Near-field Radiative Heat Transfer between Graphene Covered Biaxial Hyperbolic Materials

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Abstract

The plasmons in graphene and phonon polaritons in hyperbolic materials provide a new approach to mediate near-field radiative heat transfer (NFRHT). This work studies the NFRHT between graphene covered biaxial hyperbolic crystal α -MoO₃. The numerical results show that the coupling between plasmons in graphene and phonon polaritons in α -MoO₃ can greatly enhance the total heat flux. The spectral heat flux in the Reststrahlen bands can be suppressed or enhanced, depending on the value of the chemical potential of the graphene. What is perhaps most important here is that it is found that the surface plasmon-phonon polaritons can either enhance or suppress the heat transfer, which has not been reported in previous studies. The findings in this work can deepen our understanding of the coupling between the graphene plasmons and the phonon polaritons in the hyperbolic materials.

Keywords: Near-field radiative heat transfer; Graphene plasmons; Phonon polaritons; Hyperbolic materials.

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1. Introduction

Radiative heat transfer is a fundamental way of heat transfer, and plays an important role in the wide range of applications from energy collection to thermal management.^[1,2] When the separation distance between two objects is large (i.e. far-field region), only propagating waves contribute to heat transfer, and the maximum radiative heat transfer between two objects is determined by the black-body limit governed by the well-known Stefan-Boltzmann law. When two objects are at a distance comparable to or shorter than the characterized thermal radiation wavelength (i.e., near-field regime), both propagating waves and evanescent waves can contribute to the heat transfer. The evanescent waves of two objects can be coupled to provide a path for photons to tunnel through the gap, which is called photon tunneling.^[3,4] The evanescent waves produce more tunneling photons than that of propagating waves. As a result, the near-field radiative heat transfer (NFRHT) can significantly exceed the black-body limit.^[5-10] It has been demonstrated that the enhanced heat flux of NFRHT has potential applications in thermophotovoltaics,^[11-14] thermal rectification,^[15,16] noncontact refrigeration,^[17,18] thermal transistors,^[19] and so on. Therefore, it is of great significant to study NFRHT.

It has been demonstrated that surface polaritons, such as surface plasmon polaritons (SPPs) of metallic surfaces, or surface phonon polaritons (SPhPs) of polar dielectric materials, can mediate photon tunneling.^[20-30] Recent years, the studies of hyperbolic metamaterials show that NFRHT can be greatly enhanced over a broad frequency region via exciting hyperbolic phonon polaritons (HPPs).^[30-40] However, most of the hyperbolic metamaterials studied previously are artificial structures constructed with periodically stacked subwavelength metallic and dielectric layers. The hyperbolic property is no longer maintained when the tangential wave vector component is greater than π/Λ (Λ is the unit period of metamaterial).^[40] For natural uniaxial hyperbolic materials, such as hexagonal boron nitride (hBN), this limitation can be ignored because the lattice constant is on the order of sub-nanometer,^[41,42] thereby the natural hyperbolic materials have unique advantages. As a natural biaxial hyperbolic crystal, α -MoO₃ has wider hyperbolic bands.^[43,44] It has been proved that the NFRHT of two semi-infinite α -MoO₃ crystals is much larger than that of two semi-infinite hBN crystals due to the excitation of hyperbolic volume phonon polaritons (HVPPs) and hyperbolic surface phonon polaritons (HSPPs).^[45] However, the research on NFRHT between α -MoO₃ has not yet been exploited, and it deserves further study.

As a two-dimensional (2D) material, graphene can support a large number of resonances to promote photon tunneling.^[46-50] In recent years, due to its excellent electronic and optical properties, graphene has attracted extensive attention. It has

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been suggested that graphene plasmons could couple with other plasmons and phonon polaritons, leading to a further mediation of NFRHT.^[11,51-60] Particularly, Zhao and Zhang have shown that the surface plasmons in graphene could couple with the phonon polaritons in hBN films to form both surface plasmon-phonon polaritons (SPPPs) and hyperbolic plasmon-phonon polaritons (HPPPs), while the former could enhance the photon tunneling and the later could suppress the photon tunneling.^[61] The difference between SPPPs and HPPPs is that the later preserves the hyperbolic-waveguide-mode features.^[61] As far as we know, the coupling mechanism between phonon polaritons in α -MoO₃ and plasmons in graphene is not clear. Both graphene and α -MoO₃ exhibit excellent performance in NFRHT, but the combination of them has not been studied yet. Therefore, it is imperative to investigate the influence of graphene on α -MoO₃ regarding NFRHT.

