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976nm symmetrical one-dimensional photonic crystals enhance black phosphorus absorption

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Abstract: *In this paper, a one-dimensional photonic crystal with a defective layer is designed, and the single-layer BP is embedded in the CeO_2 and SiO_2 structure of the one-dimensional photonic crystal, and the electric field distribution and magnetic field distribution in the one-dimensional photonic crystal are studied. The electric field intensity distribution at the defect layer of the one-dimensional photonic crystal is significantly enhanced. The magnetic field strength of the upper and lower layers of the defect layer is enhanced cons. Changes in the wavelength of incident light affect the absorption rate of one-dimensional photonic crystals. When the wavelength of incident light is 976 nm, the absorption rate of one-dimensional photonic crystals is robust. The absorption rate change of a 976 nm symmetrical one-dimensional photonic crystal was studied by changing its incidence angle based on its wavelength. Numerical simulation results show that the absorption rate of one-dimensional photonic crystals can be controlled by adjusting the wavelength of the incident light and can also be actively controlled by adjusting the angle of incidence, which increases the channel of interaction between light and matter. The one-dimensional photonic crystal containing the defective layer has a maximum absorption rate of 56.65% at a wavelength of 976 nm and an incidence angle of 0°. This simple sheet structure can be applied to various optical devices, such as ultra-fast light switches, solar cells, and other fields.*

Keywords: *One-dimensional photonic crystal, electric field distribution, magnetic field distribution, absorption rate, nonlinearity*

1. Introduction

Since the first discovery of graphene, its excellent electrical and optical properties have attracted widespread attention. Because of its wideband absorption and high carrier mobility, graphene has attracted much attention in the field of ultrafast fiber lasers. Grzegorz et al. made a composite film using thin layers of graphene and PMMA, applied them to annular cavity-doped erbium fiber lasers, and achieved an ultra-short pulse output of 406 fs at 1561.5 nm.[1] [1] With the development of material preparation technology, such as mechanical peeling technology, CVT technology, CVD technology, and hydrothermal technology, a variety of new two-dimensional materials with excellent photoelectric properties have emerged, which have shown many excellent photoelectric properties that traditional semiconductors do not have due to the quantum limitations of the longitudinal scale, which significant attracts the interest of optoelectronic devices based on two-dimensional materials. However, the optical path of the thickness at the atomic layer level limits the light absorption of the two-dimensional material, which is a crucial factor in the low response rate of the photoelectric devices of the intrinsic two-dimensional material. In recent years, the interaction between light and matter has been regulated by micro-nano photonic structure, thereby enhancing the absorption of two-dimensional materials, which is becoming a new development trend to improve the performance of two-dimensional material optoelectronic devices.

As an essential member of the two-dimensional material family, black phosphorus has received widespread attention with its two-dimensional layered structure similar to graphene. Its layers interact with each other through weak van der Waals forces. Therefore, thin layers of black phosphorus can be obtained through low-cost processes like mechanical peeling. Zhang et al. used this peeling technique to budget nm of black phosphorus. They prepared a field-effect transistor based on this thin layer with carrier mobility f up to $1000cm^2V^{-1}S^{-1}$[1] [2] With the continuous optimization of the preparation process of black phosphorus, it has been widely used in the fields of light energy storage and biological

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sensing.[1] [3] Recently, Liu et al. prepared a BP/PMMA composite film and applied it as a saturable absorber to a 1.5 micron Q fiber laser, achieving a single pulse energy of the most significant pulse energy known. [1] [4] This energy is at leasttwo2 orders of magnitude lower than the single pulse energy of a pulsed solid-state laser. This is because PMMA films are organic polymer films, so the ability to withstand high power is minimal; when the pump power increases, the film will be burned due to poor heat dissipation capacity, limiting the peak power of black phosphorus pulsed fiber lasers.

