Perovskite Hybrid Surface Plasmon Waveguide

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Abstract
A novel perovskite hybrid surface plasmon waveguide structure is designed. Its physical model is established, and its theoretical basis is introduced in detail. Based on the finite element method, the mode characteristics, quality factor, and gain threshold of the waveguide structure are analyzed with geometric parameters. The results show that the optical field constraint of the waveguide can reach a good deep sub-wavelength level under the optimal operating wavelength of 1550 nm. By adjusting the waveguide design parameters, the high-quality factor, low energy loss, low threshold limit, and ultra-small effective mode field area are obtained. Compared with the hybrid waveguide structure proposed in the current research results, this structure has stronger optical field limiting ability and microcavity binding ability. The waveguide structure can provide theoretical and technical support for the development of new efficient nanolaser devices and has a good application prospect.

Keywords Perovskite · Hybrid surface plasmonic waveguide · Finite element method · Mode characteristic · Quality factor

Introduction
With the rapid development of micro-nano technology, traditional electronic devices can not meet the requirements of high speed and high capacity of modern information technology. In this way, the advantages and applications of photonic devices have brought opportunities. However, due to the influence of light diffraction limit, the maximum radial size of traditional photonic devices is only in the order of wavelength, which makes it difficult to achieve miniaturization and high integration, and becomes the bottleneck of the development of integrated optics. The surface plasma polaritons [1] (SPPs) waveguides’ technologies have attracted extensive attention of many researchers. SPP is a surface electromagnetic wave mode generated by the interaction of external photons and free electrons on the metal surface. Because of its ability to control the diffraction, it can improve the characteristics of the laser. In the existing surface plasmon waveguide structures, the waveguide performance can not be perfected, and there is a certain contradiction between the characteristic parameters. For example, although the metal–insulator-metal [2, 3] waveguide has strong optical field limitation ability, its transmission loss is very large, resulting in a very small transmission distance. The long-range surface plasmonic waveguides [4] can achieve low-loss and long-distance optical propagation, but at the expense of the field limiting ability. The hybrid plasmonic waveguide (HPW) structures have been proposed and widely studied in order to achieve low transmission loss and strong optical field limitation [5–7].

In recent years, the hybrid surface plasmonic waveguides with various structures have been proposed one after another [8, 9]. Following Oulton’s proposal of a typical hybrid surface plasmonic waveguide [10], Lv et al. proposed a HPW structure consisting of a silver substrate, CdS nanowires, and MgF2 dielectric layer between them and analyzed the mode characteristics and gain threshold of the structure [8]. Zhu used air as a low refractive index medium to study the mode characteristics of the waveguide structure and explained the coupling mechanism between the SPP mode and nanowire waveguide mode [9]. Based on the above structures, Bian Y.S. proposed several hybrid surface plasmonic waveguide structures and applied them to fabricate sub-wavelength-constrained nanolasers [10], such as the coupled nanowire surface plasmonic lasers. Therefore, further study of this waveguide structures and give full play to its advantages are of great significance for realizing the miniaturization, integration, and high-speed of photonic devices.
In order to improve the mode confinement capability of HPW, reduce the transmission loss of the waveguide and optimize the transmission performance of the plasma waveguide, this paper introduces a two-dimensional material perovskite (CH$_3$NH$_3$PbI$_3$) into the hybrid waveguide structure.

The general structural formula of perovskite is ABX$_3$, where A is a large radius cation (such as Ca$^{2+}$ and Ba$^{2+}$), B is a small radius cation (such as Ti$^{4+}$ and Zr$^{4+}$), and X is a halogen anion (such as C$^-$, Br$^-$, and I$^-$). The perovskite structure is characterized by a tetrahedron with the A-site ion as the vertex, an octahedron with the B-site cation as the center, and X anion as the vertex. Its cubic crystal structure gives it special physical and chemical properties. CH$_3$NH$_3$PbI$_3$ is a typical ABX$_3$ structure. It has strong light absorption capacity, which is an important characteristic that should be possessed as a photovoltaic material. As a direct band gap semiconductor material, the optical absorption range of the composite perovskite material extends from the near-infrared region to the whole visible region and shows a high absorption coefficient ($> 10^5$ cm$^{-1}$).

Perovskite materials also have long carrier lifetime and diffusion length, showing good carrier transport characteristics. The exciton binding energy of the composite perovskite is only tens of millivolts, so it is easy to separate into holes and electrons to form free carriers. And electron–hole pairs are generated almost instantaneously under the excitation of light.

