deviate the p-type doped region form the center of the waveguide by 1 μm. When the optical field is applied, a larger refractive index change area can be generated, and the phase shifting effect can be increased. Taking into account, the low carrier concentration in intrinsic diamond and the low migration efficiency of internal carriers, in order to improve its migration efficiency, the intrinsic layer was background doped and the concentration was set to p-type $1 \times 10^{14} \text{cm}^{-3}$. To compare the effect of voltage on its carriers, keep the p terminal at 0 potential, apply voltages of –8 V, 0 V, and 8 V to the n terminal to analyze the changes of internal carriers, refractive index, and phase.

### 2.2 Principle of phase shifter

In this paper, diamond is doped to produce a p–n junction structure. By changing the applied voltage, the carrier concentration inside the waveguide is changed, and then the refractive index inside the waveguide is changed, finally achieving the effect of phase shifting. The relationship between the change of refractive index and carriers is based on the Drude-Lorenz formula, and the formula for the change of refractive index with carriers is [27]

$$\Delta n(\text{carrier}) = \frac{-e^2}{8\pi^2 c^2 \varepsilon_0 n} \frac{\Delta N_e}{m_{ce}} + \frac{\Delta N_h}{m_{ch}}.$$  \hfill (2)

And, the formula for the change of carrier absorption rate of the waveguide material is

$$\Delta \alpha = \frac{\pi \lambda}{\mu_e \mu_h} \left( \frac{\Delta n}{n} + \frac{\Delta \alpha}{\alpha} \right),$$  \hfill (3)

where $e$ is the charge of electrons, $\lambda$ is the wavelength of light, $c$ is the speed of light, $\varepsilon_0$ is the vacuum dielectric constant, $\Delta N_e$ is the change in electron concentration, $\Delta N_h$ is the change in hole concentration, $m_{ce}$ is the effective mass of electrons, $m_{ch}$ is the effective mass of the hole, $\mu_e$ is the electron movement rate, and $\mu_h$ is the hole migration rate.

### 2.3 The relationship between refractive index change and phase

In the p–n type phase shifter, the p-type region and the n-type region will be combined with each other, and electrons and holes will mutually diffuse due to the concentration gradient, resulting in a built-in electric field. The built-in electric field will cause the carriers to drift in the opposite direction, and when the two kinds of carrier motions reach equilibrium, a stable space charge distribution will be formed, and a layer will be formed in the middle with no electrons and no holes, which is called the depletion region. The width of the depletion zone is

$$\Delta = \sqrt{\frac{\mu_e \mu_h}{e N_s}}.$$  \hfill (4)

where $\varepsilon_s$ is the dielectric constant of the material, $N_p$ and $N_n$ are the concentrations of p-type doping and n-type doping, respectively, $e$ is the electron charge, and $V_D$ is the built-in potential difference. Its relationship with the doping concentration is

$$V_D = \frac{kT}{e} - \frac{n_i}{N_p + N_n},$$  \hfill (5)

where $kT/e$ is the thermal voltage and $n_i$ is the concentration of intrinsic carriers. However, after a forward current is applied, the original internal built-in electric field is weakened, the internal current increases, and the electrons and holes combine to cause a change in the carrier concentration inside, resulting in a change in the refractive index. And, the relational formula of the phase change brought about by the change of refractive index is [28]

$$\Delta \phi = \frac{\pi}{\lambda} \Delta n_{eff} L,$$  \hfill (6)

So, the change of phase ($\Delta \phi$) is related to the change of refractive index $\Delta n_{eff}$ and length $L$ of the phase shifter. This shows that in addition to analyzing the carrier distribution of the phase shifter, the length of the phase shifter also needs to be considered.

### 3. Results and discussion

Figure 2(a) shows the carrier distribution when p type doping concentration is $4 \times 10^{17} \text{cm}^{-3}$, n type doping concentration is $1 \times 10^{18} \text{cm}^{-3}$, and the loading voltage is 0 V. As shown in Figure 2(a), the red area is the distribution of electrons, and the blue area is the distribution of holes.
It can be seen from Figure 2(a) that when no voltage is applied, the internal carrier distribution is relatively uniform, and only the built-in electric field generated by the diffusion movement of the carriers is contained in the internal carriers. From Figure 2(b), we can see that the light is well confined inside the waveguide. Moreover, no matter if 8 V reverse voltage or –8 V forward voltage is applied, the electric field strength is the same as when no voltage is applied, that is, the light is well confined in the waveguide, so we will not show it in the follow-up. And, Figure 2(c) depicts the carrier distribution inside the waveguide marked with length a in Figure 2(a), the distribution of carriers inside the waveguide is more consistent with our presets. It can be seen from Figure 2(c) that between 6.5 and 7.5 μm, electrons and holes will mutually diffuse each other due to the concentration gradient, and the electrons migration rate is faster than the hole migration rate, so the carrier concentration has a significant decline process. And between 7.5 and 9 μm, the p-type and n-type regions will form a built-in electric field due to the mutual diffusion of the concentration gradient, and the existence of the built-in electric field will cause the carriers to drift in the opposite direction. When these two movements reach an equilibrium, a stable charge distribution region with neither electrons nor holes will be formed, so the carrier concentration has an equilibrium stage. Under this carrier distribution condition, the refractive index inside the waveguide is shown in Figure 2(d). From Figure 2(d), it can be seen that the refractive index of the p-type region is significantly reduced, the refractive index of the n-type region is slightly reduced. This is because the change in the refractive index is related to the carrier concentration and the relationship is formula (2). Due to the high carrier concentration on both sides and the low concentration in the middle, the refractive index changes on both sides are relatively large. And due to the low carrier concentration between 8 and 9 μm, especially the depletion layer is formed between 7.5 and 9 μm, the refractive index is close to that of intrinsic diamond.

