Dynamic Tuning of Near-Field Radiative Thermal Rectification

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Taking advantage of phase-transition and reconfigurable metamaterials, dynamic control of nanoscale thermal modulation can be achieved through the near-field radiative thermal rectification devices. Herein, an active-tuning near-field thermal rectifier using reconfigurable phase-transition metamaterials is explored. The rectifier has two terminals separated by vacuum, working under a controllable operational temperature around the critical temperature of the phase-transition material VO₂. One of the terminals is a stretchable structure made of polydimethylsiloxane (PDMS) thin film and grating consisting of various types of phase-transition material. The effects of various inclusion forms and all the related geometric parameters are well analyzed. The controllable nanoscale thermal modulation can be achieved and the ultrahigh rectification ratios of 23.7 and 19.8, the highest values ever predicted, can be obtained for two deformation scenarios, respectively. It will shed light on the dynamic tuning of small-scale thermal transport and light manipulation.

1. Introduction

Active control of heat transfer is an important and challenging topic in thermal engineering and it attracts much attention recently. The thermal rectifiers based on conduction mechanism have been presented in several articles. However, because of the presence of Kapitza resistances and the speed of phonons, the performance of these types of thermal diodes has been restricted. Alternatively, thermal rectification based on radiative heat transfer is proposed. Some works have been conducted in both far-field and near-field limits experimentally and theoretically. Extensive studies have realized thermal rectification by utilizing polar materials and phase-transition materials.

In the near-field regime, the radiative heat transfer exceeds the blackbody limit by several orders of magnitude because of the tunneling of evanescent waves and coupling of surface phonon or plasmon polaritons, thus outstanding thermal rectification can be realized. Thermal diode is one of the thermal rectifiers that modulate thermal transport: the heat flux in one direction is much larger than the one in the opposite direction depending on the temperature gradient. To evaluate the performance of a thermal diode, the rectification ratio R is defined as

$$R = \frac{Q_F}{Q_R}$$

where Q_F and Q_R refer to the forward and reverse heat fluxes, respectively. Ito et al. experimentally investigate the far-field radiative thermal rectifier utilizing the phase-transition material VO₂ and tune its operating temperature by doping tungsten. Yang et al. show numerical results of thermal rectification based on VO₂ and discuss the influence of film thickness. Huang et al. combine two phase-change materials, VO₂ and LCSMO, to improve the thermal rectification ratio to a higher value of 7.7 according to the aforementioned definition. In addition to the plate–plate structure, some microstructures and nanostructures, such as surface grating, are also introduced to further enhance the rectifier performance.

The phase-transition materials modulate the heat transfer due to their temperature-dependent thermal and optical properties, which renders a phase-transition-based thermal device must operate around its critical temperature of phase change. In addition to the temperature dependence, the modulation of thermal transport can also be achieved by changing the configuration of a thermal device when subjected to mechanical strain. Biehs et al. present a theoretical study that the twisting angle between two grating structures can modulate the net heat flux up to 90% at room temperature. Ghani et al. propose a near-field thermal modulator exhibiting sensitivity to mechanical strain. Liu et al. demonstrate a noncontact thermal modulator based on the mechanical rotation and a modulation contrast greater than 5 can be achieved. Though the studies on thermal rectifier driven by mechanical force are not much, reconfigurable metamaterials that can dynamically manipulate electromagnetic properties have aroused a lot of attention recently, paving the way for a deeper study on nanoscale radiative thermal rectification.

Here, we combine the comprehensive effects of phase transition and reconfigurable structures and propose a near-field stretchable radiative thermal diode based on the phase-transition material vanadium dioxide (VO₂) and the soft host material polydimethylsiloxane (PDMS) with a tunable rectification. A comprehensive design is shown in Figure 1a and it has two terminals separated by a distance in nanoscale, which is less than the thermal wavelength of interest. The passive terminal is composed of 1 μm BN layer on top of 1 μm gold layer. The other terminal is referred to as the active terminal. The VO₂ film is deposited on top of a stretchable PDMS layer. In addition, VO₂ nanoparticles
2. Theoretical Fundamentals

The expressions for the radiative heat fluxes across the near-field thermal diode are obtained through the dyadic Green’s function formalism.[33] The heat flux between planar objects can be calculated by

\[ Q = \int_0^\infty \frac{da\sqrt{\frac{\omega}{\pi}}} {2r} \left[ \Theta(a, T_1) - \Theta(a, T_2) \right] \int_0^\infty \frac{k_i dk_i}{2\pi} Z(\omega, k_i) \]  