The CH$_3$NH$_3$PbI$_3$ crystal is a common light absorption layer material for perovskite solar cells. It has the advantages of narrow band gap, high extinction coefficient, and good light absorption capacity [11]. The dielectric loss of the CH$_3$NH$_3$PbI$_3$ crystal prepared in vacuum will increase with the increase of frequency due to its strong light absorption ability and easier carrier passage. And the CH$_3$NH$_3$PbI$_3$ crystal has a small dielectric constant, which indicates its good conductivity. This paper uses the characteristics of the CH$_3$NH$_3$PbI$_3$ crystal to propose a novel perovskite hybrid surface plasmonic waveguide structure and investigates the influence of its geometric parameters on the mode characteristics of the waveguide. The results show that the structure has excellent waveguide characteristics at the working wavelength of 1550 nm, such as ultra-low transmission loss, lower mode field area, and higher quality factor, which improves the comprehensive performance of the nanolaser.

**Physical Model Establishment and Theoretical Research**

**Design of Waveguide Structure**

The structure of the novel perovskite hybrid surface plasma waveguide is shown in Fig. 1. The structure is composed of triangular semiconductor waveguide Si, air layer Air, ring-shaped perovskite material (CH$_3$NH$_3$PbI$_3$), circular metal silver pillar Ag, and U-shaped substrate SiO$_2$ from bottom to top. Because Ag has the characteristics of low absorption coefficient and low transmission loss, Ag is chosen as the metal material in the structure. Si provides some gain. The thickness of SiO$_2$ is $h_2$, the thickness of perovskite is $h_1$, $h_1=0.5$ nm, and the radius of Ag is $r$. In the experimental production, in order to avoid non-zero radius fillets and singularities [12], the tip of the triangular waveguide is rounded, and the curvature radius of the tip corner is $r_m$. At the same time, the metal Ag and the vertex of the triangular gain medium are in the same vertical direction, which enhances the coupling between the mode fields. Between the perovskite layer and the semiconductor waveguide is an air layer with a width of $t$. The working wavelength of the structure is set to 1550 nm. The refractive index of Si, SiO$_2$, Ag, and CH$_3$NH$_3$PbI$_3$ are 3.455, 1.445, 0.1453 + 11.3587i, and 2.243 + 0.019i [13].

**Definition and Mathematical Expression of Characteristic Parameters**

The mode characteristic is an important index to reflect the characteristics of the hybrid surface plasmonic waveguide. The mode characteristics [14] studied in this paper include the concepts of the effective index ($n_{eff}$), normalized mode scaling factor ($SF$), confinement factor ($\Gamma$), gain threshold ($g_{th}$), and quality factor ($Q$).

The normalized effective mode area is the proportion of effective mode area $A_{eff}$ in diffraction limit mode area $A_0$. The relationship [15] is shown in Eq. (1):

$$A = A_{eff} / A_0$$

(1)

The expression of effective mode area $A_{eff}$ in Eq. (1) is as follows:
\[ A_{\text{eff}} = \left( \int |E|^2 \, dx \, dy \right) / \left( \int |E|^4 \, dx \, dy \right) \]  
\[ E \] is the electric field strength. The diffraction limit mode area \( A_0 \) is defined as
\[ A_0 = \lambda^2 / 4 \]  
The confinement factor \( \Gamma \) is defined as the ratio of the electric field energy in Si to the total energy of the mode waveguide [16], which is used to characterize the field strength limiting ability of the gain dielectric nanowires. The mode characteristics of the hybrid surface plasmon waveguide can be obtained by the finite element method.

The quality factor \( Q \) is used to evaluate the characteristics of the optical resonator in the laser. The higher the quality factor is, the lower the pumping value needed to excite the laser is, and the stronger the binding ability of the microcavity to photons is. The expression of quality factor \( Q \) [17] is
\[ Q = 2\pi f \frac{\epsilon}{P_\delta} \]  
\[ \epsilon = n_0 hfV \]  
\[ P_\delta = -\frac{d\delta}{dt} = -\frac{dn}{dt} \theta \cdot hfV = n_0 \frac{hfV}{\tau R} \]  
\[ Q = \frac{2\pi f \tau R}{\frac{L}{\delta \cdot c}} \]  
\( f \) is the frequency of the light field in the cavity, \( \epsilon \) is the total energy stored in the cavity, \( P_\delta \) is the energy lost in unit time, \( n_0 \) is the photon number density when \( t = 0 \), \( h \) is the Planck constant, \( V \) is the volume of the cavity, \( n \) is the

Fig. 2 Electric field distribution, (a), (b) normalized electric field distribution of the designed fundamental mode of the waveguide, (c), (d) denotes (a) normalized electric field distribution along horizontal and vertical dashed lines
photon number density in the cavity, \( r R \) is the time constant of the cavity, \( \delta \) is the cavity loss, and \( L \) is the length of the cavity. This article only considers the mirror loss of the resonator and ignores other losses of the resonator.