The photon crystal structure has received widespread attention for its precise manipulation of electromagnetic waves. Because the materials it composes (such as SiO_2, HfO_2, CeO_2, etc.) have ultra-high damage resistance thresholds, it is applied to ultrafast fiber lasers. It may become a potential solution to improve the damage resistance threshold of saturable absorbers. Periodic photonic crystals produce an energy band structure like a semiconductor, which selectively controls the propagation of electromagnetic waves. In nature, photonic crystals come in the form of structural coloring and animal reflectors, and in different forms, they are expected to be helpful in a range of applications. The one-dimensional photonic crystal structure is a microstructure in which dielectric constants are distributed periodically in one dimension in space. Its main feature is that light waves of specific frequencies are suppressed during propagation, forming photon band gaps. One-dimensional photonic crystals can be made by layers deposited or adhered together.

This paper uses BP's unique optical properties to design a one-dimensional defect photonic crystal. Precisely, the refractive index curve and extinction coefficient curve of BP is calculated based on first principles. The one-dimensional photonic crystal of symmetrical defective layer (BP) is established in the finite element simulation software Comsol. The optical characteristics of the photonic crystal of the one-dimensional inferior layer are studied, as well as the electric field distribution and magnetic field distribution inside the photonic crystal, which provides a theoretical basis for the preparation of related optical devices.

2. Model and calculation results

2.1. First-principles computation of BP

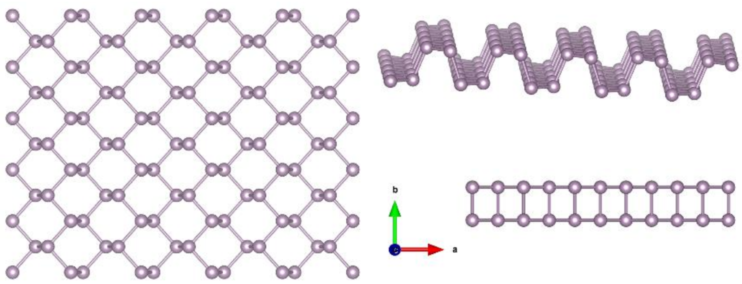

Figure 1: Schematic diagram of black phosphorus (5×5 supercell) in different axes

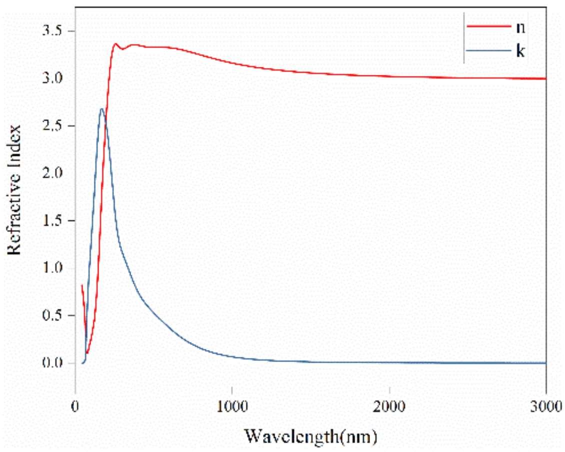

Figure 2: Refractive index coefficient curve and extinction coefficient curve of BP

The crystal structure of black phosphorus mainly consists of simple cubes, oblique and orthogonal. Among them, the black phosphorus of the orthogonal design has been widely studied for its good

