Journal of Quantitative Spectroscopy & Radiative Transfer 200 (2017) 100–107

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

Pattern-free thermal modulator via thermal radiation between Van der Waals materials

Xianglei Liu[a,b,*], Jiadong Shen[a], Yimin Xuan[a]

[a] School of Energy and Power Engineering, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China
[b] Key Laboratory of Thermo-Fluid Science and Engineering, Xi'an Jiaotong University, Ministry of Education, Xi'an, 710049, China

ARTICLE INFO

Article history:
Received 21 March 2017
Revised 10 June 2017
Accepted 10 June 2017
Available online 13 June 2017

Keywords:
Thermal modulator
Van der Waals materials
Hexagonal Boron Nitride
Hyperbolic surface phonon polaritons
Near-field radiative transfer

ABSTRACT

Modulating heat flux provides a platform for a plethora of emerging devices such as thermal diodes, thermal transistors, and thermal memories. Here, a pattern-free noncontact thermal modulator is proposed based on the mechanical rotation between two Van der Waals films with optical axes parallel to the surfaces. A modulation contrast can reach a value higher than 5 for hexagonal Boron Nitride (hBN) films separated by a nanoscale gap distance. The dominant radiative heat exchange comes from the excitation of both Type I and Type II hyperbolic surface phonon polaritons (HSPhPs) at the vacuum-hBN interface for different orientations, while the large modulation contrast is mainly attributed to the mismatching Type I HSPhPs induced by rotation. This work opens the possibility to design cheap thermal modulators without relying on nanofabrication techniques, and paves the way to apply natural Van der Waals materials in manipulating heat currents in an active way.

1. Introduction

The manipulation of heat currents analogous to that of electric currents has attracted considerable interest in recent years due to its increasingly crucial role in thermal information processing, thermal management of nanoelectronics, and heat-to-electricity conversion, to name a few [1–3]. Extensive thermal devices like thermal diodes [4–7], transistors [8–13], switches [14,15], logic gates/circuits [16–19], and memories [20–24] have been experimentally and theoretically proposed via controlling the heat currents, which lies in the heart of aforementioned applications. At an early stage, the investigations on thermal modulation were mainly confined to heat conduction [25] by engineering phonon transport in bulk materials [26–29] and nanostructured materials [30–34] in virtue of the maturity of theories and experiments of heat conduction. Nevertheless, the thermal modulation based on manipulating phonons may have some limitations, such as much lower speed of phonon transport and the inevitable existence of local Kapitza resistances reducing phononic heat flow dramatically [35].

Alternatively, photons, another important energy carriers, are also promising to serve as a candidate for thermal modulation. Near-field thermal radiation has been demonstrated theoretically and experimentally to vastly exceed the blackbody limit governed by Stefan-Boltzmann law by several orders of magnitude due to the contribution of photon tunneling [36–40], especially when surface plasmon/phonon polaritons (SPPs/SPhPs) [41–46], non-resonance hyperbolic modes [47,48] or hyperbolic surface plasmon/phonon polaritons (HSPPs/HSPhPs) [45,49,50] are excited. This efficient radiative energy transport has been recently employed in thermal modulation [51–58]. Modulating the radiative heat flux can be achieved by changing the gap distance between two substances. Nevertheless, this method tends to have some shortcomings. For example, in the deep near field, the radiative heat flux is very sensitive to the gap distance and varies as d^{-2} [59], thus the gap distance should be controlled very precisely (resolution may need to be sub-nanometer) to meet the required modulation effect. More discussions will be presented later. For the far field where neither interference effects of propagating waves nor tunneling of evanescent waves are present, the radiative heat flux may still reduce with the gap distance for objects with finite surface area since the view factor will decrease. Nevertheless, the macroscale gap space may inhibit the applications in micro/nanoscale devices. Recently, Biehs et al. [60] proposed to modulate the radiative heat flux by acting on the relative orientation of two polar/metallic gratings. This alternative modulation technique can relieve the aforementioned shortcomings of modulators based on varying gap distances to some extent. The modulator tends to have a good performance at a nanoscale gap distance, for which the fabrication of gratings will be an enormous challenge given that the roughness and imperfections should be guaranteed to be within a few nanometers.

