Plasmonic thermal transport in graphene nanodisk waveguides

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(Received 13 May 2017; published 16 October 2017)

DOI: 10.1103/PhysRevB.96.165428

I. INTRODUCTION
Thermal activation of electromagnetic (EM) surface modes, such as surface plasmon-polaritons or surface phonon-polaritons, can lead to a thermal radiation flux at sub-wavelength gaps that is orders of magnitude larger than the Planck black-body limit. The strong near-field coupling in materials that support surface polaritons suggests a new form of thermal transport mediated by guided EM modes. While optical losses are essential for enhanced near-field radiative heat transfer, they limit mode propagation in waveguides. As such, the thermal conductivities of polaritonic waveguide arrays have been predicted to be small, with maximum values of $1 \times 10^{-8}$ W m$^{-1}$ K$^{-1}$ for surface plasmons in a copper nanosphere array and 0.04 W mm$^{-1}$ K$^{-1}$ for surface phonon-polaritons in a silicon carbide nanospheroid array.

The emergence of graphene as a platform for terahertz plasmon-enhanced thermal transport is assessed by predicting their heat capacities, thermal conductivities, and thermal diffusivities in a variety of configurations. The conclusions are presented in Sec. V.

II. METHODS
A. Graphene optical conductivity

The optical response of graphene is dictated by the two-dimensional optical conductivity, $\sigma$, which is controlled by the electron concentration, or equivalently, the Fermi level $E_f$ above the Dirac point. Fermi levels up to 1 eV have been realized by electrical gating. According to the random phase approximation, the optical conductivity of graphene in the local limit is given by

$$\sigma(\omega) = \frac{2e^2k_BT}{\pi\hbar^2} \frac{i}{\omega + i\tau} \ln[2\cosh(E_f/2k_BT)]$$
$$+ \frac{e^2}{4\hbar} \left[ H(\omega/2) + \frac{4i\omega}{\pi} \int_0^{\infty} \frac{H(x) - H(\omega/2)}{\omega^2 - 4x^2} \, dx \right],$$

where

$$H(x) = \frac{\sinh(\hbar x/k_BT)}{\cosh(E_f/k_BT) + \cosh(\hbar x/k_BT)}.$$

Here, $e$ is the electron elementary charge, $k_B$ is the Boltzmann constant, $T$ is the temperature, $\hbar$ is the reduced Planck constant, $\omega$ is the angular frequency, and $\tau$ is the impurity-limited lifetime. The first term on the right-hand side is not restricted by the separation between disks because the calculations are based on analytical expressions for the interactions between all plasmon modes.
side corresponds to the contribution from intraband transitions and the second term corresponds to the contribution from interband transitions.

Interband transitions become important at photon energies, $\hbar \omega$, satisfying the condition $\hbar \omega / E_f > 1$ [23]. Optical losses due to interband transitions are given by $\tau = \mu E_f / \epsilon_2^2$, where $\mu$ is the electron mobility and $v_f = 10^6 \text{ m/s}$ is the Fermi velocity [22]. We consider a mobility of 10 000 cm$^2$ V$^{-1}$ s$^{-1}$, which is a conservative value compared with the largest mobilities observed in high-quality suspended graphene ($\mu > 15 000 \text{ cm}^2 \text{ V}^{-1} \text{s}^{-1}$) [21].

At room temperature ($E_f / k_B T > 1$), Eq. (1) can be simplified to [8,23]

$$\sigma(\omega) = \frac{e^2 E_f}{\pi \hbar^2} \frac{i}{\omega + i \tau^{-1}} + \frac{e^2}{4\hbar} \left[ \Theta(h\omega - 2E_f) + \frac{i}{\pi} \ln \left| \frac{\hbar \omega - 2E_f}{\hbar \omega + 2E_f} \right| \right],$$

(2)

where $\Theta$ is the step function.

### B. Plasmonic band structure

The transport properties of guided surface plasmon modes in a periodic one-dimensional co-planar disk array are obtained from an eigenvalue problem that is described in Sec. S1 of Ref. [24]. The formulation considers the Coulombic (i.e., electrostatic) interactions between disks using the semi-analytical model from Ramirez et al. [6] [Eq. (S10)]. The solution is given by a set of complex eigenfrequencies $\tilde{\omega}_p$, whose real part $\omega_p$, defines the dispersion relation and whose imaginary part represents the mode's temporal losses through the relation $\tau_p = [2\Im(\tilde{\omega}_p)]^{-1}$. At low temperatures ($E_f / k_B T > 1$) and surface plasmon energies $\hbar \omega_p$, satisfying the condition $\hbar \omega_p / E_f < 1$, the second term on the right-hand side of Eq. (2) becomes negligible and $\tau_p = \tau$.