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photoelectric effect. The structure of the orthogonal monolayer of black phosphorus is shown in Figure 1. It is arranged in a folded arrangement in the x-direction and contains two atomic layers and two p-p bonds. The short bond connects two P atoms in the same plane, and the long bond connects the two P phosphorus atoms in the z-direction. This article obtained BP unit-cell through the Materials Project and single-layer BP using VESTA. In this paper, the single-layer BP is optimized using the Cambridge Sequential Total Energy Package (CASTEP) module in the First Principles computing software Materials studio, using ultra-soft pseudo-potential processing core electrons, the valence electron configuration is: P-$3s^2$ $3p^3$, and the exchange-correlation between valence electrons uses a generalized gradient approximate generalized gradient The PBE functional in approximation (GGA) is processed, and the highly symmetric k-point is selected to integrate the Brillouin region. The k-point grid is set to 4×1×3, the fast Fourier transform mesh is set to 20×64×27, and the plane wave c truncation energy in the calculation E_{cut}=300 eV, the minimization algorithm is Two-Point Steepest Descent (TPSD), The convergence criteria are: the total energy change on each atom is more minor than 5.0×10^{-6} eV, the maximum stress is 0.02 GPa, the inter-atom interaction force is less than 1×10^{-2} eV/Å, and the atomic displacement is more minor than 5×10^{-4} Å. According to the optimized crystal structure, the refractive index coefficient curve and extinction coefficient curve of BP is calculated, as shown in Figure 2. It is not difficult to find that the refractive index of BP reaches its maximum value at 253 nm.

2.2. Comsol simulates a 976nm symmetrical one-dimensional photonic crystal

The structural model of the one-dimensional photonic crystal composed of CeO_2 and SiO_2 is shown in Figure 3, where the blue part is CeO_2, the purple part is the SiO_2, and the black line is BP. There are 6 cycles on each side of the BP. This article sets the CeO_2 width W_0, thickness d_1, refractive index n_1= 2.2, SiO_2 width W_0, thickness d_2, refractive index n_2 = 1.458. According to the formula of photonic crystals are:

$$2n_2d_2 = \lambda/2$$

$$n_1d_1 + n_2d_2 = \lambda/2$$

$$n_1 sin\theta_1 = n_2 sin\theta_2$$

Therefore, for the wavelength λ = 976 nm, the refractive index $n_2 = 1.458$the thickness of the SiO_2 can be found d_2=168.04 nm; Then according to the refractive index of $n_1d_1 + n_2d_2 = \lambda/2$, the refractive index n_1 of the CeO_2 is 2.2, the thickness of the CeO_2 can be found d_1=111.36 nm. Subsequently, according to the different angles of incidence, the refraction angle can be further solved by $n_1 sin\theta_1 = n_2 sin\theta_2$.

Therefore, for the 976 nm center wavelength studied in this paper, there are d_1=111.36 nm and d_2=168.04 nm. The width of the substrate SiO_2 remains consistent with the width of the superstructure, that is, theW_0, and the thickness d_0 = 1 μm. Since single-layer black phosphorus is almost negligible compared to CeO_2 and SiO_2, to reduce the number of meshes, this article sets BP to surface current. Periodic condition 1 satisfies equation $E_{dst} = E_{src}e^{-ik_F\cdot(r_{dst}-r_{src})}$, $H_{dst} = H_{src}e^{-ik_F\cdot(r_{dst}-r_{src})}$; Periodic condition 2 satisfies the equation $E_{dst} = E_{src}e^{-ik_F\cdot(r_{dst}-r_{src})}$, $H_{dst} = H_{src}e^{-ik_F\cdot(r_{dst}-r_{src})}$.

