We present a theory of the phononic thermal (Kapitza) resistance at the interface between graphene or another single-layer two-dimensional (2D) crystal (e.g. MoS$_2$) and a flat substrate, based on a modified version of the cross-plane heat transfer model by Persson, Volokitin and Ueba [J. Phys.: Condens. Matter 23, 045009 (2011)]. We show how intrinsic flexural phonon damping is necessary for obtaining a finite Kapitza resistance and also generalize the theory to encased single-layer 2D crystals with a superstrate. We illustrate our model by computing the thermal boundary conductance (TBC) for bare and SiO$_2$-encased single-layer graphene and MoS$_2$ on a SiO$_2$ substrate, using input parameters from first-principles calculation. The estimated room temperature TBC for bare (encased) graphene and MoS$_2$ on SiO$_2$ are 34.6 (105) and 3.10 (5.07) MWK$^{-1}$m$^{-2}$, respectively. The theory predicts the existence of a phonon frequency crossover point, below which the low-frequency flexural phonons in the bare 2D crystal do not dissipate energy efficiently to the substrate. We explain within the framework of our theory how the encasement of graphene with a top SiO$_2$ layer introduces new low-frequency transmission channels which significantly reduce the graphene-substrate Kapitza resistance. We emphasize that the distinction between bare and encased 2D crystals must be made in the analysis of cross-plane heat dissipation to the substrate.

In our theory, we do not assume that the 2D crystal has any extended volume in the out-of-plane direction.
like in conventional mismatch models. Indeed, this approach offers us the unique advantage of directly linking the flexural nature of the 2D crystal to phonon transmission to the substrate. Moreover, this allows us to incorporate the effects of a superstrate, such as a top gate oxide layer, on heat dissipation to the substrate, and enables us to understand the difference in heat dissipation to the substrate by a bare 2D crystal and that by its encased counterpart. Our theory predicts that encased 2D crystals have a significantly higher thermal boundary conductance (or lower Kapitza resistance), consistent with empirical trends observed across different experiments. In spite of the simplicity of the model, its numerical predictions of the TBC are in very good agreement with published experimental data for graphene and MoS$_2$, using numerical parameters obtained from first-principles calculations and published elasticity parameters.

The organization of our paper is as follows. We begin with the derivation of our theory of flexural phonon-mediated interfacial heat transfer for bare and encased graphene, and show how our theory is obtained by modifying the model by Persson, Volokitin and Ueba [13]. We then discuss how the damping function for flexural phonons, a key element of our theory, can be approximated and how the interfacial spring constant can be estimated in density functional theory (DFT) calculations. We apply the theory to estimate the TBC values for bare and SiO$_2$-encased graphene and MoS$_2$, and compare them with published experimental [14, 15, 18, 19] and simulation [20] data. Excellent agreement is obtained between our predicted TBC values and the various experimental and simulation data. We also discuss the physics underlying the higher TBC of SiO$_2$-encased graphene and MoS$_2$, and interpret it in terms of the additional low-frequency transmission channels due to coupling to the superstrate. Finally, we give an overall picture of the heat dissipation pathways in supported 2D crystals and discuss how the TBC may change when the different components are modified.

II. THEORY OF HEAT TRANSFER

A. Bare single-layer 2D crystal and solid substrate

The point of departure in the formulation of our theory is Ref. [13] by Persson, Volokitin and Ueba. We begin with a self-contained introduction to the essential elements of Ref. [13], following closely the treatment in Ref. [13]. Suppose we have a single-layer 2D crystal supported by a flat substrate as shown in Fig. 1 with the $z$-axis perpendicular to the substrate surface. The normal stress acting on the 2D crystal at position $r = (x, y)$ and time $t$ is

$$\sigma_{\text{int}}(r, t) = -K[u_{2D}(r, t) - u_{\text{sub}}(r, t)]$$

where $u_{2D}$ and $u_{\text{sub}}$ are respectively the out-of-plane displacement of the 2D crystal and the substrate surface, and $K$ is the spring constant per unit area characterizing the interaction, typically van der Waals, at the interface. If we take the Fourier transform of $u(r, t)$, i.e.,

$$u(q, \omega) = (2\pi)^{-3} \int d^3r \int dt \ u(r, t)e^{i(q \cdot r - \omega t)}$$

where $q$ and $\omega$ are respectively the crystal momentum and frequency, then we have

$$\sigma_{\text{int}}(q, \omega) = -K[u_{2D}(q, \omega) - u_{\text{sub}}(q, \omega)] \quad (1)$$