To account for the effects of the substrate in supported disk arrays, we consider the disks to lie between two regions with dielectric constants $\epsilon_1$ (above the array) and $\epsilon_2$ (the substrate). Unless noted, $\epsilon_1 = 1$, which corresponds to vacuum. The separation between disks is maintained at $\Delta x / D \geq 1.1$, where $\Delta x$ and $D$ are the disk center-to-disk center separation and the disk diameter. Under these conditions, quantum effects such as electron tunneling can be ignored [25].

### III. PLASMONIC PROPERTIES

#### A. Dispersion relation and decay length

The dispersion relation of a one-dimensional array of highly-doped graphene disks ($E_f = 1.0 \text{ eV}$, $D = 100 \text{ nm}$, and $\Delta x = 110 \text{ nm}$) over a substrate with $\epsilon_2 = 2.4$ are plotted in Fig. 1(a). This Fermi level was chosen to show the upper limit of the wave-guiding properties in terms of doping by electrostatic gating. The dielectric constant of the substrate represents the average value for SiO$_2$ for the frequency spectrum considered in Fig. 1(a) [26]. The plasmonic bands can be classified according to the radial ($k = 0, 1, \ldots$) and angular ($l = 0, \pm 1, \pm 2, \ldots$) indices of the localized surface plasmons in a single graphene disk [6]. Here, only the modes corresponding to the lowest radial mode ($k = 0$) are presented.

![Figure 1](image-url)

**FIG. 1.** (a) Dispersion relation and (b) decay lengths of the lowest radial modes ($k = 0$) for a one-dimensional periodic co-planar array of graphene disks ($E_f = 1.0 \text{ eV}$, $D = 100 \text{ nm}$, and $\Delta x = 110 \text{ nm}$). The dispersion for EM-waves propagating in vacuum ($\epsilon_1 = 1.0$) and in a dielectric substrate ($\epsilon_2 = 2.4$) are included in (a) as a reference, where $v_\epsilon$ is the speed of light in vacuum. The inset of (b) shows the decay length in terms of number of cycles completed, $L_p / \lambda_{sp}$, for the fundamental dipole modes, $(l, l) = (0, \pm 1)$.

Modes with $k > 0$ have group velocities close to zero and their contributions to thermal transport can be ignored, as revealed by analysis of the frequency-dependent thermal conductivity accumulation (see Sec. IV A). For each angular mode with $l > 0$, longitudinal and transverse polarizations are observed, where the modes on each disk oscillate parallel and perpendicular to the direction of propagation. The dispersion relations of EM waves in vacuum and in the dielectric substrate are also plotted. These linear bands show the large degree of confinement of the fundamental dipole modes ($k, l) = (0, \pm 1$), as their dispersion lies mostly outside of the light cone.

The $1/e$ decay lengths, $L_p$, are obtained from

$$L_p = \tau_p v_s,$$

(3)

where $v_s = \frac{d\omega_p}{dk_p}$ is the group velocity of the surface plasmon and $k_p$ is its wavenumber. As our model is based on the electrostatic approximation, radiation damping effects, i.e., surface plasmon decay through retardation of EM waves and radiation reaction, are ignored. Thus the mechanisms of plasmon decay are directly related to the optical losses dictated by intraband and interband transitions from Eq. (1).

Using Eq. (3), the decay lengths of the modes from Fig. 1(a) are plotted in Fig. 1(b). The longitudinal fundamental dipole modes have the largest decay lengths, with a maximum of 3.1 $\mu$m. The transverse fundamental dipole modes have a maximum decay length of 1.2 $\mu$m. Surface plasmon modes
with \( l > 1 \) show smaller decay lengths as the magnitude of \( l \) increases due to a reduction in their group velocities. The number of wave-cycles completed, \( L \Delta x / \lambda_p \), for \( l = \pm 1 \), where \( \lambda_p = 2\pi / k_p \) is the surface plasmon wavelength, is plotted in the inset to Fig. 1(b). The longitudinal and transverse modes reach a maximum of eight and three cycles before decaying.

