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A thermally tunable terahertz bandpass filter with insulator-metal phase transition of VO_2 thin film*

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A terahertz bandpass filter with the sandwich structure consisting of thermally tunable vanadium dioxide (VO_2) thin film, silica substrate and subwavelength rectangular Cu hole arrays is designed and theoretically analyzed. The results show that the transmittance of the filter can be actively tuned by controlling the temperature of VO_2, the narrow band terahertz (THz) waves with the transmittance from 85.2% to 10.5% can be well selected at the frequency of 1.25 THz when the temperature changes from 50 ℃ to 80 ℃, and the maximum modulation depth of this terahertz bandpass filter can achieve 74.7%.

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Many kinds of terahertz (THz) modulators and filters, such as photonic crystals[1,2], metamaterials[3,4], subwavelength metallic hole arrays[5,6], liquid crystal materials[7,8], and silicon semiconductors[9], are presented and demonstrated. However, the transmission bandwidth, modulation depth and rate are still limited by the dielectric constants, losses, and response time of the materials used in the devices. Therefore, it is necessary to develop the higher-speed and lower-loss THz functional materials and novel device structures.

Subwavelength hole arrays composed of metals and dielectric substrates have been extensively studied in the THz regime, since Ebbesen et al[10,11] discovered the phenomenon of extraordinary transmission through subwavelength metallic hole arrays. Theoretical and experimental researches show that subwavelength metallic hole arrays have good bandpass filtering features with high peak transmittances and low losses in THz regime[12,13]. However, the transmittances and resonance frequencies of such devices are difficult to be further tuned once the metallic structures are processed. Therefore, subwavelength metallic hole arrays can only act as passive THz devices.

On the other hand, vanadium dioxide (VO_2) undergoes a phase transition from insulator to metal, which can be triggered by temperature[14], electrical field[15] and light[16]. This phase transition is caused by a structural transition from a monoclinic insulated phase to a tetragonal metallic phase[17], and meanwhile the conductivity of VO_2 will be exponentially changed, which hence results in abrupt several orders of magnitude changes in electrical and optical properties. VO_2 film in the insulating phase has a very high transmittance for THz waves, while the film in the metallic phase has a very low transmittance, which has been confirmed by the simulations and experiments[18]. In this work, we take this advantage to further modulate subwavelength metallic hole arrays in THz regime, and propose a terahertz bandpass filter with the sandwich structure consisting of thermally tunable VO_2 thin film, silica substrate, and subwavelength rectangular Cu hole arrays. The transmittance of this filter is expected to be actively tuned by controlling the temperature of the VO_2 film.

VO_2 thin film exhibits a reversible phase transition from a low-temperature insulating phase to a high-temperature metallic phase at the critical temperature close to 68 ℃ in the heating transition and 66 ℃ in the cooling transition[19]. The heating and cooling transitions are accompanied by a hysteresis temperature of $\Delta T= 2$ ℃. For the heating transition, when the temperature is increased towards and beyond the transition temperature, the phase transition is initiated at seed points, and then the metallic domains grow and spread in the thin insulating VO_2 film. Consequently, the insulating and metallic domains are coexisting in the process of phase transition. The effective dielectric function of VO_2 film in such a phase transition process has been described most widely with two kinds of effective medium theories (EMTs) which are the

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Bruggeman EMT and the Maxwell-Garnett EMT. The polycrystalline VO_2 film is predicted well by the Maxwell-Garnett EMT[19]. On the other hand, the Bruggeman EMT is more suitable to describe the epitaxial VO_2 film[20]. Mandal et al suggest that the epitaxial VO_2 film has greater dynamic tunable transmittance with its phase transition. Among them, we chose the Bruggeman EMT to simulate the epitaxial VO_2 film in THz regime. The effective dielectric function of VO_2 thin film is expressed as follows[21]:

$$\varepsilon_{\mathrm{eff}} = \frac{1}{4}\Big\{\varepsilon_{\mathrm{i}}(2-3f)+\varepsilon_{\mathrm{m}}(3f-1)+ \sqrt{\left[\varepsilon_{\mathrm{i}}(2-3f)+\varepsilon_{\mathrm{m}}(3f-1)\right]^2+8\varepsilon_{\mathrm{i}}\varepsilon_{\mathrm{m}}}\Big\}, \tag{1}$$