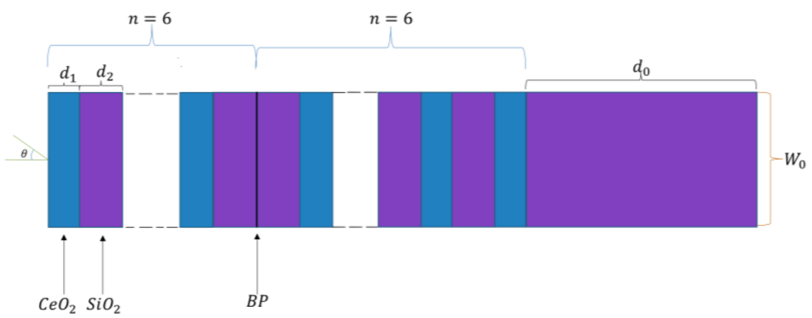

Figure 3: One-dimensional photonic crystal model

The first parametric sweep is performed for the established model to obtain the wavelength of light corresponding to the highest absorption rate. The scan results are shown in Figure 4. It can be seen from the figure that in the visible and near-infrared spectral ranges, the transmittance of one-dimensional photonic crystals containing the black phosphorus defect layer is greater than 80%. For this one-dimensional photonic crystal structure, the reflectance will mutate between 760 nm and 976 nm, and the reflectance of the one-dimensional photonic crystal at 760 nm is about 60%. The transmittance is close to 40%. This is mainly due to the periodic effect of this photonic crystal structure, so it produces similar transmission and reflection effects at a fixed wavelength near the center wavelength. Similarly, at 840 nm, as the wavelength of the incident light increases, the reflectance and transmittance of one-dimensional photonic crystals change exponentially. At the central wavelength of 976 nm studied in this paper, the absorption rate of one-dimensional photonic crystals reached its maximum. Since one-dimensional s crystals transmit the one-dimensional photonic crystals designed in this paper, their transmittance also reaches a maximum value of 976 nm. According to the relationship between transmittance, reflectivity, and absorption rate, we can judge that the reflectivity reaches the minimum value, which helps the one-dimensional photonic crystal be applied to annular cavity transmission fiber lasers. Figure 4. shows that the absorption rate of one-dimensional photonic crystals is as high as 56.65%. Compared with the absorption rate of 7.1% of monolayer black phosphorus, this structure significantly enhances the absorption efficiency of black phosphorus.

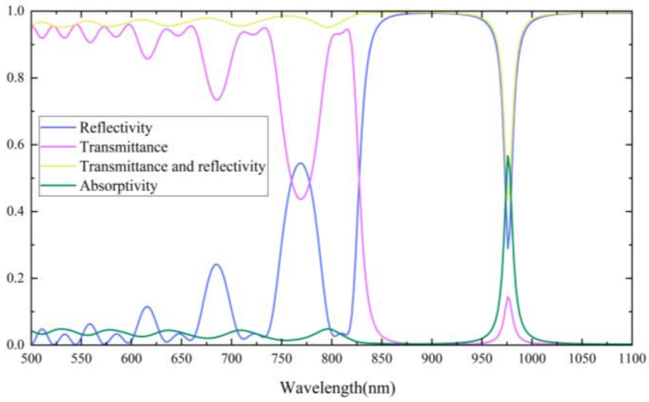

Figure 4: The relationship between absorption rate and wavelength in one-dimensional photonic crystals

Further, this paper analyzes the relationship between the wavelength of incident light and the angle of incidence and absorption rate. The parametric sweep wavelength range is set to 965-985 nm, and the rise of incidence range is set to $(0°, 30°)$. The final scanned 2D drawing surface is shown in Figure 5. It is not difficult to find from the figure that as the θ increases, the most vital absorption position of the one-dimensional photonic crystals emits a blue shift. It is easy to understand from the phase conditions of one-dimensional photonic crystal resonance that it keeps the phase shift of $\delta = 2\pi\theta/\lambda$ unchanged. The resonance wavelength must be blue shifted. At the same time, with the increase of the incident wavelength, the absorption of one-dimensional photonic crystals increased first, then decreased, reaching a maximum value at 976 nm designed in this paper, which further confirmed the rationality of the structure created in this paper. In addition, in the large extensive range of $0°$ to $30°$, the wavelength change of incident light has a more significant impact on the absorption rate of one-dimensional photonic crystals, and the incident light angle will also have an impact on the absorption rate of one-dimensional photonic crystals, and the effect is most evident in the range of 0°-10°.

