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The influence of the two-dimensional sinusoidal gratings on the near-field radiative heat flux between two doped silicon films

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ABSTRACT

The near-field radiative heat flux between two two-dimensional sinusoidal grating surfaces made of doped-silicon is investigated by the finite difference time domain (FDTD) method. The parameter Λ , which is defined as the ratio of the amplitude to the period of the two-dimensional sinusoidal grating surface, is used to characterize the surface feature. When the amplitude is much smaller than the period, the surface effect is not significant to modify the near-field radiative heat flux between two smooth films. However, when the amplitude is comparable with the period, the near-field radiative heat flux between two smooth films can be enhanced remarkably. The coupling of the localized surface modes between the may be responsible for the variation of the near-field radiative heat flux when the parameter Λ is changed. Moreover, the effect of the lateral displacement of the films on the near-field radiative heat flux is also studied. The results indicate that the near-field radiative heat flux will achieve the maximum value when the peaks of the sinusoidal gratings are aligned. This work will be valuable to research on contactless thermal management in nanoscale.

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1. Introduction

When the distance between two emitting objects is less than or comparable with the dominated wavelength of the thermal emission, the radiative heat flux can exceed the Planck's blackbody limit by orders of magnitude [\[1\]](#page--1-0). This radiative heat transfer is called near-field radiative heat transfer. In the past decades, researchers have extensively investigated the near-field radiative heat transfer between two smooth surfaces based on the scattering matrix theory, dyadic Green's function (DGF) method and the fluctuational electrodynamics theory $[1-9]$. The underlying mechanisms for enhancing the near-field radiative heat flux have been attributed to the photon tunneling effect and coupling of surface polaritons (SPs) [\[10–12\].](#page--1-0) The theoretical research is well supported by experiment research in recent years, exhibiting that experimental prediction agrees well with the theoretical prediction by the fluctuating electrodynamics in the sub-wavelength scale, even for the extremely near-field radiative heat flux [\[13–21\]](#page--1-0). Benefitting from the above fundamental studies, numerous applications have been proposed by the researchers, such as thermal based data

recording [\[22\],](#page--1-0) thermal rectification [\[10,23,24\],](#page--1-0) energy harvesting [\[25–27\]](#page--1-0) and thermal imaging [\[28\].](#page--1-0)

Recent decades, the technologies of nanofabrication enable the further explorations of the near-field radiative heat transfer without limited to the plane surface. The artificial materials with periodic patterned surface, for example gratings, can exhibit intriguing physical properties in the near-field radiation transfer [\[29\]](#page--1-0). Biehs et al. [\[30\]](#page--1-0) have theoretically investigated the near-field heat transfer between two gratings, illustrating the relative orientation and distance effects on the heat flux. The results show that the net heat flux can be modulated up to 90% by changing the angle between the optical axes at room temperature. Liu et al. [\[31\]](#page--1-0) have investigated the near-field radiative heat transfer between two graphene covered corrugated silica plates, indicating that graphene can promote the radiative heat flux between the gratings and alleviate the sensitivity of the radiative heat flux to lateral shift. Yang et al. [\[32\]](#page--1-0) have theoretically demonstrated the near-field radiative heat flux between two one-dimensional periodic metallic gratings by rigorous coupled-wave analysis (RCWA). They have found that the radiative heat flux between the gratings can be additionally enhanced by the magnetic polaritons excited between the grating ridges except for the coupling of the surface plasmon polaritions. The findings give a new method to spectrally control the near-field radiative heat transfer between two metallic gratings.

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Nevertheless, the existing work concentrate mainly on the rectangle gratings and hence it is fascinating that how the nonrectangular gratings affect the near-field radiative heat flux. In the presented work, the two-dimensional sinusoidal grating is used to estimate the non-rectangular grating effects on the nearfield radiative heat flux by the FDTD method.

The FDTD method, which has been successfully employed to tackle the electromagnetic scattering problems, is also a powerful tool to deal with the near-field radiative heat flux problems of any periodic nanostructure [\[33–36\]](#page--1-0). In this paper, a brute-force approach based on the FDTD method [\[37\]](#page--1-0) is employed to compute the near-field radiative heat flux between two closely spaced doped-silicon films in the vacuum. The surface morphology of the film is characterized by two-dimensional sinusoidal grating surface, where the parameter Λ is used to characterize the surface feature and is defined as the ratio of the amplitude to the period of the two-dimensional sinusoidal grating surface. The effects of the structural parameters (including lateral displacement) of the surfaces on the near-field radiative heat flux are investigated. The results indicate that the near-field radiative heat flux between two closely spaced doped-silicon films can be enhanced due to the coupling of the localized surface modes when the parameter Λ is increased. This work will be valuable to research on contactless thermal management in nanoscale.