where f is the volume fraction of metallic domains, and ε_{i} and ε_{m} are the dielectric functions of the insulating and metallic domains, respectively. The dielectric function ε_{m} of the metallic phase VO_2 follows the simple Drude form[19, 21]:

$$\varepsilon_{\mathrm{m}}(\omega) = \varepsilon_{\infty} - \frac{\omega_{\mathrm{p}}^2}{\omega^2+\mathrm{i}\gamma\omega}, \tag{2}$$

where ε_{∞} represents the high-frequency dielectric function, and $\omega = 2\pi v$ is the cyclic frequency. The plasma fre-quency $\omega_{\mathrm{p}} = \sqrt{Ne^2/\varepsilon_0 m^*}$ depends on the intrinsic carrier density N, the electronic charge e, the vacuum permittivity ε_0, and the effective mass m^* of free carriers. The damping constant γ is related to the mobility μ of the charge carriers through $\gamma = e/m^*\mu$. According to the previous research[22], we use the high-frequency dielectric function of $\varepsilon_{\infty} = \varepsilon_{\mathrm{i}} = 9$, the free-carrier concentration of $N = 1.3\times10^{22}\ \mathrm{cm}^{-3}$ and the effective mass of the charge carriers of $m^* = 2m_{\mathrm{e}}$, where m_{e} is the mass of free electron, and the carrier mobility is $\mu = 2\ \mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$. For the temperature modulation, the volume fraction f of metallic phase is given by the Boltzmann function[19]:

$$f(T) = f_{\max}\left\{1-\frac{1}{1+\exp\left[(T-T_0)/\Delta T\right]}\right\}, \tag{3}$$

with the phase transition temperature T_0 and the hysteresis temperature ΔT. According to the experimental result in Ref.[19], the volume fraction of the metallic domain at the highest temperature is considered as $f_{\max} = 0.95$. The dielectric function is related to the conductivity and the effective conductivity σ_{eff} obeys the following relationship[23]:

$$\sigma_{\mathrm{eff}} = -\mathrm{i}\varepsilon_0\omega(\varepsilon_{\mathrm{eff}}-1). \tag{4}$$

In Fig.1 we can see that the conductivity of VO_2 film varies from 10.62 S/m to 2.76×10^5 S/m when the temperature changes between 50 °C and 80 °C, which is consistent with the previous experimental results[14, 20]. Next, we will design and simulate the THz bandpass filter with periodic subwavelength rectangular Cu hole arrays based on VO_2 thin film utilizing the phase transition curves and the parameters.

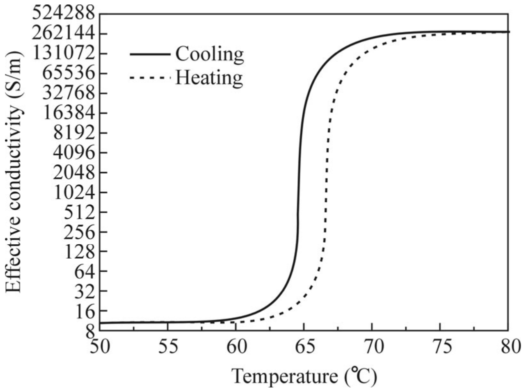
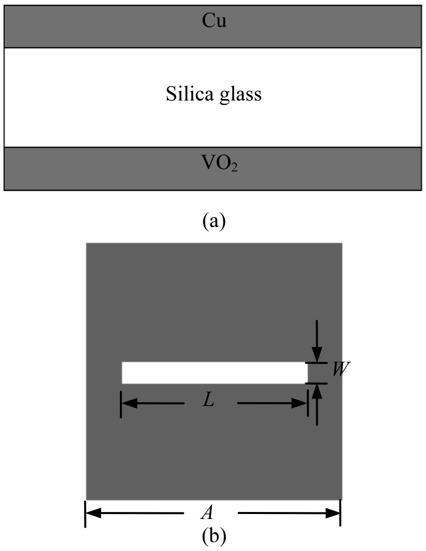


Fig.1 The effective conductivity of VO_2 film vs. temperature in the heating (T_0=68 °C) and cooling (T_0=66 °C) processes with the hysteresis of ΔT=2 °C, calculated with the Bruggeman EMT