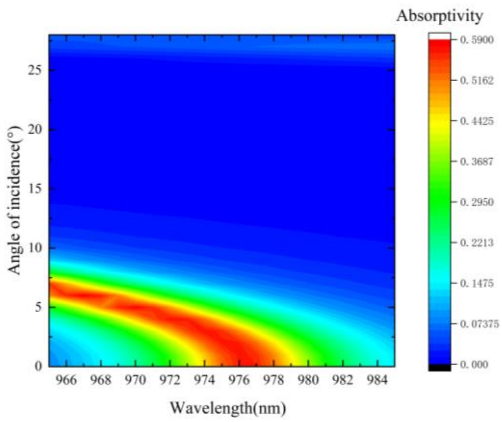

Figure 5: Relationship between the wavelength of incident light and the angle of incidence and absorption rate

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In order to determine the root cause of BP absorption enhancement, this paper plots the electric field intensity with a position change curve. The corresponding result is shown in Figure 6(a). The internal electric field intensity of the photonic crystal fluctuates with the increase of arc length; the overall trend first increases and then weakens and tends to zero. There is a maximum electric field intensity at about 1.7 microns of arc length, that is, the location of the defect layer. This paper analyzes the electric field distribution at different locations inside the photonic crystal under 976 nm illumination, and the corresponding results are shown in Figure 6(b). The yellow part of the figure is the location of the defect layer, and the electric field mode distribution can be observed from the constitution; the electric field intensity reaches the maximum at the site of the defect layer, and there is almost no electric field distribution at the bottom of the one-dimensional photonic crystal. At the defect layer location, the interaction between light and matter is significantly enhanced, which in turn causes a significant increase in BP absorption rate.