* Corresponding author.
E-mail address: xliu@nuaa.edu.cn (X. Liu).

http://dx.doi.org/10.1016/j.jqsrt.2017.06.010
0022-4073/

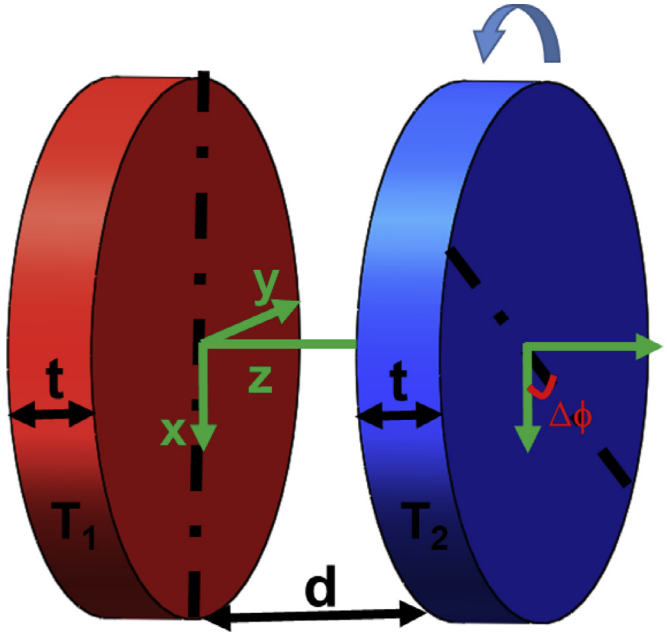

Fig. 1. Schematic of the pattern-free thermal modulator based on Van der Waals films with a thickness of t separated by a vacuum gap of d and relatively twisted by an angle of $\Delta\phi$. The black dash-dotted lines denote the optical axes. Temperatures of hBN films are $T_1 = 310$ K and $T_2 = 290$ K as default.

Here, this paper proposes a noncontact thermal modulator without requiring patterning objects into nanostructures based on natural Van der Waals materials, i.e., layered materials with strong in-plane covalent bonding and weak interlayer van der Waals interactions. Two common Van der Waals materials, i.e., hexagonal Boron Nitride (hBN) and graphite, are considered here. The modulator is applicable for varying gap spacing ranging from deep near field to far field. The modulation contrast can be higher than 5 for nanometer thick hBN films at a nanoscale gap spacing. The underlying mechanism of the high modulation performance will be analyzed in detail.

2. Theory and computation

The proposed thermal modulator is depicted in Fig. 1, in which two Van der Waals films are separated by a vacuum gap, with optical axes of both films parallel to the surfaces (perpendicular to the energy flow direction). The two optical axes, denoted by black dash-dotted lines, have an orientation angle of ϕ_1 and ϕ_2, respectively, and $\Delta\phi = \phi_1 - \phi_2$. ϕ_1 is set to be zero as default, and ϕ_2 is adjustable by external mechanical rotation. d and t are the vacuum gap distance and film thickness, respectively, and T_1 and T_2 are the temperature of emitter and receiver, respectively. According to the coordinate system in Fig. 1, the dielectric function can be written as [60]

$$\varepsilon_{\mathrm{hBN}} = \begin{pmatrix} \varepsilon_{\parallel}\cos^2\phi_{\mathrm{i}} + \varepsilon_{\perp}\sin^2\phi_{\mathrm{i}} & (\varepsilon_{\perp} - \varepsilon_{\parallel})\sin\phi_{\mathrm{i}}\cos\phi_{\mathrm{i}} & 0 \\ (\varepsilon_{\perp} - \varepsilon_{\parallel})\sin\phi_{\mathrm{i}}\cos\phi_{\mathrm{i}} & \varepsilon_{\parallel}\sin^2\phi_{\mathrm{i}} + \varepsilon_{\perp}\cos^2\phi_{\mathrm{i}} & 0 \\ 0 & 0 & \varepsilon_{\perp} \end{pmatrix}, \tag{1}$$

where i represents 1 or 2, $\parallel$ and $\perp$ denote the electric field parallel and perpendicular to the optical axis, respectively. hBN and graphite, as two common naturally existing Van der Waals materials, are taken into consideration here to investigate the thermal modulation effects. The dielectric functions of hBN for ordinary ($\varepsilon_{\perp}$) and extraordinary ($\varepsilon_{\parallel}$) waves can be calculated using Lorentz model as [61]