**B. Effect of radiation damping on the plasmonic band structure**

Radiation damping, i.e., retardation of EM waves and radiation reaction, is neglected in our electrostatic model [Eq. (S8)]. Its effect is evaluated in this section by comparing the frequencies and decay lengths of the fundamental dipole modes \([k, l = (0, \pm 1)]\) predicted from our model with those obtained when the full dipole-dipole interactions are included. Higher-order modes cannot couple to light in the free space and are thus unaffected by radiation damping. The full dipole-dipole interaction model is based on the exact solution of the EM fields emitted by an electric dipole [Eq. (S11)]. This approach has been used to represent the interactions between graphene nanodisks when \( \Delta x / D > 1.5 \) [27,28]. To study arrays with \( \Delta x / D < 1.5 \), we built a model [Eq. (S18)] that considers electrostatic interactions of a disk with its nearest-neighbor and full dipole-dipole interactions with the other disks in the array. This added level of detail provides better accuracy in predicting the plasmonic band structure. In comparison with our electrostatic model, inclusion of the full dipole-dipole interactions results in a nonlinear eigenvalue problem that does not allow for nondimensionalization [29]. Thus a separate calculation is needed for every disk array configuration. The electrostatic model, on the other hand, allows for the extraction of multiple band structures from a single nondimensional dispersion (see Sec. III C). This nondimensionalization is particularly advantageous when multiple plasmonic band structures are required, as in the determination of the plasmonic thermal properties discussed in Sec. IV.

The surface plasmon frequencies and decay lengths of the longitudinal and transverse fundamental dipole modes obtained from the full dipole-dipole interaction and from our electrostatic model are plotted for arrays with disks of diameter of 100 nm in Fig. 2(a) and 500 nm in Fig. 2(b). In these plots, \( E_f = 1.0 \text{ eV} \) and \( \Delta x / D = 1.1 \). We consider the case of suspended disk arrays \((\varepsilon_1 = \varepsilon_2 = 1)\) as the full dipole-dipole interaction model is constructed on the basis of dipole arrays lying in a homogeneous host. The frequencies predicted for a disk diameter of 100 nm show no difference. The decay lengths show a deviation of at most 5% as a consequence of changes in the mode lifetime (Fig. S2(a)), which is a result of the radiation damping of modes below the light line [29,30]. For a disk diameter of 500 nm, the deviation is at most 0.4% for the frequencies. The difference is characterized by a dip in the dipole-dipole prediction at the crossing between the light line and the transverse polarization band. It is a result of the coupling of dipole modes with light traveling in the free space due to a lower degree of confinement [29]. The coupling with light in the free space also affects the mode lifetimes, as shown in Fig. S2(b). As a result of these changes in the frequencies and lifetimes, the decay lengths predicted with the electrostatic model for \( D = 500 \text{ nm} \) show a larger discrepancy than for \( D = 100 \text{ nm} \).

**FIG. 2.** Surface plasmon dispersion relations and decay lengths of the fundamental dipole modes \([k, l = (0, \pm 1)]\) for an array of graphene nanodisks in vacuum with \( \Delta x / D = 1.1 \), \( E_f = 1.0 \text{ eV} \), \( \varepsilon_1 = \varepsilon_2 = 1 \), and (a) \( D = 100 \text{ nm} \) and (b) \( 500 \text{ nm} \). The lines correspond to the full dipole-dipole interaction model from Eq. (S18) and the open circles correspond to the electrostatic model from Eq. (S8).

The average relative error between both models for disk arrays \((E_f = 1.0 \text{ eV} \text{ and } \varepsilon_1 = \varepsilon_2 = 1)\) with diameters of 100, 200, 500, and 1000 nm and separations \( \Delta x / D \) of 1.1, 1.6, and 1.9 are provided in Table I. For disk diameters of 100 and 200 nm, the deviation is less than 1% in the frequencies and less than 12% in the decay lengths. For the larger disk diameters, the frequencies remain within 1% agreement, but the decay lengths deviate by up to 23% \((D = 500 \text{ nm})\) and 68% \((D = 1000 \text{ nm})\). The deviation is the result of the lower degree of confinement as the disk size increases. Our electrostatic model is thus an efficient and accurate way to predict the plasmonic properties in disk arrays with diameters smaller than 200 nm. At larger disks diameters, the model continues to offer accurate predictions of the frequencies but loses accuracy for the decay lengths. The suitability of the electrostatic model for thermal conductivity prediction is investigated in Sec. IV A.

**C. Nondimensionalization**

Under the electrostatic approximation, the plasmonic eigen-modes of coupled nanostructures can be directly extracted...
from a nondimensional Hermitian eigenvalue problem [31]. Inspection of Eq. (S8) shows that in the case of graphene nanodisk arrays, the nondimensional eigenfrequency $\Omega_p$ is strictly dependent on the nondimensional parameters $k_p \Delta x$ and $\Delta x/D$, where $\Omega_p$ is given by

$$\Omega_p = \sqrt{\frac{i \omega_0 \epsilon_0 \epsilon_h D}{2 \sigma}}. \tag{4}$$

Here, $\epsilon_0$ is the permittivity in vacuum and $\epsilon_h = (\epsilon_1 + \epsilon_2)/2$ is the average dielectric constant. This transformation allows us to reduce the number of independent variables that define the plasmon frequency, i.e., $\omega_0 = f(k_p, \Delta x, D, \epsilon_h, \sigma)$. For a given $\Delta x/D$, multiple dispersion relations can be extracted from a single $\Omega_p$ dispersion. The dispersion relation given by $\Omega_p$ can be fitted using an electrostatic dipole-dipole interaction model (see Appendix).