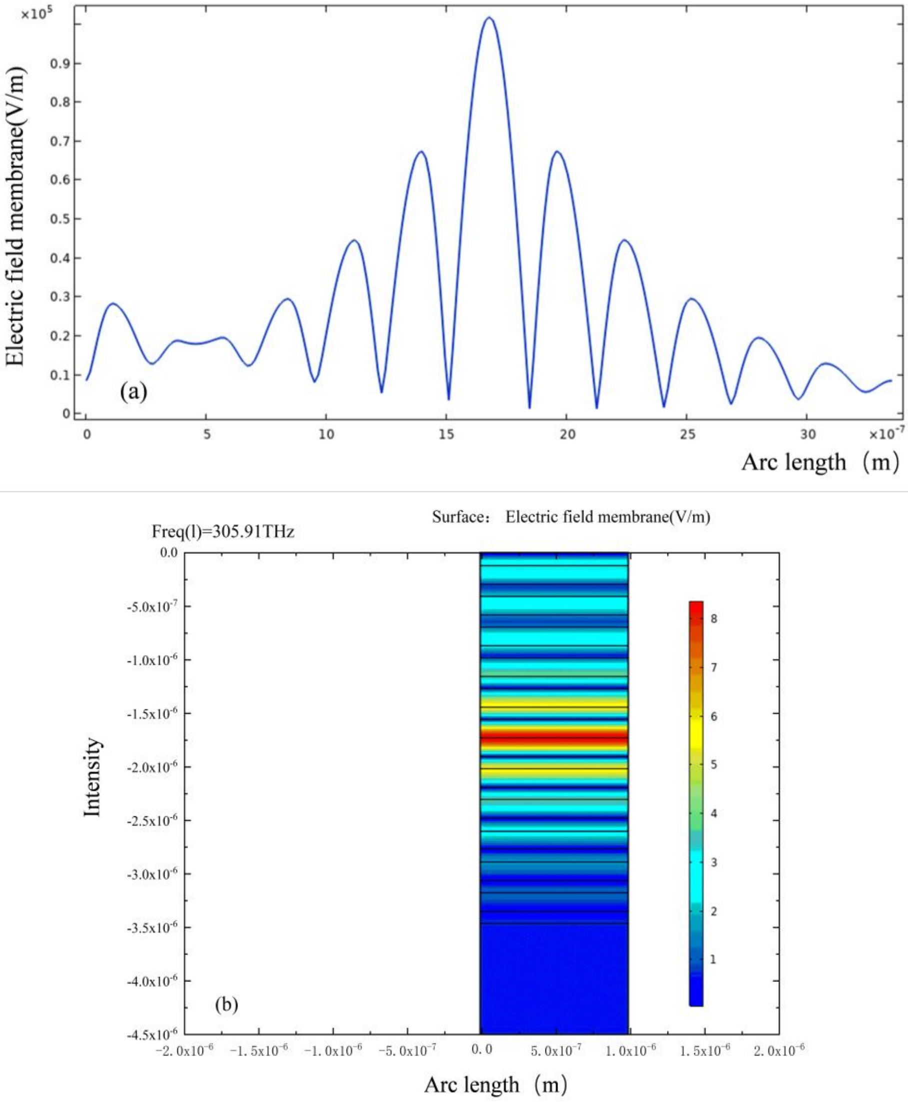

Figure 6: (a) Curve of electric field strength with position, (b) Distribution of electric fields inside photonic crystals

After analyzing the electric field intensity, the distribution of magnetic field strength in one-dimensional photonic crystals is further explored, as shown in Figure 7. The center of the two red lines in the figure is the location of the defect layer, and the distribution of the magnetic field strength in the photon crystal can be observed, at this time, the magnetic field strength does not reach the maximum value at the defect layer, which is due to the magnetic field relative to the electric field. There is a phase delay, so the magnetic field strength on both sides of the defect layer is enhanced, and the magnetic field strength at the defect layer is minimal.

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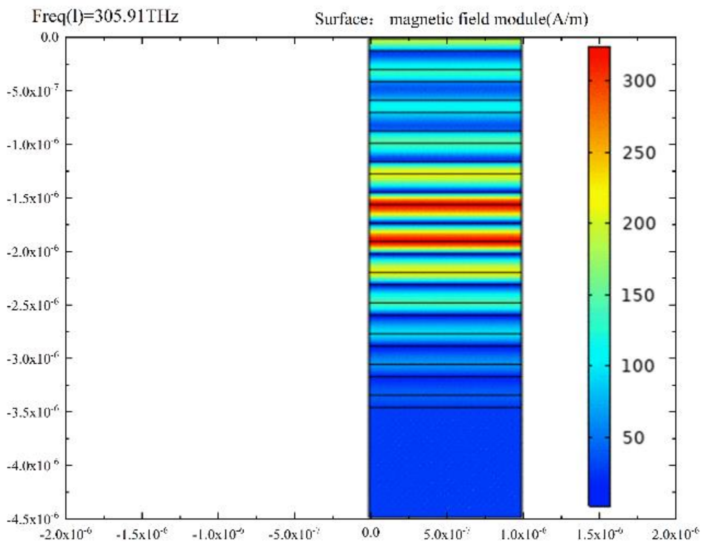

Figure 7: The distribution of magnetic fields inside photonic crystals

3. Conclusion

As the wavelength of light changes, the reflectivity, transmittance, and absorption rate of one-dimensional photonic crystals will also change accordingly. When the wavelength of light is 976 nm, the absorption rate of one-dimensional photonic crystals reaches the strongest, which meets the design requirements. As the angle of incident light increases, the absorption rate of one-dimensional photonic crystals shifts blue. At the same time, as the incident wavelength increases, the absorption of one-dimensional photonic crystals increases first and decreases until it disappears. And at an incident angle of 0° and an incident light wavelength of 976 nm, there is a maximum absorption rate of 56.65%, significantly higher than the 7.1% of monolayer black phosphorus. It shows that the one-dimensional photonic crystals we designed greatly enhance the absorption of BP. Among them, the wavelength change of incident light has a more significant impact on the absorption rate of one-dimensional photonic crystals. The angle of incident light also affects the absorption rate of one-dimensional photonic crystals. The result is most evident in the range of 0°-10°. Moreover, the curve of the change of electric field intensity with position is plotted to determine the overall distribution of electric field intensity in one-dimensional photonic crystals. In addition, the root cause of absorption enhancement is that the electric field is enhanced at the defect layer position and the magnetic field is weakened at the defect layer position. The one-dimensional photonic crystals designed in this paper can be widely used in other two-dimensional materials and have excellent application space.

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