(1)

where \( T_1 \) and \( T_2 \) are the temperatures of two objects. \( \Theta(a, T) = (\hbar a / 2) \coth(\hbar a / 2k_b T) \) is the energy of the harmonic oscillator. \( \int_0^\infty \frac{k_i dk_i}{2\pi} Z(\omega, k_i) \) is known as the spectral transmissivity in radiative transfer between media 1 and 2 with gap \( L \), where \( k_i \) is the parallel component of wavevector and \( Z(\omega, k_i) \) is known as the energy transmission coefficient. For our proposed 1D grating structure of PDMS and VO2, the second order approximation of the effective medium theory is used to obtain the effective dielectric properties.[34]

Effective medium approximation is only valid as the grating period \( \Lambda \) is much less than the wavelength \( \lambda \). In addition, the prerequisite for using the approximation in near-field radiative heat transfer is that the gap \( L \) between the two objects is larger than the grating period.[34] In this work, the grating period (50 nm) is much less than the thermal wavelength around 341 K (≈8.5 μm) and is smaller than the gap (100 nm) as well. Therefore, all these criteria are satisfied. To calculate the effective dielectric function of a composite medium containing nanoparticles in a host material, the Clausius–Mossotti equation is applied.[35]

When the temperature of VO2 is lower than its critical temperature (341 K), it is in the anisotropic insulator state. We can use the classical oscillator formula \( \varepsilon(\omega) = \varepsilon_\infty + \sum_{i=1}^{N} \frac{\varepsilon_{i}}{\omega_{i} - \omega} - \frac{\varepsilon_{i}}{\omega_{i} + \omega} \) to determine dielectric functions of the ordinary mode \( \varepsilon_0 \) and the extraordinary mode \( \varepsilon_e \). The experimental values for calculation are given in the work of Barker et al.[36] As the temperature is above 341 K, VO2 is in the isotropic metallic state. The Drude model is used to calculate the dielectric function \( \varepsilon(\omega) = \frac{-\omega_0^2}{\omega^2 + i\gamma} \).

The dielectric function of gold can be found in the study by Johnson and Christy.[37] Query provide the refractive indices of PDMS[38] and that of BN is given by Palik.[39]

3. Results and Discussions

To give a brief evaluation of the thermal rectification performance of the four active terminal structures proposed in Figure 1b, the heat flux dependence on the temperature difference is plotted in Figure 2. The temperature of the active terminal is set as \( T_1 = 341 K + \Delta T \). The passive terminal has its temperature \( T_2 = 341 K -\Delta T \). Here, 341 K is the critical temperature of VO2. When \( T_1 > T_2 \) (referred to as forward bias), VO2 is in metallic phase; when \( T_1 < T_2 \) (reverse bias), VO2 is in insulator phase with its optical axis normal to the surface.[12]

The right side of Figure 2 (with yellow background) is referred to as the forward bias (\( \Delta T > 0 \)) with heat flux \( Q_F \) and left side referred to as the reverse bias (\( \Delta T < 0 \)) with heat flux \( Q_R \). It can be seen that \( Q_F \) is much larger than \( Q_R \), showing a clear thermal-diode feature, especially for the grating structures with

![Figure 1](image-url)  

**Figure 1.** a) Schematic of a reconfigurable near-field thermal diode using phase-transition metamaterials. b) Four structural cases for the active terminal. PDMS film thickness \( h_2 = 60 \text{ nm} \) for all four cases. (I) PDMS grating with thickness \( h_2 = 100 \text{ nm} \), period \( \Lambda = 50 \text{ nm} \), filling ratio \( \phi = w/\Lambda = 0.5 \), \( w \) is the width of the grating strip, particle radius \( r = 3 \text{ nm} \), and volume fraction \( \phi_f = 0.3 \), which is the volume ratio between the nanoparticles and the PDMS grating strip. (II) VO2 film with thickness \( h_3 = 100 \text{ nm} \). (III) \( h_2 = 100 \text{ nm}, h_3 = 250 \text{ nm} \); \( \Lambda \) and \( \phi \) are the same as case I. (IV) \( h_2 \) and \( h_3 \) are the same as case III; \( r, \phi_f, \Lambda, \phi \) are the same as case I.

![Figure 2](image-url)  

**Figure 2.** Forward and reverse radiative heat fluxes \( Q_F \) and \( Q_R \) versus the temperature difference between active and passive terminals at a 100 nm separation for four different cases.
VO₂ film deposited (case III and IV). They have much better thermal rectification performances than the thin-film structure (case II). In addition, the inclusion of VO₂ nanoparticles does not play an important role in heat modulation, which can be concluded from the following two aspects. First, case I exhibits the weakest thermal rectification among the four cases. Second, curves for case III and IV almost overlap, showing little impact from the nanoparticle inclusion.