The structural illustration of the THz bandpass filter is shown in Fig.2. Cu rectangular hole arrays (200 nm thick) are supported on the upper surface of silica-glass substrate (1.1 mm thick), and the thin-film VO_2 (also 200 nm thick) is added on the lower surface of the substrate (Fig.2(a)). The dimension of a single Cu rectangular hole is 70 μm (L)×10 μm (W) with a lattice period A of 100 μm, as shown in Fig.2(b). Thus, this filter is expected not only to have a bandpass filtering feature of subwavelength metallic hole arrays, but also to have the THz thermally tunable transmittance of VO_2 film in the temperature range from 50 °C to 80 °C.



(a)

(b)

Fig.2 The structural illustration of the THz bandpass filter: (a) The structure of the device; (b) The single Cu rectangular hole with the parameters of L=70 μm, W=10 μm and A=100 μm

The transmission spectra of the THz bandpass filter are calculated with the finite-difference time domain (FDTD) method at various temperatures. In the simulations, the dielectric constant of the silica-glass substrate is taken as 3.84[24]. Since no free carrier would be possibly excited by heating the silica-glass and the THz conductivity of Cu is almost not affected by temperature change[25], the tunability of the device can only be derived from the VO_2 film rather than the Cu hole arrays or glass substrate.

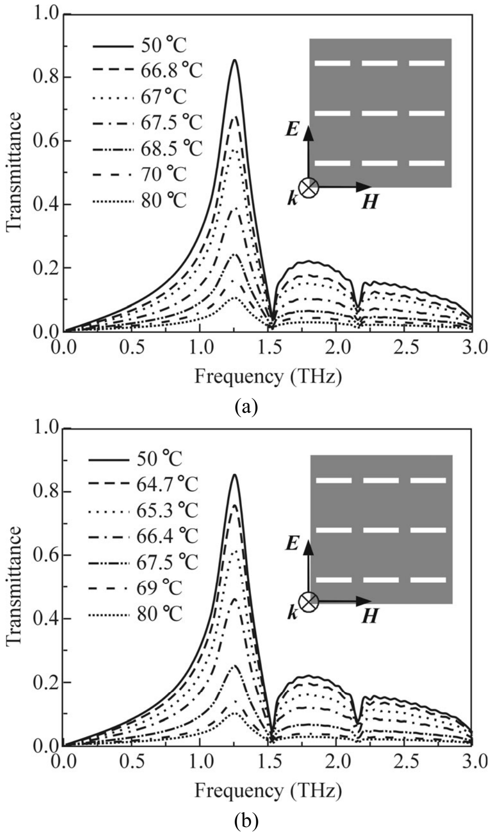
In Fig.3(a), a high transmittance of 85.2% is obtained at 1.25 THz with the full width at half maximum (FWHM) of about 255 GHz at the low temperature of 50 °C. In this case, the effective conductivity σ_{eff} of VO_2 film is 10.62 S/m, and the device exhibits an excellent bandpass filtering function. Once the device is heated, the THz transmittance of VO_2 is decreased due to the insulator-metal transition. When the temperature approaches 67.5 °C, the conductivity of VO_2 film exponentially increases to 4.33×10^4 S/m, and the transmittance peak falls to 40.3% at 1.25 THz with the FWHM of 277 GHz. At the temperature of 80 °C, the conductivity of VO_2 film is 2.76×10^5 S/m and the transmittance peak is then dramatically decreased to 10.5% with the FWHM of 303 GHz. On the contrary, as shown in Fig.3(b), during the cooling process, the transmission peak will be increased again from 10.5% to 85.2% as the temperature is decreased. Therefore, a modulation depth of 74.7% can be obtained by controlling the temperature of the device.