The gain threshold \( (g_{th}) \) is defined as the minimum gain required for laser to achieve lasing. If its value is smaller, the gain required for laser to achieve lasing is smaller. The gain threshold calculation formula \([18]\) is

\[
g_{th} = \left[ k_0 a_{eff} + n n(1/R)/L_1 \right]/\Gamma(n_{eff}/n_{wire}) \tag{8}
\]

Among them, \( L \) is the length of the resonator, \( L = 30 \mu\text{m} \), \( R \) is the reflectivity of the end face, \( R = (n_{eff} - 1)/(n_{eff} + 1) \). \( n_{wire} \) is the refractive index of the gain medium \( \text{Si} \), and \( n_{eff}/n_{wire} \) is the enhancement part of the mode effective refractive index. \( a_{eff} \) is the propagation loss of the pattern. In the analysis, only the case of uniform non-absorption is considered, and the internal absorption and scattering loss of the gain medium are ignored.

**Analysis of Propagation Characteristics of the Waveguides**

**Electric Field Distribution of Waveguide**

Based on the finite element method, the fundamental mode of waveguide structure is simulated and designed by using the modal analysis module of COMSOL Multiphysics \([19]\) simulation software, a normalized electric field distribution map of the fundamental mode of the structure \( (r_m = 20 \text{ nm}, t = 5 \text{ nm}, r = 50 \text{ nm}) \) can be obtained, as shown in Fig. 2a. As is apparent from Fig. 2, the electric field energy is mainly concentrated in the air gap between the perovskite layer and the semiconductor waveguide,
and a part of it penetrates into the graphene layer. Figure 2b, c corresponds to the normalized electric field distribution at the horizontal and vertical dashed lines in Fig. 2a, respectively. It can be seen from the figure that the electric field at the gap in both the horizontal and vertical directions is obvious. The enhancement is due to the fact that the SPP mode and the semiconductor waveguide mode are coupled to each other in the low refractive index dielectric layer, so that the low refractive index dielectric layer generates energy storage like a capacitor, thereby realizing energy confinement and highly localized enhancement effect, thereby achieving sub-wavelength constrained laser emission. The electric field of the excited SPP wave decays exponentially on the side of the interface and has a peak at the interface.

Influence of the Ag Metal Radius and Fillet Radius on Waveguide Characteristics

The changes of geometric parameters have a certain influence on the performance of the hybrid surface plasmonic waveguide. The best performance of the waveguide can be obtained by changing the geometric parameters. Firstly, the influence of metal radius \( r \) and fillet radius \( r_m \) on the mode characteristics of hybrid waveguide structure is studied. The width of air gap is fixed at \( t = 5 \) nm, and \( r = 40 \) nm, 50 nm, 60 nm, and 70 nm, respectively. The different characteristics of the structure are analyzed when the fillet radius \( r_m \) changes in the range of 2–40 nm. The simulation results are shown in Fig. 3.

As can be seen from Fig. 3, the radius of the metallic Ag has a great influence on the mode characteristics of the waveguide structures with different rounded radius. In Fig. 3a, b, with the increase of the fillet radius \( r_m \), the increase of the high index medium region results in the increase of the effective index of the mode. At this time, the light confined in the air layer begins to diffuse to both sides, resulting in the increase of transmission loss. With the increase of \( r \), the coupling between the mode field and the perovskite surface mode field in the high refractive index dielectric layer becomes smaller, and its normalized mode field area shows an increasing trend. As can be seen from Fig. 3c, with the continuous increase of \( r_m \), the locality of the field increases, and the area of the normalized mode field continues to decrease. Its value is always less than 0.0045, indicating that the structure can well achieve the deep sub-wavelength mode field limitation. When \( r_m = 40 \) nm and \( r = 40 \) nm, the minimum value is reached, and the effective mode field area is 0.0032. The increase of the limiting factor in Fig. 3d is mainly due to the increase of the overlap area between the metal and the gain medium.