The effect of the nanoparticle inclusion is discussed in more details based on case I, as nanoparticle is the only inclusion form of the phase-transition material in this case. The rectification ratio is calculated at active terminal temperature \( T_1 = 331 \) K for reverse bias and \( 351 \) K for forward bias, and passive terminal temperature \( T_2 = 341 \) K. This temperature profile is applied for the cases in Figure 3, 4, and 5. Here, the grating height of PDMS is 400 nm, the period is 50 nm, and the filling ratio is 0.5. It can be observed from Figure 3 that the rectification ratio increases monotonically with volume fraction of nanoparticles, but it is quite limited. Due to the Maxwell–Garnett–Mie theory, the volume fraction threshold value is around 33%, though higher volume fraction of nanoparticles is not feasible in real case as nanoparticles are easy to aggregate. If high volume fraction of VO₂ is needed, VO₂ can be involved as the host material rather than doped nanoparticles. Therefore, the doping process has little meaning. As we change the radius \( r \) from 1 to 5 nm, the rectification ratio \( R \) almost remains the same, so it can be concluded that radius is not a crucial factor in the thermal rectification. In one word, the nanoparticle is not a good inclusion form of phase-transition materials to realize a sharp thermal rectification, so in this work, case III is chosen as an ideal structure and VO₂ is involved in the diode in the form of thin films.

The effects of all the related geometric parameters on the variation of rectification ratio are analyzed for case III. The parameters include the height of the PDMS substrate \( h_1 \), the height of PDMS grating \( h_2 \), the thickness of VO₂ film \( h_3 \), period \( \Lambda \), filling ratio \( \phi \), and separation distance \( L \). Figure 4a shows a larger rectification ratio can be obtained at smaller \( h_1 \) in three given combinations of \( h_2 \) and \( h_3 \). Thinner PDMS substrate is preferred but a feasible value should be chosen for a practical device. As long as \( h_2 \) is thick enough (>200 nm), the rectification ratio remains quite stable above 17, while \( h_2 \) has little impact on the rectifier, which can be observed in both Figure 4b,c. So here, \( h_2 \) is introduced in the diode mainly for an easy stretching rather than enhancing rectification. There is an optimal value for \( h_3 \), beyond which \( R \) will decrease. The period is not a crucial parameter compared with filling ratio as \( \Lambda \) is much smaller than the dominant thermal wavelength. When the filling ratio decreases, it optimizes the rectification ratio significantly. It is found in the inset of Figure 4e that \( R \) rises up to 30 when the filling ratio \( \phi \) is 0.04, impractically small, and goes down to zero when \( \phi = 0 \), though such small filling ratio cannot be realized actually. The dependence of the rectification ratio on the filling ratio is due to the change in dielectric properties of the grating structure, thus influencing the surface waves across the interfaces. Also, it is easy to understand that when filling ratio is close to 1, the grating structure behaves like a thin film, which exhibits a weaker rectification shown in Figure 2. Figure 4f displays the dependence of rectification ratio on the separation distance. It is easy to understand that \( R \) increases at a smaller gap because of the strong variation in the intensity of evanescent waves, which is the fundamental mechanism of an ultrahigh near-field thermal rectification.[19] The effect of evanescent waves become less dominant when gap \( L \) increases, and it is negligible in the far-field thermal radiation. Based on the aforementioned complete analysis and considering the condition of the effective medium approximation \( (L > \Lambda) \), a set of optimal parameters is determined: \( h_1 = 60 \) nm, \( h_2 = 100 \) nm, \( h_3 = 260 \) nm, \( \Lambda = 50 \) nm, \( \phi = 0.2 \), \( L = 100 \) nm, and an ultrahigh rectification ratio of 18 can be obtained compared with previous studies.[7,9,12,19]

More significantly in this work, nanoscale thermal rectification is demonstrated as the active terminal is subjected to mechanical strain. As VO₂ has a much larger Young’s modulus than PDMS, it is assumed that VO₂ does not undergo any deformation. As in the original state, the active terminal has period \( \Lambda \) and grating width \( w \). Here, two scenarios for deformation are considered as shown in Figure 6. The first one is an ideal scenario. The PDMS grating width \( w \) remains unchanged as the period elongates from \( \Lambda \) to \( \Lambda + \Delta \Lambda \). However, from a more practical perspective, the PDMS grating must undergo deformation to some extent. It is assumed that the top width of the PDMS grating \( (w_0) \) remains unchanged and the bottom width \( (w_b) \) elongates in the same proportion to the substrate, which means the filling ratio is the same before and after deformation \( (w/\Lambda = w_0/(\Lambda + \Delta \Lambda)) \). The shape of the PDMS grating strip can be viewed as an isosceles trapezoid after deformation, which represents the real situation to some extent, though not exactly accurate, so it is known as the ideal actual scenario in this work. The change in \( h_1 \) and \( h_2 \) upon deformation is considered due to the fact that the Poisson’s ratio for PDMS is 0.5, meaning the volume of PDMS remains constant during stretching or compression.