The equation of motion for the 2D crystal is

$$\rho \frac{\partial^2 u_{2D}(r, t)}{\partial t^2} + \rho \gamma \frac{\partial u_{2D}(r, t)}{\partial t} + \kappa \nabla^2 \nabla^2 u_{2D}(r, t) = \sigma_{\text{int}}(r, t) + \sigma(r, t) \quad (2)$$

where $\rho$ and $\kappa$ are the mass density per unit area and the bending stiffness of the uncoupled 2D crystal, respectively and $\gamma$ is the damping coefficient representing the intrinsic damping of the flexural motion. On the RHS of Eq. (2), $\sigma(r, t)$ represents the stochastic force from thermal fluctuation within the 2D crystal, in addition to the interface force from the substrate. The Fourier transform of Eq. (2) yields the algebraic expression

$$- (\rho \omega^2 + i \rho \gamma \omega - \kappa q^4) u_{2D}(q, \omega) = \sigma_{\text{int}}(q, \omega) + \sigma(q, \omega) \quad (3)$$

or

$$u_{2D}(q, \omega) = u_l(q, \omega) - D_{2D}(q, \omega) \sigma_{\text{int}}(q, \omega) \quad (4)$$

where

$$D_{2D}(q, \omega) = \lim_{\eta \to 0^+} (\rho \omega^2 + i \rho \gamma \omega - \kappa q^4 + i\eta)^{-1}$$

is the retarded Green’s function [21] for the flexural motion of the 2D crystal at the interface, and $u_l(q, \omega) = -D_{2D}(q, \omega) \sigma_l(q, \omega)$ is the stochastic component of the flexural motion due to thermal fluctuation. Equation (4) describes the flexural response of the 2D crystal to a periodic harmonic stress exerted at the interface and the

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![Figure 1: Schematic representation of the bare single-layer 2D crystal (graphene or MoS$_2$) and the substrate. The springs represent the weak van der Waals interaction at the interface. The simulation parameters are also displayed.](image-url)
stochastic force. We modify Eq. (5) to take into account frequency-dependent damping by setting $\gamma$ as a function of $\omega$, i.e. $\gamma = \gamma(\omega)$. The key difference between our model and the one in Ref. [13] is our inclusion of the damping term represented by the self-energy of the flexural phonons (in the 2D crystal). Physically, this means that the excitation of flexural modes but the energy of these phonons) in the 2D crystal. Given the stochastic thermal fluctuation in the interface. One can also write $\langle |u_l(q, \omega)|^2 \rangle$ as the Fourier transform of the autocorrelation function of the displacement $\langle u_l(r, t)u_l(0, 0) \rangle$, i.e.,

$$\langle |u_l(q, \omega)|^2 \rangle = \frac{A\tau}{(2\pi)^3}C_{uu}(q, \omega)$$

where $C_{uu}(q, \omega) = \frac{1}{(2\pi)^3} \int d^2q \int d\omega \frac{\omega K^2 \text{Im} D_{sub}(q, \omega)\langle |u_l(q, \omega)|^2 \rangle}{[1 - K(D_{2D}(q, \omega) + D_{sub}(q, \omega))]^2}$

and $N(\omega, T) = \text{exp}(\hbar \omega/k_B T) - 1^{-1}$ is the Bose-Einstein occupation function for frequency $\omega$ at temperature $T$. The heat current from the 2D crystal to the substrate due to the thermal fluctuations in the 2D crystal is $J_{2D\rightarrow \text{sub}} = \langle \Delta E_{2D\rightarrow \text{sub}} \rangle/(A\tau)$. Thus, Eq. (11) gives us the expression for the average power dissipated from the 2D crystal to the substrate:

$$J_{2D\rightarrow \text{sub}}(T) = \frac{4}{(2\pi)^3} \int d^2q \int_0^\infty d\omega \hbar \omega N(\omega, T)$$

$$\times \frac{K^2 \text{Im} D_{2D}(q, \omega) \text{Im} D_{sub}(q, \omega)}{[1 - K(D_{2D}(q, \omega) + D_{sub}(q, \omega))]^2}.$$
Using the same procedure, a similar expression can be obtained for the average power dissipated from the substrate to 2D crystal, $J_{\text{sub} \rightarrow 2D}(T)$. Therefore, the thermal boundary conductance $G$ for the interface \cite{13} is $G(T) = \lim_{\delta T \to 0} [J_{2D \rightarrow \text{sub}}(T + \delta T/2) - J_{\text{sub} \rightarrow 2D}(T - \delta T/2)]/\delta T$, giving us

$$G(T) = \frac{4K^2}{(2\pi)^3} \int d^2q \int_0^\infty d\omega \hbar \omega \frac{\partial N(\omega, T)}{\partial T} \times \frac{\text{Im}D_{\text{sub}}(q, \omega)\text{Im}D_{2D}(q, \omega)}{|1 - K[D_{\text{sub}}(q, \omega) + D_{2D}(q, \omega)]|^2}. \quad (14)$$

We can express Eq. (14) in the more familiar Landauer form

$$G(T) = \frac{1}{(2\pi)^3} \int d^2q \int d\omega \hbar \omega \frac{\partial N(\omega, T)}{\partial T} \Xi(q, \omega) \quad (15)$$

where

$$\Xi(q, \omega) = \frac{4K^2\text{Im}D_{\text{sub}}(q, \omega)\text{Im}D_{2D}(q, \omega)}{|1 - K[D_{\text{sub}}(q, \omega) + D_{2D}(q, \omega)]|^2}. \quad (16)$$

is the transmission function at $(q, \omega)$. If we assume that $\text{Im}D_{\text{sub}}(q, \omega) \geq 0$ and $\text{Im}D_{2D}(q, \omega) \geq 0$, we can show in Appendix A that $0 \leq \Xi(q, \omega) \leq 1$ which is exactly the property needed for a transmission coefficient.