At low temperatures ($k_B T/E_f \ll 1$), $\sigma$ is given by Eq. (2). Assuming only intraband transitions (i.e., $\hbar \omega_{l,P}/E_f < 1$), Eq. (4) can be simplified to

$$\Omega_p \approx \omega_p/\omega_R, \tag{5}$$

where

$$\omega_R = \sqrt{\frac{2E_f e^2}{\pi \hbar^2 \epsilon_0 \epsilon_h D}} \tag{6}$$

is the characteristic plasmon frequency. With this result, a nondimensional expression for the decay length is given by

$$\frac{L_p}{\tau \omega_R D} = \frac{\Delta x}{D} \frac{d \Omega_p}{d (k_p \Delta x)}, \tag{7}$$

where we replace $\tau_p$ by $\tau$ as only intraband transitions are present (see Sec. II B).

The characteristic plasmon frequency provides a reference of the frequency range of the plasmonic band structure. For example, for the conditions of the dispersion relation plotted in Fig. 1(a), $\omega_R = 44 \text{ THz}$, which is within the frequency range of the lowest bands. Based on the conditions used to derive Eqs. (5) and (7) (i.e., low temperature and only intraband transitions), a criterion to evaluate the validity of the proposed scaling relations is $\chi_T \equiv \hbar \omega_R k_B T/E_f^2 \ll 1$.

The nondimensional dispersion for $\Delta x/D = 1.1$ for the transverse and longitudinal fundamental dipole modes is plotted in Fig. 3(a) for a selection of $E_f$, $D$, and $\epsilon_2$. The results are compared with the exact solution from Eq. (4), which is plotted as black circles. The simplified expression for the frequency remains valid when $\hbar \omega_R k_B T/E_f^2 < 0.02$ (less than 1% relative error). For $D = 100 \text{ nm}$, $E_f = 0.1 \text{ eV}$, and $\epsilon_2 = 1$ (case 3), which has $\chi_T = 0.28$, a deviation of up to 8% is present.

The nondimensional decay lengths corresponding to the dispersion curves from Fig. 3(a) are plotted in Fig. 3(b). There is no exact solution to compare to for the decay length, as Eq. (7) was obtained for the specific conditions of low temperature and only intraband transitions. The three curves that satisfy the criterion $\chi_T \ll 1$ fall within a range of 3%. The case 3 curve, which has $\chi_T = 0.28$, is redshifted by 8% and reduced in magnitude by 42% with respect to the others.

IV. GUIDED SURFACE PLASMONS AS HEAT CARRIERS

A. Heat capacity and thermal conductivity of disk arrays

We now evaluate the thermal transport properties of surface plasmons in one-dimensional co-planar graphene disk arrays using dispersion relations and decay lengths as obtained in Sec. III. The results were obtained using the scaling rules from Eqs. (5) and (7) at a temperature of 300 K.

The volumetric heat capacity ($J \text{ m}^{-3} \text{ K}^{-1}$) due to surface plasmons in the disk array, $C_t$, is calculated from [32]

$$C_t = \frac{2}{A} \sum_{l,p} \int \hbar \omega_{l,p}^2 D_p(\omega_{l,p}^2) \frac{d\epsilon_{BE}}{dT} d\omega_{l,p}, \tag{8}$$

where $A$ is the disk’s cross sectional area ($A = D t$, where $t$ is the thickness of a graphene layer), $D_p(\omega_{l,p}^2)$ is...
the thermal conductivities for all three cases are two and eight orders of magnitude larger than previous predictions of 0.04 W m\(^{-1}\) K\(^{-1}\) [35].

Of these three diameters, the heat capacity is the largest for 500 nm throughout the \(\Delta x/D\) domain, which is a result of competing effects. This phenomenon is demonstrated in the inset of Fig. 4(a), where the heat capacity is plotted as a function of \(D\) for \(\Delta x/D = 1.1, 1.2,\) and 1.3. As the diameter is reduced, the heat capacity in all three curves increases until reaching a maximum at \(D = 234\) nm. To elucidate the origin of the maximum, Eqs. (5) and (7) are used to obtain a set of scaling rules for the parameters in Eq. (8). For example, the density of states can be rewritten in the form

\[
D_p(\omega_p) = \frac{1}{\pi D\omega_r} \left( \frac{D}{\Delta x} \right)^{d(\omega_p/\Delta x)} \frac{d(\delta_p/\Delta x)}{d\omega_p}.
\]