Next, the change rule of gain threshold and figure of merit of the laser model is analyzed. Figure 4a, b shows the influence of gain threshold \( r \) and quality factor \( r_m \) of the laser model on the change of metal radius and fillet radius. It can be seen from Fig. 4a that as the radius of the metal increases, the quality factor increases. When \( r_m = 2 \) nm and \( r = 70 \) nm, the maximum quality factor is 1890.49. Due to the monotonically increased transmission loss, the gain threshold also shows an increasing trend. The minimum threshold of the structure designed in this paper can reach 0.0395. Compared with the ordinary waveguide structure, the gain threshold is reduced by an order of magnitude.

Influence of Air Gap Width \( t \) on Waveguide Characteristics

When \( r_m = 40 \) nm, a smaller normalized mode field area and a larger quality factor can be obtained. In order to further study the characteristics of the designed structure, the fixed fillet

![Fig. 4](image-url)
radius is 40 nm, and the main characteristics of the laser model are analyzed by changing the air gap $t$. It can be seen from Fig. 5 that as $t$ increases, the coupling between modes becomes weaker, and the effective refractive index and transmission loss have the same decreasing trend. Because the transmission loss and the normalized mode field area are a pair of contradictory physical quantities, the normalized mode field area is gradually increasing. However, its value is still very small, which can well achieve the deep sub-wavelength limitation of the light field.

Figure 6a, b shows the effect of gap width $t$ on the quality factor and gain threshold. From Fig. 6a, b, with the increase of $r$ and $t$, the quality factor is gradually increasing, but the gain threshold shows a decreasing trend. When $r = 70$ nm and $t = 2$ nm, the minimum gain threshold is 0.039.

Through the above simulation, the characteristic parameters, gain threshold, and quality factor of the waveguide are integrated. In order to improve the laser performance and realize the sub-wavelength constraint, the waveguide with $r_mS = 40$ nm, $t = 2$ nm, and $r = 70$ nm is selected to achieve the highest comprehensive performance. At this time, the transmission loss is 0.0024, the effective mode field area is 0.0014, the gain threshold is 0.039, and the quality factor is 1717.66. By introducing a layer of perovskite material in the hybrid surface plasmon waveguide, the waveguide structure has low transmission loss while maintaining the ability to confine the optical field. The reason is that the perovskite material has a large light absorption coefficient, and the absorption layer of a good optoelectronic device needs to have strong absorption in a wide spectral range, which can reduce material consumption and energy loss. In addition, the exciton binding energy of the perovskite material is relatively small, and the carrier mobility is relatively high. Based on these characteristics, the introduction of perovskite materials into the waveguide structure can greatly improve the performance of the waveguide.

Fig. 5 The trend of mode characteristics of hybrid surface plasmon waveguide with gap width $t$ and $r$
A novel perovskite hybrid surface plasmon waveguide is presented in this paper. Through simulation analysis, it has excellent waveguide characteristics at a communication wavelength of 1550 nm. Changing the parameters $r$, $r_m$, and $t$ of the waveguide to obtain the best structure of the waveguide is $r = 70$ nm, $r_m = 40$ nm, and $t = 2$ nm. The transmission loss at this time is 0.0024. Compared with other hybrid waveguide structures, the transmission loss is reduced by an order of magnitude. The effective mode area is 0.0014, so that the electromagnetic wave mode is tightly confined in the air between the semiconductor and the perovskite layer, realizing the sub-wavelength confinement of light. When this structure is applied to a laser, the laser performance is greatly improved, and the most appropriate waveguide characteristics can be obtained by adjusting the waveguide parameters. The gain threshold can reach 0.039, which greatly reduces the gain required by the laser to achieve lasing. The quality factor is 1717.66, and the ability of the microcavity to confine photons is 5 times that of the ordinary waveguide structure. These characteristics indicate that the perovskite hybrid surface plasmon waveguide structure proposed in this paper has great potential for high-performance waveguides in the sub-wavelength range and provides a certain theoretical basis and method for the development of a new generation of nanophotonic devices. With the development of micro nanofabrication technology, it is possible to realize all-optical integration in the future and then develop new micro-nanophotonic devices with small size, low power consumption, and high speed.

Author Contributions Wenchao Li, Jiawei Wu, and Xin Li contributed to the conception of the study; Wenchao Li, Jiawei Wu, and Zhiquan Li contributed significantly to analysis and manuscript preparation; Jiawei Wu performed the data analyses and wrote the manuscript.

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Data Availability The datasets used or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Consent to Participate Informed consent was obtained from all individual participants included in the study.

Consent for Publication The participant has consented to the submission of the case report to the journal.

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