To illustrate the stretching or compression process for the active terminal, the strain is defined as the change in period over the period of grating \( (\Delta \Lambda/\Lambda) \). For the deformation in scenario 2, the grating strip can be considered approximately as a composition of multiple layers of rectangular gratings, with increasing filling ratio from top to bottom. Here, 50 layers are used in the
calculation and it is enough to get converging solutions. As seen in Figure 5, the rectification ratio increases along with strain in both scenarios. It increases much slower for scenario 2 compared with scenario 1, and the reason is that the grating structure in scenario 1 tends to cover less space on the substrate, i.e., smaller filling ratio, upon deformation. It is concluded that a smaller filling ratio contributes to a larger rectification ratio. Using the data from Figure 5. Strain-dependent thermal rectification for two scenarios with the corresponding changes in heights ($\Delta h_1$ and $\Delta h_3$) while considering the Poisson’s ratio of the soft host material PDMS in stretching.

Figure 4. The effects of geometric parameters on the rectification ratio $R$ for case III: a) height $h_1$, b) height $h_2$, c) height $h_3$, d) period $\Lambda$, e) filling ratio $\phi$, and f) gap $L$. The inset of figure (e) shows a trend of rectification values at small filling ratios. For all the unspecified parameters in these six figures, they are set as $h_1 = 60$ nm, $h_2 = 100$ nm, $h_3 = 260$ nm, $\Lambda = 50$ nm, $\phi = 0.2$, $L = 100$ nm. The active terminal temperature is 331 K for reverse bias and 351 K for forward bias, and the passive terminal temperature is 341 K.

Figure 5. Strain-dependent thermal rectification for two scenarios with the corresponding changes in heights ($\Delta h_1$ and $\Delta h_3$) while considering the Poisson’s ratio of the soft host material PDMS in stretching.

Figure 6. Three states of the active terminal of a reconfigurable near-field thermal diode. Top: the active terminal in its original state. Middle: scenario 1 (constant $w$) for an ideal stretching and compression deformation due to mechanical strain. Bottom: scenario 2 (constant $w$) for an ideal actual deformation due to mechanical strain.
Wu et al.\(^\text{[40]}\) the PDMS film will break at the strain of 128%, which is set to be the stretching limit in this work. The area beyond the limit with yellow background cannot be reached actually. At the stretching limit, the rectification ratio for scenario 1 and 2 are 23.7 and 19.8, respectively. Above all, an increasing trend of radiative thermal rectification effect is observed when a reconfigurable near-field thermal diode undergoes deformation.

4. Conclusion

In conclusion, many studies have been conducted on realizing thermal rectification in both far-field and near-field radiation by utilizing phase transition or varying configurations. In this work, a dynamic tuning of near-field thermal diode using reconfigurable and phase-transition metamaterials is explored. It is designed in a nano-grating structure and works around the critical temperature of phase-transition material VO\(_2\). The best inclusion forms of VO\(_2\) in thermal diodes are studied and it is found that inclusion as thin films outperforms nanoparticles. The geometric parameters of the thermal diode may play an important role in enhancing rectification, such as the thickness of VO\(_2\) film and the filling ratio of the grating. With the determined optimal parameters, an ultrahigh rectification ratio of 18 in the original state is obtained. In addition, the effect of mechanical strain on the rectifier is well analyzed. Two scenarios are considered for the deformation process and a rising trend of rectification ratio is presented upon deformation as well as the highest rectification ratio equals to 23.7 to date. More study can be carried out on designing structures more sensitive to mechanical strain and temperature gradient. This work verifies the possibility of improving thermal rectification through reconfigurable nanostructures utilizing phase-transition metamaterials. It sheds light on the high-performance thermal diodes and motivates promising applications in dynamic control of nanoscale thermal transport. More future work will be addressed in thermal rectification by radiative thermal diode, such as studying alternative phase-transition and host materials, designing nanostructures of active/passive terminals, and exploring other heat modulation mechanisms.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

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