Here, the terms \(D/\Delta x\) and \(d(\omega_p/\Delta x)/d\omega_p\) are invariant under changes to \(D\) when \(\Delta x/D\) is fixed, while the term \(1/\pi D\omega_r\) scales as \(D^{-1/2}\). Therefore the density of states scales with the diameter as \(D^{-1/2}\). From the same analysis, we find that \(\omega_p\) scales as \(D^{-1/2}\). Thus, as the diameter increases, the frequency spectrum is redshifted, increasing the contribution from \(df_{BE}/dT\). This effect competes with the overall reduction in \(h\omega_p D_p(\omega_p)d\omega_p\), which scales as \(D^{-3/2}\).

The thermal transport properties are evaluated under the assumption of diffusive transport [2,3]. This approximation requires that the disk array be longer than the maximum surface plasmon decay length. It has been argued that thermal transport in plasmonic nanostructure arrays may be superdiffusive under certain conditions [4]. Although that behavior is not considered in our diffusive model, its predictions should provide a good estimate of the thermal transport properties.

In the diffusive regime, the array thermal conductivity, \(k_t\), can be calculated from [2]

\[
k_t = \frac{2}{A} \sum_{l,p} \int C(\omega_p) |l|^2 \omega_l \omega_p \sigma l_p \omega_p d\omega_p,
\]

where \(C(\omega) = h\omega D_p(\omega)df_{BE}/dT\) is the frequency-dependent heat capacity [see Eq. (8)]. In writing Eq. (10), we have taken the decay length to be the surface plasmon mean free path, as it represents the distance traveled by a plasmon before its energy dissipates due to interband and intraband transitions (and radiation damping effects, when considered).

The thermal conductivities of the same arrays considered in Fig. 4(a) are plotted in Fig. 4(b) and are of \(O(1 \text{ W m}^{-1} \text{ K}^{-1})\). At \(\Delta x/D = 1.1\), the thermal conductivities for all three cases are two and eight orders of magnitude larger than previous predictions of 0.04 W m\(^{-1}\) K\(^{-1}\) for suspended SiO\(_2\) nanosphere arrays at a temperature of 500 K (Ref. [3]) and \(1 \times 10^{-8}\) W m\(^{-1}\) K\(^{-1}\) for copper nanosphere arrays at a temperature of 900 K [2]. For a given diameter, the thermal conductivity decays monotonically with increasing \(\Delta x/D\), which is a result of the weaker near-field coupling between disks. For a given \(\Delta x/D\), the thermal conductivity for an array with disks of diameter 500 nm is always larger than the other two cases, i.e., thermal conductivity does not change monotonically with the diameter.

In the inset of Fig. 4(b), the thermal conductivity is plotted for \(\Delta x/D = 1.1, 1.2,\) and 1.3 as a function of the disk diameter.

The plasmonic density of states per unit length, and \(f_{BE} = 1/[\exp(h\omega_p/k_B T) - 1]\) is the Bose-Einstein distribution. A graphene thickness of 0.5 nm is chosen based on previous studies of graphene plasmonic nanostructures [8,12]. We note that studies of thermal transport in graphene often use a thickness of 0.34 nm, which is based on the layer separation in graphite [33,34].

In Fig. 4(a), the heat capacity is plotted for doped graphene disk arrays \((E_F = 1.0 \text{ eV})\) on a dielectric substrate \((\varepsilon_2 = 2.4)\) as a function of the separation between disks \(\Delta x/D\) at disk diameters of 100, 500, and 1000 nm. There is a monotonic increase of the heat capacity as \(\Delta x\) is reduced. This increase is a result of stronger near-field coupling, which increases the number of thermally-activated modes. The heat capacities are \(O(0.1 \text{ J m}^{-3} \text{ K}^{-1})\), small in comparison to the phonon heat capacity of a continuous graphene sheet of \(1.6 \times 10^4\) J m\(^{-3}\) K\(^{-1}\) [35].
Similar to the heat capacity, there is a maximum due to the presence of competing effects. From Eqs. (5) and (7), $L_p$ and $v_s$ scale as $D^{1/2}$. Thus the increased mode population for larger disks, represented by a larger contribution from $d_{fBE}/dT$, competes with the decay in the overall contribution from $\tau_{op}D_p(\omega_p)L_p\tau v_s d\omega_p$, which scales as $D^{-1/2}$.