In this work, we studied the NFRHT between biaxial hyperbolic crystal covered with graphene. The numerical results show that the coupling of surface plasmon polaritons in graphene and phonon polaritons in α -MoO₃ can greatly enhance the NFRHT. The spectral heat flux in the Reststrahlen bands can be suppressed or enhanced, depending on the value of the chemical potential of the graphene. It is found that the HPPPs always suppress the heat transfer, while the SPPPs can enhance or suppress the heat transfer. We believe that our work helps to understand the interaction between graphene and biaxial hyperbolic materials.

2. Theory and methods

Fig. 1 Schematic of the near-field radiative heat transfer between bulk α -MoO₃ covered with graphene.

In this paper, we study the NFRHT between bulk α -MoO₃ covered with graphene, as shown schematically in Fig. 1, where the vacuum gap is d . The temperatures of the emitter and the receiver are T_1 and T_2 , respectively. In the mid-infrared and far-infrared, the conductivity of graphene can be approximately written by Equation (1):

$$\sigma_s = \frac{e^2 \mu}{\pi \hbar^2} \frac{\tau}{1 - j\omega\tau} \quad (1)$$

where e is the elementary charge, $\hbar$ is the reduced Planck constant, ω is the angular frequency, τ is the relaxation time, and μ is the chemical potential. Here, $\tau = 10^{-13}$ s is chosen for all the calculations. In the calculation, the graphene can be

treated as a layer of thickness ($\Delta = 0.3$ nm) with an effective permittivity $\epsilon_{eff} = 1 + \frac{j\sigma_s}{\epsilon_0 \omega \Delta}$.^[61]

Fig. 2 The real parts of three permittivity components of α -MoO₃.

The α -MoO₃ is a natural biaxial hyperbolic material, whose permittivity tensor can be expressed as $\text{diag}(\epsilon_x, \epsilon_y, \epsilon_z)$. The explicit expression of ϵ_x , ϵ_y , and ϵ_z can be found in literature.^[45] The whole Reststrahlen band, covering from 1.03×10^{14} to 1.89×10^{14} rad/s, can be divided into five bands according to the signs of three permittivity components, as shown in Fig. 2. There is $\epsilon_y < 0$ from 1.03×10^{14} to 1.55×10^{14} rad/s, $\epsilon_x < 0$ and $\epsilon_y < 0$ from 1.55×10^{14} to 1.60×10^{14} rad/s, $\epsilon_x < 0$ from 1.60×10^{14} to 1.81×10^{14} rad/s, $\epsilon_x < 0$ and $\epsilon_z < 0$ from 1.81×10^{14} to 1.83×10^{14} rad/s, $\epsilon_z < 0$ from 1.83×10^{14} to 1.89×10^{14} rad/s. The HPPPs and SPPPs are possible to be excited in the whole Reststrahlen band.

Based on the fluctuation-dissipation theorem and the reciprocity of the dyadic Green's function, the NFRHT between media 1 and 2 can be expressed as

$$q = \frac{1}{4\pi^2} \int_0^\infty [\Theta(\omega, T_1) - \Theta(\omega, T_2)] d\omega \int_0^\infty \xi(\omega, \beta) \beta d\beta \quad (2)$$

where $\Theta(\omega, T)$ is the mean energy of a Planck oscillator, β is the parallel wavevector component. $\xi(\omega, \beta)$ is called the photon tunneling probability or energy transmission coefficient, whose explicit expression can be found in literature.^[45] The energy transmission coefficient can be obtained by solving the reflection and transmission coefficients using the 4×4 transfer matrix method.^[42] In the calculations, the temperatures of the emitter and the receiver are set as 300 and 0 K, respectively. In addition, the vacuum gap is maintained at $d = 20$ nm.