Generally, the transmittance of the filter mainly depends on the sizes of the rectangle Cu hole arrays. It should be noted that the two minimum values in the transmittance curves occur at the frequencies of 1.53 THz and 2.16 THz, respectively, which is considered to be caused by the resonant excitation of surface plasmons (SPs) in subwavelength Cu hole arrays. The SP modes excited in the array can be approximately given as[26,27]:

$$\omega_{\text{SP}}^{m,n} \cong cG_{mn}\big/\sqrt{\varepsilon_{\text{d}}}\ , \tag{5}$$

where $\omega_{\text{SP}}^{m,n}$ is the resonance frequency of the SP mode given by the momentum relationship, c is the speed of light in vacuum, $G_{mn}=(2\pi/A)\sqrt{m^2+n^2}$ is the grating momentum wave vector for two-dimensional square hole arrays, A is the lattice period of the array, m and n are integers of the SP modes, and ε_{d} is the dielectric constant of medium contact with the metal. Thus, the SP modes [m, n] are excited in the interface of Cu and silica-glass at 1.53 [±1, 0] THz and 2.16 [±1,±1] THz, respectively, when A is selected as 100 μm.

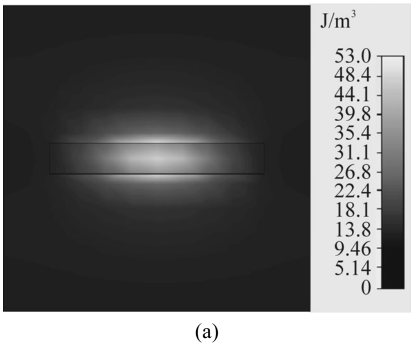
In order to further investigate the influence of the temperature on the transmittance of the filter, the electric energy density distributions on the Cu surface of one unit cell of the sandwich filter with the structural parameters defined in Fig.2(b) for 1.25 THz wave are calculated at 50 °C, 67.5 °C and 80 °C as shown in Fig.4(a), (b) and (c), respectively. At the low temperature of 50 °C, the THz waves at frequency of 1.25 THz are concentrated in the rectangular hole in the center of the device with the maximum power density of 53 J/m^3, because the thin insulating film VO_2 is nearly transparent to the THz waves. As the temperature is increased to 67.5 °C, the VO_2 film undergoes a phase change, with the effective conductivity of 4.33×10^4 S/m. Accordingly, the maximum power density is decreased to 9.32 J/m^3 at 1.25 THz, and the THz waves through the device are significantly reduced. When the temperature is further increased to 80 °C, the conductivity of the thin metallic film VO_2 approaches 2.76×10^5 S/m and the maximum power density is deduced to 1.11 J/m^3. These results indicate that the transmittance of the device is mainly determined by the thermally tunable VO_2 thin film.



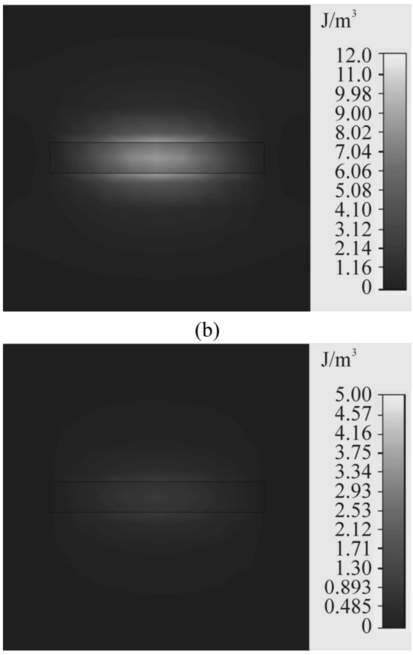
(a)

(b)

Fig.3 THz transmission spectra of the filter at various temperatures calculated with the FDTD method: (a) The heating process; (b) The cooling process (Inset: the polarization direction of the terahertz wave)



(a)



(b)

(c)

Fig.4 Electric energy density distributions on the Cu film side of a unit cell at 1.25 THz at the temperatures of (a) 50 ℃, (b) 67.5 ℃ and (c) 80 ℃ during the heating process

In summary, we propose a THz bandpass filter with subwavelength rectangular Cu hole arrays and thermally tunable VO_2 thin film added on the surface of silica glass like a sandwich. This device provides the narrow band THz waves with the transmittance from 85.2% to 10.5% at 1.25 THz, which is related to the variation in the effective conductivity of VO_2 thin film as a result of thermal-triggered insulator-metal transition. Therefore, this device is a thermally controllable intensity modulator in the THz regime, which has potential applications in the fields of THz imaging, sensing and communications.

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