The data plotted as open circles in Fig. 4(b) corresponds to thermal conductivities predicted from the dispersion relations extracted form Eq. (S18), which includes radiation damping. For that calculation, we considered light traveling in a host material with a dielectric constant $\varepsilon_h = (\varepsilon_1 + \varepsilon_2)/2 = 1.7$. The two sets of results follow the same trend and our electrostatic model becomes more accurate as the gap between disks and the disk diameter decrease. The discrepancy is due to radiation damping effects on the plasmonic properties of the fundamental dipole modes, as discussed in Sec. III B. For a disk diameter of 100 nm, the error ranges from 5.4% at $\Delta x/D = 1.1$ to 8.0% at $\Delta x/D = 1.5$. For disk diameters of 500 and 1000 nm, the error ranges from 8.0 to 23% and 9.0 to 28%. The errors are smaller than those for the decay lengths provided in Table I because higher-order modes, which are accurately predicted by the electrostatic model, contribute to thermal transport.

We analyze mode-dependent contributions to the thermal conductivity by evaluating the frequency-dependent thermal conductivity accumulation,

$$k_i(\omega) = \frac{2}{A} \int_0^\infty \sum_{l,p} C(\omega_{\omega_p}^l) L_p^l V_2^l d\omega_{\omega_p}^l,$$  \hspace{1cm} (11)

for arrays with 100- and 500-nm diameter disks and $\Delta x/D = 1.1$. The results are plotted in Figs. 5(a) and 5(b).

![FIG. 5. Frequency-dependent thermal conductivity accumulation, $k_i(\omega)$, for $\Delta x/D = 1.1$, $E_f = 1.0$ eV, $\varepsilon_2 = 2.4$, and (a) $D = 100$ and (b) 500 nm. The contribution from each band is labeled by its angular index $l$.](image)

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for arrays with 100- and 500-nm diameter disks and $\Delta x/D = 1.1$. The results are plotted in Figs. 5(a) and 5(b). All modes (including those with $k > 0$) were considered in this calculation. The fundamental dipole modes are the main heat carriers, with longitudinal modes dominant over transverse modes. The contribution of $k > 0$ modes to the net thermal conductivity is less than 0.1% as a consequence of their small group velocities. For the disk array with $D = 500$ nm, there is a higher number of modes carrying heat ($l = \pm 1, \pm 2, \pm 3, \pm 4, \pm 5$) in comparison with the case for $D = 100$ nm ($l = \pm 1, \pm 2$), which is a result of the larger thermal activation when the diameter increases. Thus varying the disk diameter (or $E_f$ or $\varepsilon_2$) allows for direct control of the number of thermally activated modes.

### B. Fermi-level tuning of thermal transport

We now explore the tuning the thermal conductivity by varying the Fermi level up to 1 eV, as can be achieved from electrical gating. In Fig. 6(a), the thermal conductivity dependence on the Fermi level is plotted for disk arrays with $\Delta x/D = 1.1$, $\varepsilon_2 = 2.4$, and $D = 100$, 500, and 1000 nm. For a diameter of 100 nm, the thermal conductivity decreases with $E_f$ until it reaches a maximum at $E_f = 0.65$ eV, which indicates the existence of competing effects. As explained by Eqs. (5) and (7), when $E_f$ is reduced, the plasmonic spectrum redshifts and the decay length is reduced. Thus similar to the competing effects associated with changing the disk diameter [see Fig. 4(b)], the increased population of thermally activated modes competes with the reduction in $\tau_{op}$ and $L_p$. For diameters of 500 and 1000 nm, the maximum thermal conductivity is reached at Fermi levels larger than 1 eV, so that the thermal conductivity increases monotonically over the accessible range.

The effect of the Fermi level on the thermal diffusivity, $\alpha_t$, is now analyzed. As surface plasmons are supported by the conduction electrons in graphene, the heat capacity of electrons, $C_t^e$, also needs to be considered, which is given by [32]

$$C_t^e = \frac{1}{3} \pi^2 D_e(E_f) \frac{k_B T}{l},$$  \hspace{1cm} (12)

where $D_e(E) = 2E/(\pi \hbar^2 v_f^2)$ is the electron density of states in graphene [22]. As a reference, for $E_f = 0.1$–1.0 eV and $T = 300$ K, the electronic heat capacity ranges from 350 to 3500 J m$^{-3}$ K$^{-1}$, which is three to four orders of magnitude larger than the plasmonic heat capacity.

The thermal diffusivity is thus calculated as $\alpha = k_i/(C_t + C_t^e)$ and is plotted as a function of the Fermi level in Fig. 6(b). For a disk diameter of 100 nm, the thermal diffusivity reaches a maximum of $1.2 \times 10^{-3}$ m$^2$/s at $E_f = 0.275$ eV. For diameters of 500 and 1000 nm, the thermal diffusivity grows monotonically over the accessible range of $E_f$, reaching values of $1.1 \times 10^{-3}$ and $1.3 \times 10^{-3}$ m$^2$/s at $E_f = 1.0$ eV. These values are ten times larger than the largest values reported for metals, suggesting fast response to temperature fluctuations [36].