3. Results and discussion

3.1 Bulk α -MoO₃

Here, we first analyze the phonon polaritons excited in the bulk α -MoO₃. According to the theoretically analysis for phonon polaritons in hyperbolic materials, the regions in the wavevector space where HVPPs and HSPPs can exist are totally determined by the signs of three permittivity components, i.e., ϵ_x , ϵ_y , and ϵ_z .^[39, 62] Eight cases are clearly shown in Fig. 3. Here we first discuss the case when the sign of ϵ_z is positive. There are no phonon polaritons excited when

the signs of three permittivity components are all positive, as shown in Fig. 3(a). The HVPPs can be excited in all azimuthal angles when the signs of ε_x and ε_y are negative, as shown in Fig. 3(b). The HVPPs can be excited in limited regions when there is a strong in-plane anisotropy, i.e., ε_x and ε_y have opposite signs, as shown in Fig. 3(c) and 3(d). In addition, the boundary lines are governed by $k_y = \pm \sqrt{\frac{-\varepsilon_x}{\varepsilon_y}} k_x$.^[39] When ε_z is negative, the HVPPs or HSPPs can be excited in all azimuthal angles when the signs of ε_x and ε_y are all positive or negative, as shown in Fig. 3(e) and 3(f), respectively. When ε_x and ε_y have opposite signs, as shown in Fig. 3(g) and 3(h), both HVPPs and HSPPs can be possible to be excited. Moreover, the regions in the wavevector space where HVPPs and HSPPs can exist are complementary. In addition, the asymptotes are governed by $k_y = \pm \sqrt{\frac{-\varepsilon_x}{\varepsilon_y}} k_x$, and thus the angle θ can be obtained according to the asymptotes, i.e., $\theta = 2 \tan^{-1} \sqrt{\frac{-\varepsilon_x}{\varepsilon_y}}$.

Fig. 3 Schematic of the regions in the wavevector space where HVPPs and HSPPs can exist. The boundary lines for HVPPs and HSPPs are $k_y = \pm \sqrt{-\varepsilon_x/\varepsilon_y} k_x$.

Fig. 4 Schematic of the regions in the Reststrahlen bands where HVPPs and HSPPs can be excited.

According to the signs of the three permittivity components of α -MoO₃, the HVPPs and HSPPs can be excited in different band, as shown in Fig. 4. We present the regions where the HVPPs can be excited using the black grid. In the bands from 1.03×10^{14} to 1.55×10^{14} rad/s and from 1.60×10^{14} to 1.81×10^{14} rad/s, only HVPPs can be excited in a limited range of azimuthal angle, which is determined by the boundary line $\theta = 2 \tan^{-1} \sqrt{\frac{-\varepsilon_x}{\varepsilon_y}}$. In the bands from 1.55×10^{14}

to 1.60×10^{14} rad/s and from 1.83×10^{14} to 1.89×10^{14} rad/s, the HVPPs can be excited in the whole azimuthal angles. In the bands from 1.81×10^{14} to 1.83×10^{14} rad/s, both HVPPs and HSPPs can be excited, and the boundary line between them is determined by Equation $\theta = 2 \tan^{-1} \sqrt{\frac{-\varepsilon_x}{\varepsilon_y}}$. The HSPPs can only be excited in the region below the boundary line.

Fig. 5 Energy transmission coefficient varying with wavevector components at different angular frequencies: (a) 1.3×10^{14} , (b) 1.58×10^{14} , (c) 1.7×10^{14} , and (d) 1.82×10^{14} rad/s.

To vividly show the excitation of phonon polaritons, here we plot the energy transmission coefficient at four different typical angular frequencies. As shown in Fig. 5a and 5c, only HVPPs can be excited at angular frequencies 1.3×10^{14} and 1.7×10^{14} rad/s. In addition, the HVPPs are excited on the upper and lower sides of the origin at an angular frequency of 1.3×10^{14} rad/s, while these are excited on the left and right sides of the origin at an angular frequency of 1.7×10^{14} rad/s. The asymptotes are denoted by two green dashed lines and are found to be in excellent agreement with the borders of the bright color regions. The angles between the asymptotes are respectively 49° and 64° . As shown in Fig. 5b, the HVPPs can be excited in the whole azimuthal angles at an angular frequency of 1.58×10^{14} rad/s. We have checked that the energy transmission coefficient in the band from 1.83×10^{14} to 1.89×10^{14} rad/s is similar to that shown in Fig. 5(b).