2. Theoretical formulation and calculation model

The DGF is used to relate the elementary electric and magnetic currents to the electric and magnetic fields created by them [\[7\].](#page--1-0) The electric $\,E\,$ field and magnetic H field induced by the electric current \int^e can be written as [\[6,7\]](#page--1-0)

$$
\overrightarrow{E}(\overrightarrow{r},\omega) = j\omega\mu_0 \int_{V'} dV \overline{\overline{G}}^{ee}(\overrightarrow{r},\overrightarrow{r}',\omega) \cdot \overrightarrow{J}^e(\overrightarrow{r}',\omega)
$$
 (1)

$$
\vec{H}(\vec{\mathbf{T}},\omega) = \int_{V'} dV \overline{\vec{G}}{}^{me}(\vec{\mathbf{T}},\vec{\mathbf{T}}',\omega) \cdot \vec{J}^{\cdot e}(\vec{\mathbf{T}}',\omega)
$$
 (2)

where *j* is the imaginary unit. $\overline{\overline{G}}^{ee}(\overrightarrow{r}, \overrightarrow{r}', \omega)$ is the electric type DGF and $\overline{\overline{G}}^{\text{me}}(\overrightarrow{r}, \overrightarrow{r}, \omega)$ is the magnetic-electric type DGF [\[7\].](#page--1-0) The electro-
magnetic wave of the thermal emission is induced by the fluctuatmagnetic wave of the thermal emission is induced by the fluctuating electric currents within the emitting objects. Base on the fluctuation–dissipation theorem (FDT), the correlation function of the fluctuating electric currents $\overrightarrow{J}^e(\overrightarrow{r}, \omega)$ within the nonmagnetic
isotropic materials can be expressed as [1, 3] isotropic materials can be expressed as [\[1–3\]](#page--1-0)

$$
\langle \vec{J}_{\alpha}^{\,e}(\vec{\Gamma}',\omega) \vec{J}_{\beta}^{\,e}(\vec{\Gamma}'',\omega') \rangle
$$

=
$$
\frac{\omega \varepsilon_0 \text{Im}[\varepsilon_r(\omega)]}{\pi} \Theta(\omega,T) \delta(\vec{\Gamma}'-\vec{\Gamma}'') \delta(\omega-\omega') \delta_{\alpha\beta}
$$
(3)

where $\langle \rangle$ represents the ensemble average of the fluctuating currents and ε_0 is vacuum permittivity. Im $[\varepsilon_r(\omega)]$ and T are the imaginary part of the relative permittivity and temperature of emitter, respectively. The Dirac delta functions $\delta(\vec{r}' - \vec{r}'')$ and $\delta(\omega - \omega')$
represent the incoherance of spatial and frequency. The Kronecke Þ represent the incoherence of spatial and frequency. The Kronecker delta function $\delta_{\alpha\beta}$ indicates the incoherence of the amplitude directions of the fluctuating electric current. $\Theta(\omega, T) =$ $\hbar\omega/|\exp(\hbar\omega/k_B/T)-1|$ is the average energy of the Planck's oscillator at temperature T and frequency ω .

With the DGF method and FDT, the expression of the radiative heat flux Q_z is expressed as [\[4,37\]](#page--1-0)

$$
Q_z = \frac{2k_0^2}{\pi} \int \Theta(\omega, T_1) - \Theta(\omega, T_2) d\omega
$$

$$
\int_{V'} Re \left[j \varepsilon_r'' \cdot \sum_{\alpha = x, y, z} \left(G_{xx}^{ee} G_{yx}^{me*} - G_{yx}^{ee} G_{xx}^{me*} \right) \right] dV'
$$
 (4)

where k_0 is the wave vector in vacuum, T_1 and T_2 are the temperatures of the emitter and receiver. According to Eq. (4), the radiative heat flux can be obtained if the dyadic Green's functions are known.

The analytical expressions of the Green's functions for layered structures can be easily obtained by means of the scattering matrix method [\[4,7\].](#page--1-0) Nevertheless, the exact expressions of the Green's functions for the complicated structures can hardly be derived analytically. Fortunately, the Green's functions of the complicated structures can be numerically computed by the FDTD method [\[36\]](#page--1-0). By using the spectrum of the excitation point source $\hat{J}_{g}^{e}(\mathbf{r}', \omega)$ to normalize the Fourier transform of the fields $\Omega_{i}(\mathbf{r}, \mathbf{t})$, the component of electric type Green tensor is expressed as [\[36\]](#page--1-0)

$$
G_{ix}^{ee}(\mathbf{r},\mathbf{r}',\omega) = \frac{\Omega_i(\mathbf{r},\omega)}{\int_{\alpha}^e(\mathbf{r}',\omega)} = \frac{F[\Omega_i(\mathbf{r},\mathbf{t})]}{F[\int_{\alpha}^e(\mathbf{r}',\mathbf{t})]}
$$
(5)

where $i, \alpha \in \{x, y, z\}$. F[] represents the Fourier transform operator, Ω is the symbol for the electric and magnetic field. The point sources distributed within the emitting object are computed by FDTD with an ergodic method. Then the radiative heat flux can be figured out by adding up the resulted Poynting vectors of each simulation.

3. Schematic diagram and some default definitions

The Fig. 1(a) depicts the schematic structure of the twodimension sinusoidal grating. The surface profile of the film is described by the sinusoidal function along the x and y directions, which can be mathematically described as

$$
z_{\text{surface}} = z_b + A \cdot \sin\left[\frac{2\pi}{L} \cdot (x - r_x)\right] \cdot \sin\left[\frac{2\pi}{L} \cdot (y - r_y)\right] \tag{6}
$$

where A and L are the amplitude and the period of the twodimensional sinusoidal grating, respectively. r_x and r_y are respectively the relative lateral displacements along the x and y directions, which can be recorded by binary array (r_x, r_y) . As is shown in Fig. 1 (a), the plane $(z = z_b)$ and the thickness d of the grating are

Fig. 1. Schematic diagrams of the structures.

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