$$\varepsilon_m = \varepsilon_{\infty,m}\left[1 + \frac{\omega_{\mathrm{LO},m}^2 - \omega_{\mathrm{TO},m}^2}{\omega_{\mathrm{TO},m}^2 - \mathrm{i}\gamma_m\omega - \omega^2}\right], \tag{2}$$

where m represents $\parallel$ or $\perp$. The corresponding parameters are obtained from Ref. [61]. While for graphite, $\varepsilon_{\perp}$ and $\varepsilon_{\parallel}$ can be achieved in Ref. [62,63].

The fluctuation-dissipation theory combined with the dyadic Green function is used to calculate the radiative heat flux exchanged between two films as [60]

$$\mathrm{Q} = \frac{1}{4\pi^2}\int_0^{\infty}[\Theta(\omega, T_1) - \Theta(\omega, T_2)]d\omega \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\xi(\omega, k_x, k_y)dk_x dk_y, \tag{3}$$

where $\xi(\omega, k_x, k_y)$ is the energy transmission coefficient with k_x and k_y as the tangential wavevectors along x and y coordinates, respectively. $\Theta(\omega, T) = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$ is the mean energy of Planck's oscillator. The energy transmission coefficient can be obtained as [64,65]

$$\xi(\omega, k_x, k_y) = \begin{cases} \mathrm{Tr}[(R_2^* - R_2)D(R_1 - R_1^*)D^*]e^{-2|k_z|d}, & \sqrt{k_x^2 + k_y^2} > k_0 \\ \mathrm{Tr}[(I - R_2^* R_2)D(I - R_1 R_1^*)D^*], & \sqrt{k_x^2 + k_y^2} < k_0 \end{cases}, \tag{4}$$

where $k_0 = \omega/c$ is the wavevector in vacuum, $k_z = \sqrt{k_0^2 - k_x^2 - k_y^2}$ is the tangential wavevector along z axis in vacuum, $D = (I - R_1 R_2 e^{2ik_z d})^{-1}$, $R_{1,2}$ is a 2×2 reflection coefficient matrix, and * signifies the complex conjugate. The four elements of matrix $R_{1,2}$ represent the scattering of s/p polarized plane waves into s/p counterparts, expressed in Ref. [66].

3. Results and discussion

3.1. Modulation contrast of hBN films

Fig. 2(a) plots the near-field radiative heat flux normalized to the case at $\Delta\phi = 0°$ as a function of the rotation angle at $d = 10$ nm for hBN bulks and 10-nm-thick films. As can be clearly seen, the radiative heat flux drops monotonically with the rotation angle for both hBN bulks and films, and the lowest radiative heat flux occurs at $\Delta\phi = 90°$, which is due to the increasing mismatch of radiative properties of the two objects. The minimum normalized radiative heat flux of hBN films achieves 0.285, which is much lower than that of hBN bulks with a value of 0.476. If defining the modulation contrast as the ratio of radiative heat flux at $\Delta\phi = 0°$ to that at $\Delta\phi = 90°$, apparently, the modulation contrast increases from 2.10 for hBN bulks to 3.50 for 10-nm-thick hBN films.

To investigate modulation effects for varying gap spacing, the absolute radiative heat flux between hBN bulks versus d is illustrated in Fig. 2(b) for both $\Delta\phi = 0°$ and 90°. The radiative heat fluxes for both orientations increase monotonically with decreasing gap distance owing to increasing contributions of the tunneling of evanescent waves. Therefore, it is feasible to design a modulator based on varying gap distance. Taking the case with $d = 10$ nm, $t = 10$ nm, and $\Delta\phi = 0°$ as an example, the radiative heat flux changes by 18.6% per nanometer while by 0.28% per degree when adjusting the rotation angle slightly. To this sense, the controllability of thermal modulators based on mechanical rotation tends to be better. As denoted by the red solid line in Fig. 2(b), when $d > 10$ μm, the radiative heat flux for both cases is independent of the gap distance, as a result, the modulation contrast saturates to the value of 1.08. With decreasing d, a small dip of modulation contrast occurs around $d = 3.6$ μm, which can be attributed to the more rapid increase of the radiative heat flux for $\Delta\phi = 90°$ than