Figure 3 shows the distribution of lateral carrier concentration and refractive index after a reverse voltage of 8 V is applied, that is, a voltage of 8 V is applied to the n-pole. From Figure 3(a), it is observed that the carrier concentration in the middle depletion zone has changed greatly, especially in the equilibrium stage. This can be clearly seen from the logarithmic distribution of electron concentration in the illustration. And Figure 3(b) shows the refractive index distribution inside the waveguide both when 8 V and no voltage is applied. It can be seen from the figure that after the carrier concentration is changed, the refractive index distribution is basically similar to that when no voltage is applied, except that there are certain changes in the two regions, which are represented by the dashed region 1 and the dashed region 2 in the figure. The magnified two regions are shown in Figure 3(c,d), respectively. It can be found in Figure 3(c) that the real part of the refractive index of the waveguide in the area of the dashed region 1 is $R_1^0 = 2.400232$ and the imaginary part is $I_1^0 = 7.903 \times 10^{-5}$ when no voltage is applied. The change in the real part of the refractive index after applying a voltage of 8 V is $R_1^1 = 2.400248$, and the imaginary part is $I_1^1 = 7.901 \times 10^{-5}$. However, the real part of the

![Figure 2](image_url)

Figure 2. (a) The logarithmic distribution of electron-hole concentration when $V=0$ V, where the red region represents the distribution of the logarithm of the electron concentration, and the blue region represents the distribution of the logarithm of the hole concentration; (b) electric field intensity distribution when $V=0$ V; (c) lateral carrier concentration distribution inside the waveguide marked with length a in (a); and (d) the distribution of refractive index inside the phase shifter when no bias is applied.
refractive index in Figure 3(d) is $R_2 (\text{neff}) = 2.381171$ and the imaginary part is $I_2 (\text{neff}) = 1.835 \times 10^{-5}$ when no voltage is applied. And the changes in the dashed region 2 after applying 8 V reverse voltage are $R_2 (\text{neff}) = 2.381183$ and $I_2 (\text{neff}) = 1.831 \times 10^{-5}$. Therefore, the effective refractive index change inside the waveguide is $\Delta R_1 (\text{neff}) = 1.6 \times 10^{-5}$, $\Delta I_1 (\text{neff}) = 2 \times 10^{-8}$, $\Delta R_2 (\text{neff}) = 1.2 \times 10^{-5}$, and $\Delta I_2 (\text{neff}) = 4 \times 10^{-8}$. So, we can find that the largest refractive index change region is in the region 1, and we use the refractive index of the region 1 to calculate the length of the phase shifter. Thus, according to formula (6), it can be calculated,

$$
\Delta \phi = \frac{\pi}{\lambda} \Delta \text{neff} = \frac{\pi}{\lambda} \left( \Delta R \times 10^{-5} \right) \quad (7)
$$

where $\Delta \phi$ is the phase change, $\Delta \text{neff}$ is the change in the real part of the effective refractive index, $L$ is the length of the phase shifter, and $\lambda$ is the wavelength of light, here we use 7.7 $\mu$m to calculate.

Then, in the case of a reverse bias voltage of 8 V, the required length of the phase shifter for $\pi$ phase shift is $L = 241$ mm. In addition, the change of the imaginary part of the refractive index inside the waveguide will also increase the additional loss. The relationship is where $\text{Ki}$ is loss, $k_0$ is the vacuum propagation constant, $k_0 = 2\pi/\lambda$, and $\Delta I (\text{neff})$ is the change in an imaginary part of the effective refractive index, so according to the formula, the loss can be calculated to be 0.023 dB/cm, and the loss change is 0.56 dB. This means that a longer phase shifter is required when applying a reverse voltage of 8 V, and the loss is relatively large.

Moreover, we also studied the application of forward voltage to change the internal carrier situation to achieve the purpose of phase shift. Figure 4(a) shows the carrier distribution inside the waveguide after a forward voltage of $-8$ V is applied. No voltage is applied to the left, and the electron distribution changes significantly after applying a voltage of $-8$ V to the n-doped terminal on the right. After electrification, the electrons on the left side are transferred to the right side, so that the hole carrier concentration at the right end decreases, while the electron concentration increases. Compared with applying a reverse voltage, applying a forward voltage causes a more significant change in the carrier concentration. The carrier concentration has dropped significantly, especially there are two equilibrium stages between 7.5 and 9.5 $\mu$m.