Thermal diffusivity is a key property in the design of interconnects for thermotronic devices [37], as it sets the distance affected by an oscillating temperature signal (i.e., the thermal penetration depth, $\delta_{th}$). For a sinusoidal temperature
oscillation at frequency $\nu_t$, the thermal penetration depth is \[ \delta_{th} = \sqrt{\frac{\alpha_t}{\pi \nu_t}}. \] (13)

Consider an array of 100-nm diameter disks of period $\Delta x = 110$ nm and $E_f = 0.275$ eV on a quartz substrate, where $\alpha_t = 1.2 \times 10^{-3}$ m$^2$/s. At frequencies of 4 and 96 MHz, the plasmons can carry energy over distances of 10 and 2 $\mu$m. At these frequencies, the temperature signal in a quartz substrate decays at much shorter lengths of 0.7 and 0.1 $\mu$m, given its low thermal diffusivity ($5.3 \times 10^{-6}$ m$^2$/s) [36]. These frequencies are in the range of the bandwidth observed in photon-based thermal rectification [39]. Additionally, the frequencies of the thermally active plasmons modes (Fig. 5) are in the same range as the resonant frequencies for materials used in photon-based thermotronic devices [19,39–41], meaning that the near-field coupling between the disk array and such devices can be strong. Graphene disks waveguides are thus highly compatible with thermotronic devices.

V. CONCLUSIONS

We studied plasmonic thermal transport in graphene nanodisk arrays. The coupling between disks was modeled using a semi-analytical model based on the electrostatic approximation. The plasmonic band structure showed multiple nonlocalized bands and $1/e$ decay lengths as large as 3.1 $\mu$m for 100 nm disk arrays [Figs. 1(a) and 1(b)]. As shown in Table I, our electrostatic model can predict the plasmon frequencies (decay lengths) in arrays with disk diameters smaller than 200 nm to within 0.4(10)% of a model that considers radiation damping. As such, the plasmonic properties are well-described by nondimensional analysis for disk diameters below 200 nm. At low temperatures, a set of scaling rules can be derived for the dispersion relation and decay length (Fig. 3). The nondimensional models demonstrate that the frequencies and decay lengths of guided plasmon modes can be tuned by changing the disk size and separation, substrate properties, and graphene’s intrinsic optical properties, Fermi level, and electron mobility.

Heat carried by surface plasmons in disk arrays at room temperature offers tunable heat capacity and thermal conductivity up to 0.48 J m$^{-3}$ K$^{-1}$ [Fig. 4(a)] and 4.5 W m$^{-1}$ K$^{-1}$ [Fig. 4(b)] and control over the activated modes, as shown in Fig. 5. We demonstrated a Fermi level-dependent thermal conductivity and thermal diffusivity with values ranging up to 4.5 W m$^{-1}$ K$^{-1}$ [Fig. 6(a)] and $1.4 \times 10^{-3}$ m$^2$/s [Fig. 6(b)]. The thermal diffusivities are ten times larger than those of metals. We note that our calculations consider a graphene thickness of 0.5 nm. If a value of 0.34 nm is considered, which is consistent with other studies of thermal transport in graphene, the thermal conductivity and heat capacity would increase by a factor of 1.47. The thermal diffusivity is not affected by a change in the thickness.

An experimental validation of our predictions will need to take the following into account. First, current fabrication techniques affect the quality of patterned graphene samples, which is reflected in a mobility of less than 2000 cm$^2$ V$^{-1}$ s$^{-1}$ [22]. This lower mobility reduces the decay length of surface plasmons and thus also reduces the thermal transport properties. The thermal diffusivity under such conditions is still larger than that of the substrate. For mobilities $\sim 1000$ cm$^2$ V$^{-1}$ s$^{-1}$, the estimated thermal diffusivity is $\sim 10^{-4}$ m$^2$/s, which is two orders of magnitude larger than that of amorphous silica, a common substrate. Transient thermal measurement techniques such as frequency domain thermoreflectance [42] or transient thermal grating [43] may be able to resolve the larger thermal diffusivity from plasmonic transport.

Second, the performance of the guided modes will be affected by (i) defects in the array induced by misalignment or disk deformations and (ii) the coupling of surface plasmons with optical phonons in the substrate. Regarding defects, a mismatch between disks will relax the selection rules and allow for interactions between all the fundamental modes [44], opening up additional channels for thermal transport.

