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Near-field radiative heat transfer with doped-silicon nanostructured metamaterials

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The objective of this work is to evaluate different practically achievable doped-silicon (D-Si) nanostructured metamaterials (including nanowires and nanoholes, multilayers, and one-dimensional gratings) in terms of their potential for enhancing near-field radiative heat transfer at ambient temperature. It is found that both doped silicon nanowires and nanoholes may achieve an enhancement over bulk doped silicon by more than one order of magnitude in the deep submicron gap region. The enhancement is attributed to either the broadband hyperbolic modes or low-loss surface modes or a combination of both. On the other hand, polarization coupling, which can occur in the grating configuration, contributes little to the radiative transfer at the nanometer scale. This work will facilitate the application of nanostructures in more efficient non-contact thermal management, thermal imaging, and near-field thermophotovoltaics.

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1. Introduction

Near-field radiative heat transfer has attracted significant attention in recent years due to its wide potential applications in microscale thermophotovoltaic (TPV) cells [1–8], submicron thermal imaging [9–12], non-contact thermal rectifiers [13–16], thermal modulators [17–19], and local thermal management [20–22]. Planck's law of blackbody radiation breaks down when two objects at different temperatures are placed close enough, i.e., at a distance close to or smaller than the characteristic wavelength of thermal radiation [23–25]. At nanometer distances, near-field radiative heat transfer could be orders of magnitude greater than that between two blackbodies, especially when surface plasmon polaritons (SPPs) or surface phonon polaritons (SPhPs) are excited [26–29]. A number of groups have experimentally demonstrated that near-field radiation can exceed the blackbody limit using plate-plate or sphere-plate geometries [30–35].

Large heat transfer coefficients are desired for increased power throughput or heat dissipation in energy harvesting [4] or cooling [20] applications, respectively. However, the super-Planckian thermal radiation enabled by surface modes (either SPPs or SPhPs) is usually narrowband and has high loss due to the inherent resonance effects, thus precluding more efficient heat transport. Reducing material loss (e.g., by reducing the electron scattering rate) could increase the cutoff wavevector and thus helps to improve near-field heat transfer [27,36]. Another method to obtain higher radiative heat flux is to broaden the super-Planckian radiation band with the help of the resonance-free hyperbolic modes [37–41]. Hyperbolic dispersion or hyperbolic modes may exist in natural or artificial anisotropic materials in certain frequency regions, where the electromagnetic waves with large transverse wavevector can propagate inside the hyperbolic metamaterials, unlike surface modes where the electromagnetic waves propagate only along the interface and decay into both media. Hyperbolic metamaterials, no matter whether they exist in nature (such as graphite) or are artificially synthesized, exhibit hyperbolic dispersion only in certain frequency ranges and are not ideally lossless [38–42]. Therefore, achieving a great enhancement of near-field radiative thermal transport beyond bulks for more efficient thermal transport or heat dissipation is still a challenge.

Doped silicon (D-Si) has been shown to support surface modes in the infrared spectrum and can enhance near-field radiative transfer [23,27,29,43] to similar magnitude as those for SiC and SiO_2 based on narrowband phonon modes [44]. Furthermore, the doping level can be varied to tune the far-field radiative properties [45] or near-field heat transfer [46]. Recent studies have shown that doped Si nanowires can enhance near-field radiation over bulk by several times [47]. Additionally, doped Si nanowires can exhibit

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Nomenclature

c	speed of light in vacuum
$\mathbf{D}$	matrix
d	gap distance, m
f	volume filling ratio of D-Si
h	heat transfer coefficient, W/m^2 K
$\hbar$	reduced Planck constant, J s
$\mathbf{I}$	unit matrix
i	$\sqrt{-1}$
k	wavevector, m^{-1}
k_0	wavevector in vacuum, m^{-1}
k_B	Boltzmann constant, J/K
n	complex refractive index
$\mathbf{R}$	matrix formed by reflection coefficients
r	Fresnel's reflection coefficient
T	temperature, K

Greek symbols

β	transverse wavevector, m^{-1}
Δ	relative rotation angle between the gratings, rad
ε	dielectric function
λ	wavelength, m
ξ	energy transmission coefficient or transmission factor
σ	Stefan–Boltzmann constant, W/m^2 K^4
ϕ	azimuthal angle, rad
ω	angular frequency, rad/s
ω_m	surface plasmon frequency, rad/s

Subscripts

E	extraordinary wave
O	ordinary wave
p	p polarization or TM wave
s	s polarization or TE wave

hyperbolic modes and support negative refraction in a broad frequency range [48]. Different techniques have been successfully demonstrated to create controlled silicon nanostructures [49,50]. It is envisioned that D-Si nanostructures may allow near-field radiative heat transfer to be significantly enhanced by enabling hyperbolic modes or by reducing loss for surface modes.