The refractive index changes after the redistribution of carriers is shown in Figure 4(b). The area where the refractive index has changed is marked with the dashed region 1 and the dashed region 2, and is enlarged and reflected in Figure 4(c,d). It can be seen from Figure 4(c,d) that when a voltage of $-8$ V is applied, the change in the real part of the refractive index is $\Delta R_1 (\text{neff}) = 3.2 \times 10^{-4}$, $\Delta R_2 (\text{neff}) = 2.5 \times 10^{-5}$ and the imaginary part is $\Delta I_1 (\text{neff}) = 6 \times 10^{-6}$, $\Delta I_2 (\text{neff}) = 5 \times 10^{-8}$. Therefore, according to formula (6), to realize the movement of $\pi$ phase, the length of the phase shifter needs to be at least $L = 12.03$ mm. Compared with applying a reverse voltage, applying a forward voltage has a more obvious phase shift effect. In an optical waveguide, a high doping
concentration will increase the extinction coefficient. That is, the imaginary part of the complex refractive index, which will increase the signal loss inside the phase shifter, and its inhomogeneity will also affect the phase shifting effect of the waveguide. Compared with silicon-based phase shifters, for example, in [9], the length of the phase shifter required to achieve π-phase shifter is longer than that of silicon-based phase shifter when the reverse voltage is applied, but the loss is much smaller. However, we cannot compare with silicon-based phase shifter when applying forward voltage, because most of the p–n-type silicon-based phase shifters reported in the literature were applied reverse voltage, so they cannot be compared. The diamond phase shifter is still in the preliminary exploration stage, and the phase shifting efficiency needs to be further improved.

In order to optimize the phase shift effect of the waveguide phase shifter, the internal carrier distribution is optimized. The second and the third groups changed the p-type doping concentration; the fourth and the fifth groups changed the n-type doping concentration. The changes in the internal refractive index were analyzed and compared, and the appropriate internal doping concentration was selected.

Figure 5 shows the refractive index changes obtained by calculation for each group. As shown in Figure 5(a–c), when the p-type doping concentration is reduced to $1 \times 10^{17}$ cm$^{-3}$, compared with the region 2, the refractive index of the region 1 inside the waveguide is significantly increased by about $1.8 \times 10^{-5}$, while when the p-type doping concentration drops to $8 \times 10^{16}$ cm$^{-3}$, the refractive index is higher than the concentration of $1 \times 10^{17}$ cm$^{-3}$, but the difference is very small, only about $5.28 \times 10^{-6}$. The reason why the refractive index will increase significantly is that the hole carrier migration rate is lower than the electron migration rate. Therefore, when the p-type doping concentration decreases, the number of holes decreases. At this time, hole carriers dominate. After a forward voltage is applied, the ratio of the total proportion of electrons and holes occupied increases, so the refractive index increases. However, it can be seen from Figure 5(c) that when the refractive index rises to a certain level, the refractive index cannot continue to rise, but has a certain decline. At this time, a large part of the hole carriers is occupied by electrons. Occupation, due to the reduction of holes, the degree of carrier change is reduced, so the degree of change begins to decrease. For electron carriers, because of their higher migration rate, the impact is small. This also explains very well that when the n-type doping concentration is changed in Figure 5(b,d,f), the refractive index of the waveguide only changes by $4.3 \times 10^{-6}$. Nevertheless, a high doping concentration will cause an increase in the absorption rate of the waveguide. Therefore, the n-type doping concentration can be appropriately reduced while ensuring a high-efficiency change in refractive index. According to the experimental results shown in the figure above, the optimal doping concentration of n-type is finally determined to be $4 \times 10^{17}$ cm$^{-3}$.

4. Conclusion

In summary, we have carried out simulation design and optimization of the diamond mid-infrared phase shifter through theoretical design. The calculations demonstrate that when p-type doping concentration is $4 \times 10^{17}$ cm$^{-3}$
and n-type doping concentration is $1 \times 10^{18} \text{ cm}^{-3}$, the applied reverse voltage can only change the refractive index of $1.6 \times 10^{-5}$. The required phase shifter length is about 241 mm to realize $\pi$ phase shift. After a forward voltage is applied, the maximum refractive index can be changed reaching to $3.2 \times 10^{-4}$, and the length of the phase shifter is 12.03 mm. Compared with the reverse voltage, the forward voltage has a higher phase shift efficiency, but the refractive index distribution is not uniform. By optimizing the doping concentration inside the waveguide, the refractive index distribution becomes more uniform. The optimized doping concentration parameters are p-type $1 \times 10^{17} \text{ cm}^{-3}$ and n-type $4 \times 10^{17} \text{ cm}^{-3}$, respectively.

**Disclosure statement**

No potential conflict of interest was reported by the authors.

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**Figure 5.** (a) The second and the third sets of doping concentration lateral refractive index distribution; (b) the fourth and the fifth sets of doping concentration lateral refractive index distribution; (c) the second and the third sets of region 1 refractive index profile; (d) the fourth and the fifth groups of region 1 refractive index distribution; (e) the second and the third groups of region 2 refractive index distribution; and (f) the fourth and the fifth groups of region 2 refractive index distribution.
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