As shown in Fig. 5d, both HVPPs and HSPPs can be excited at an angular frequency of 1.82×10^{14} rad/s. In this case, the asymptotes can distinguish HVPPs and HSPPs very well, and the angle corresponding to the excitation of HSPPs is 19° . The behavior of energy transmission coefficient at different angular frequencies is strongly related to the signs of three permittivity component. Therefore, based on the analysis for the signs of three permittivity components, one can figure out where HVPPs and HSPPs can be excited. Note that the electromagnetic waves in the hyperbolic materials for exciting

HVPPs are propagating waves, while these for exciting HSPPs are evanescent waves.

3.2 Single graphene sheet

Fig. 6 The spectral heat flux for different chemical potential of graphene.

Here we study the heat transfer between graphene sheets mediated by the chemical potential. As shown in Fig. 6, the spectral heat flux can be enhanced in a broad band. In addition, the spectral heat flux increases with the decrease of the chemical potential. The solid ball in each line corresponds to the surface plasmon polaritons of graphene, which implies the red shift of SPP peaks with increasing the graphene chemical potential. The red shift of the SPP peaks is attributed to the change of the effective permittivity of graphene, which has been discussed in literature. [63]

Fig. 7 Energy transmission coefficient varying with wavevector components at an angular frequency of 1×10^{14} rad/s for different chemical potential: (a) 0.1; (b) 0.2; (c) 0.3; and (d) 0.4 eV.

To understand the behavior of the spectral heat flux changing with the chemical potential, the energy transmission coefficient at an angular frequency of 1×10^{14} rad/s is presented

in Fig. 7. The two bright rings correspond to the symmetric and asymmetric branches of the coupled SPPs in graphene. [61] As the chemical potential increases, the wavevector for exciting SPPs will be reduced, and thus the heat flux is suppressed. Therefore, the trend shown in Fig. 6 is attributed to the excited SPPs in graphene.

3.3 Bulk α -MoO₃ covered with graphene

Fig. 8 The spectral heat flux of bulk α -MoO₃ covered with graphene for different chemical potential.

The spectral heat flux of bulk α -MoO₃ covered with graphene is shown in Fig. 8. The spectral heat flux of bare bulk α -MoO₃ is also calculated for comparison. As can be seen clearly, the heat flux of bulk α -MoO₃ is only enhanced in the Reststrahlen band from 1.03×10^{14} to 1.89×10^{14} rad/s, due to its hyperbolicity. After adding the graphene, the heat flux can be greatly enhanced beyond the Reststrahlen band. Similar phenomenon has been observed in the hBN covered with graphene, and it is attributed to the coupling of graphene plasmons and phonon polaritons in hyperbolic materials. [61] Besides, such phenomenon has also been observed for polar materials, such as SiO₂ and SiC. [52,60,64] Out of the Reststrahlen bands, the heat flux is significantly enhanced, showing a similar trend to SiO₂, SiC, and hBN. [52,60,61,64] In the Reststrahlen band, the heat flux can be either suppressed or enhanced, depending on the value of the chemical potential of graphene. In addition, the heat flux is always suppressed around an angular frequency of 1.82×10^{14} rad/s. When the chemical potential is 0.1 eV, the heat flux can be almost enhanced in the whole band. The total heat flux for bare bulk α -MoO₃, graphene sheets, and their combination is 347, 1015, and 1888 kW/m², respectively. Therefore, the combination of biaxial hyperbolic materials and graphene can greatly enhance the NFRHT.

The trend in Fig. 8 can be understood by investigating the energy transmission coefficient. The energy transmission coefficient at an angular frequency of 1.3×10^{14} rad/s is shown in Fig. 9. Compared with Fig. 5(a), it is clear that the SPPs can be supported on the left and right sides of the origin. The asymptotes $k_y = \pm 1.15k_x$, denoted as green dashed lines, can clearly distinguish the contribution of SPPs and HPPs. Both SPPs and HPPs are supported at a smaller wavevector as the chemical potential increases. As a result, the heat flux will decrease.

Fig. 9 Energy transmission coefficient varying with wavevector components at an angular frequency of 1.3×10^{14} rad/s for a chemical potential of: (a) 0.1; (b) 0.2; (c) 0.3; and (d) 0.4 eV.