Four practically achievable nanostructures based on D-Si are considered here, namely, nanowires, nanoholes, multilayers, and one-dimensional (1D) gratings. Fluctuation–dissipation theorem is used to calculate the near-field and far-field radiative transfer, assuming that the nanostructures can be treated as an effective homogeneous medium with anisotropy. The mechanisms of enhancement or reduction of radiative transfer are elucidated by considering the frequency- and wavevector-dependent energy transmission factor.

2. Theoretical formulation

The schematics of doped-silicon nanowires (D-SiNWs), doped silicon nanoholes (D-SiNHs), multilayered metamaterials, and 1D gratings are shown in Fig. 1, where the x and y directions are assumed to extend to infinity and each medium is assumed to be semi-infinite. Both the multilayer and 1D grating structures are composed of D-Si and germanium (Ge), while nanowire and nanohole D-Si configurations are surrounded by vacuum. The filling ratio f for all aforementioned four different nanostructures is defined based on the volume fraction of D-Si, and d is the gap distance. Note that the minimum f for aligned D-SiNHs is $(1-\pi/4)$, and the maximum f for aligned D-SiNWs is $\pi/4$, due to the geometrical limitations of the circular holes and wires, assuming the 2D lattice to be square. The dielectric function of D-Si is governed by the Drude model and can be obtained from Basu et al. [51]. The dielectric function of Ge is largely independent of wavelength in the infrared region, and can be approximated as a constant with $\varepsilon_{Ge} = 16$. Local effective medium theory (LEMT) is used to obtain the anisotropic dielectric function and is combined with fluctuational electrodynamics to calculate the near-field radiative heat transfer coefficient due to its simplicity and low computational demand [17,36–42,47,52]. The aforementioned nanostructures are treated as homogenous uniaxial materials; this assumption is valid in the far field as long as the characteristic thermal wavelength is much greater than the nanostructure period. In the near field, as pointed out by some investigators, nonlocal effects would arise at the resonance frequency of surface plasmon polaritons (SPPs) or very large wavevectors [39,53,54]. Nevertheless, when the gap distance is much greater than the period of nanostructures, LEMT should be applicable in the near field as well [36]. In the present study, the period of nanostructures is assumed to be sufficiently small, so that LEMT can be applied to both the far and near fields.

In the Maxwell–Garnett theory, the effective properties of a composite medium are obtained by treating one constituent of the composite as the host and all other constituents as embedded grains (fillers), which are not in contact with one another. For D-SiNWs, vacuum is treated as the host with D-Si as the filler. For D-SiNHs on the other hand, D-Si is the host. When the electric field is along the optical axis (z direction), the dielectric function for both nanowires and nanoholes is given as

$$\varepsilon_z = 1 - f + \varepsilon_{\text{D-Si}} f \tag{1}$$

Here, ε_z is essentially governed by a diluted Drude model, since it is just the weighted average of the dielectric functions of doped silicon and vacuum. Note that Eq. (1) can be obtained from different effective medium approximations and should be valid for any f [47]. The Drude model of D-Si may be written as $\varepsilon(\omega) = \varepsilon_\infty - \omega_p^2/(\omega^2 + i\gamma\omega)$, where ε_∞ is a high-frequency constant, ω_p is the plasma frequency, and γ is the scattering rate [51]. The plasma frequency for D-SiNWs is $\sqrt{f}$ times that of D-Si; and the high-frequency term for D-SiNWs is $(1 - f + f\varepsilon_\infty)$, which varies from 1 for $f = 0$ to ε_∞ for $f = 1$. When the electric field is perpendicular to the optical axis, the ordinary dielectric function ε_x, which is equal to ε_y, of nanowires is governed by [45]

$$\varepsilon_{x,\text{NW}} = \frac{\varepsilon_{\text{D-Si}} + 1 + (\varepsilon_{\text{D-Si}} - 1)f}{\varepsilon_{\text{D-Si}} + 1 - (\varepsilon_{\text{D-Si}} - 1)f} \tag{2}$$

Note that $\varepsilon_{x,\text{NW}}$ given above can be expressed as a Lorentz model, and detailed derivations can be found from [45]. From a physical point of view, it is because the free electrons in nanowires are bounded by surrounding vacuum [48]. It is assumed that Eq. (2) is applicable to any f until it reaches the maximum limit of $\pi/4$, when the diameter of the Si wire is the same as the period of the unit cell. This is a reasonable assumption as long as the Si wires are separated from each other. For nanoholes, Si should be treated as the host and

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