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near-field radiative coupling between the array and other
plasmonic band structure can be exploited to achieve strong
long-range, tunable, and fast thermal transport. The tunable
activated surface plasmons in graphene disk arrays can lead to
reaching a constant value at $\Delta x/D \approx 2$, which corresponds to
the dipole-dipole interaction. We propose the following model for
the $a_{i}^{l,P}$ parameters:

$$a_{i}^{l,P} = c_{0} + c_{1} \left( \frac{\Delta x}{D} \right)^{c_{2}}$$  \hspace{1cm} (A2)

where $c_{0}$, $c_{1}$, and $c_{2}$ are fitting coefficients. The fitting of
Eq. (A2) to the data shown in Fig. 7(b) gives the $c_{i}$ parameters,
which are provided in Table II. The fitted model from
Eq. (A2) is plotted as continuous lines in Fig. 7(b) and shows
excellent agreement with the calculated data, with maximum
errors of 0.1% and 1.5% for the transverse and longitudinal
coupling parameters.

$\Delta z/D = 0.83$, $\Delta z/D = 1.0$, $\Delta z/D = 1.2$,
$\Delta z/D = 1.1$, $\Delta z/D = 1.5$.

FIG. 7. (a) Nondimensional dispersion relations of the fundamental dipole modes. The dispersion bands obtained from our electrostatic model are indicated by the circles, where open and filled correspond to longitudinal and transverse modes. The continuous lines are the bands obtained from fitting to Eq. (A1). (b) Fitting constants for the model of Eq. (A2).

cases, such scenarios will be detrimental for thermal transport. They can lead to an enhancement of the thermal transport, however, as we found for certain conditions in a study of two disks [6]. Coupling between optical phonons and guided plasmon modes leads to hybridization of the dispersion bands [45–47], which can potentially enhance the thermal transport properties by increasing the group velocity of the heat carriers. In cases where it may be detrimental, this coupling can be avoided by tuning the plasmonic band structure above the mid-infrared by using small nanostructure ($D < 100$ nm) and large doping levels ($E_{f} > 0.6$ eV).

In summary, our predictions suggest that thermally activated surface plasmons in graphene disk arrays can lead to long-range, tunable, and fast thermal transport. The tunable plasmonic band structure can be exploited to achieve strong near-field radiative coupling between the array and other thermotronic devices (e.g., interconnects).

ACKNOWLEDGMENTS

This work was supported by Comisión Nacional de Investigación Científica y Tecnológica (CONICYT), Becas de Doctorado en el Extranjero BECAS CHILE.


APPENDIX: FITTING OF NONDIMENSIONAL DISPERSION

The dispersion bands of the nondimensional model described in Sec. III C can be fit to a model based on the electrostatic dipole-dipole interaction of the form \cite{29}

$$\Omega_{i}^{l,P} = \left( \frac{D}{\Delta x} \right)^{3} \sum_{i=0}^{\infty} a_{i}^{l,P} \cos(ikx)$$  \hspace{1cm} (A1)

where $a_{i}^{l,P}$ are fitting parameters for the $(l,P)$ band and $P$ corresponds to the mode polarization (transverse or longitudinal). These fitting parameters depend on $\Delta x/D$.

We use Eq. (A1) to fit the nondimensional dispersion of the fundamental dipole modes, given the importance of these modes for plasmonic applications. The fitted dispersion bands are plotted as lines in Fig. 7(a) for $\Delta x/D = 1.01, 1.20$, and 1.50. A total of ten $a_{i}^{l,P}$ terms are considered, which gives an agreement of 1% with the exact results. The open (filled) circles correspond to the nondimensional longitudinal (transverse) dispersion obtained from the electrostatic model.

The $\Delta x/D$ dependence of the first five fitting parameters is plotted as circles in Fig. 7(b). The fitting coefficients for both polarizations either increase or decrease monotonically until reaching a constant value at $\Delta x/D \approx 2$, which corresponds to the dipole-dipole interaction. We propose the following model for the $a_{i}^{l,P}$ parameters:

$\phi_{\theta}^{\pi} \approx \sin(\theta) \cos(\pi \theta) \sum_{i=0}^{\infty} a_{i}^{l,P} \cos(k_{x}x)$

where $\phi_{\theta}^{\pi}$ is the electric field component for the $(\theta, \pi)$ mode. As we found for certain conditions in a study of two disks [6], coupling between optical phonons and guided plasmon modes leads to hybridization of the dispersion bands [45–47], which can potentially enhance the thermal transport properties by increasing the group velocity of the heat carriers. In cases where it may be detrimental, this coupling can be avoided by tuning the plasmonic band structure above the mid-infrared by using small nanostructure ($D < 100$ nm) and large doping levels ($E_{f} > 0.6$ eV).

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