Fig. 10 The contribution of HPPPs and SPPPs at an angular frequency of 1.3×10^{14} rad/s varying with the chemical potential of graphene.

To quantitatively estimate the contribution of SPPPs and HPPPs, we calculate the heat flux for them, and the results are shown in Fig. 10. The contributions of SPPPs and HPPPs are both decreased with the increase of the chemical potential. The spectral heat flux at an angular frequency of 1.3×10^{14} rad/s is $4.78 \times 10^{-9} \text{ J m}^{-2} \text{ rad}^{-1}$ for bulk $\alpha\text{-MoO}_3$, which is totally attributed to the excitation of HVPPs. When the chemical potential is 0.1 eV, the contribution of SPPPs and HPPPs is respectively 8.85×10^{-9} and $3.61 \times 10^{-9} \text{ J m}^{-2} \text{ rad}^{-1}$. In this case, the heat flux on the left and right sides of the origin is greatly enhanced, while that on the upper and lower sides of the origin is slightly suppressed, and thereby the total heat flux is enhanced at this angular frequency. When the chemical potential is larger than 0.1 eV, the contributions of both SPPPs and HPPPs are decreased with increasing the chemical potential. In particular, the heat flux due to the excitation of

SPPPs is decreased significantly. Consequently, the total heat flux can be suppressed when the chemical potential is large. Therefore, the coupling between graphene plasmons and phonon polaritons in $\alpha\text{-MoO}_3$ can either suppress or enhance the heat flux, depending on the chemical potential of graphene.

Fig. 11 Energy transmission coefficient varying with wavevector components at an angular frequency of 1.82×10^{14} rad/s for a chemical potential of (a) 0.1; (b) 0.2; (c) 0.3; and (d) 0.4 eV.

Fig. 12 The contribution of HPPPs and SPPPs at an angular frequency of 1.82×10^{14} rad/s varying with the chemical potential of graphene.

The energy transmission coefficient at the angular frequency of 1.82×10^{14} rad/s is shown in Fig. 11. It is clear that the SPPPs can be supported on the left and right sides of the origin, while the HPPPs can be supported on the upper and lower sides of the origin. The asymptotes $k_y = \pm 0.34 k_x$, denoted as green dashed lines, can clearly distinguish the contribution of SPPPs and HPPPs. Both SPPPs and HPPPs shrink to the

origin as the chemical potential increases. As a result, the heat flux will be decreased.

For bulk α -MoO₃, the contributions from HSPPs and HVPPs are respectively 5.66×10^{-9} and 3.51×10^{-9} J m⁻² rad⁻¹. After adding graphene, the calculated heat flux for SPPs and HPPs are shown in Fig. 12. When the chemical potential is 0.1 eV, the coupling between graphene plasmons and phonon polaritons in α -MoO₃ suppresses the radiative heat flux. The contributions of SPPs and HPPs both are decreased with the increase of the chemical potential. Specially, the heat flux coming from the left and right sides of the origin is reduced greatly.

Similar to previous studies,^[39,61] the thickness of the hyperbolic material α -MoO₃ should have an impact on the heat transfer. As presented in Ref.^[61] the thickness of hyperbolic material hBN had a great effect on the total heat flux and could offer a potential way to actively control the heat flux. However, compared with the case of semi-infinite, the physical mechanism for enhanced heat flux did not change essentially for a thickness-finite slab. Therefore, it is not very necessary to explore the effect of the thickness on the heat transfer here.

4. Conclusion

In summary, we have investigated the near-field radiative heat transfer between graphene covered α -MoO₃. The numerical results show that the coupling between plasmons in graphene and phonon polaritons in α -MoO₃ can greatly enhance the total heat flux. The spectral heat flux in the Reststrahlen bands can be suppressed or enhanced, depending on the value of the chemical potential of the graphene. It is found that the HPPs always suppress the heat transfer, which is the same as previous studies. However, it is also found that the SPPs can enhance or suppress the heat transfer, which has not been reported. The findings in this work not only deepen the understanding of coupling between graphene plasmons with phonon polaritons, but also pave the way to actively control the photon tunneling in graphene-covered hyperbolic materials.

Supporting information

Not applicable.

Conflict of interest

There are no conflicts to declare.

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