Here, we comment on the weak coupling approximation originally used in Ref. \cite{13} for evaluating Eq. (14). It is claimed \cite{13} that the denominator in Eq. (16) can be ignored when the coupling between the two solids is weak (i.e., $K$ is so small that $|K[D_{\text{sub}}(q, \omega) + D_{2D}(q, \omega)]| \ll 1$) and that the numerator in Eq. (16) is thus dominated by the pole contribution from $\text{Im}D_{\text{sub}}(q, \omega)\text{Im}D_{2D}(q, \omega)$ at the $(q, \omega)$-point where the dispersion curves for the substrate Rayleigh modes and the bending modes of the 2D crystal intersect. However, this argument does not hold because the denominator $|1 - K[D_{\text{sub}}(q, \omega) + D_{2D}(q, \omega)]|^2$ diverges along the poles of $D_{\text{sub}}(q, \omega)$ and $D_{2D}(q, \omega)$ and there are actually no singularities in $\Xi(q, \omega)$ which is strictly less than or equal to unity (see Appendix A for the proof). Therefore, the weak-coupling approximation is incorrect and the denominator in Eqs. (16) and (14) must be retained to avoid spurious singularities. Our calculations of the integral [Eq. (13)] without the weak-coupling approximation indicate that the integral in Eq. (14) converges numerically to zero if there is no damping. This is because $\Xi(q, \omega)$ is only nonzero when along the poles of $D_{\text{sub}}(q, \omega)$ and $D_{2D}(q, \omega)$ when there is no damping, i.e. $\gamma(\omega) = 0$. Elsewhere, the numerator in the RHS of Eq. (16) and hence, $\Xi(q, \omega)$ are zero. Physically, this means that a dissipative mechanism must be present for net heat transfer to take place. This invalid approximation also explains why the numerical estimate \cite{13} of the TBC for the graphene/SiO$_2$ interface is an order of magnitude too large.

### B. Single-layer 2D crystal with superstrate and solid substrate

In more practical device designs, the perpendicular electrostatic field is applied through a top gate which consists of a metal insulated from the channel by a layer of oxide such as SiO$_2$ or HfO$_2$. Top-gated graphene and MoS$_2$ field-effect transistors are known to have superior carrier density modulation and higher mobilities \cite{22, 28} because of better charge screening. However, the effect of the top oxide layer, the superstrate, on heat dissipation from the encased 2D crystal to the substrate has not been systematically studied or even considered.

Given the theory of heat transfer between the bare 2D crystal and the substrate surface, it is possible incorporate the effects of a superstrate, as shown in Fig. 2 on the 2D crystal by modifying the equation of motion in Eq. (3). Let $u_{\text{top}}(q, \omega)$ be the out-of-plane displacement of the bottom surface of the superstrate and $\sigma_{\text{top}} = g_{\text{top}}[u_{2D}(q, \omega) - u_{\text{top}}(q, \omega)]$, where $g_{\text{top}}$ is the spring constant per unit area characterizing the coupling to the superstrate, be the force per unit area exerted by the superstrate on the 2D crystal. Therefore, the equation of motion for the 2D crystal is

$$-(\rho \omega^2 + i\rho \gamma \omega - \kappa q^4)u_{2D}(q, \omega) = \sigma_{\text{int}}(q, \omega) - \sigma_{\text{top}}(q, \omega) + \sigma_{\text{f}}(q, \omega). \quad (17)$$

Like in Eq. (3), we define the surface response of the superstrate as

$$u_{\text{top}}(q, \omega) = D_{\text{top}}(q, \omega)\sigma_{\text{top}}(q, \omega) \quad (18)$$

where $D_{\text{top}}(q, \omega)$ is the retarded Green’s function for the free surface displacement of the superstrate. We combine Eqs. (17) and (18) to obtain the effective equation of motion for the 2D crystal analogous to Eq. (3)

$$-(\rho \omega^2 + i\rho \gamma \omega - \kappa q^4 - P(q, \omega))u_{2D}(q, \omega) = \sigma_{\text{int}}(q, \omega) + \sigma_{\text{f}}(q, \omega) \quad (19)$$

where $P(q, \omega) = g_{\text{top}}[1 - g_{\text{top}}D_{\text{top}}(q, \omega)]^{-1}$ is the ‘self-energy’ contribution from coupling to the superstrate. Therefore, we define the effective retarded Green’s function for the flexural motion of the covered 2D crystal as

$$\overline{D_{2D}(q, \omega)} = |\rho \omega^2 + i\rho \gamma \omega - \kappa q^4 - P(q, \omega)|^{-1}. \quad (20)$$

In the case of a top oxide layer, $D_{\text{top}}(q, \omega)$ may have the same functional form as Eq. (7). In fact, if the superstrate is of the same material as the substrate, we can set $D_{\text{top}}(q, \omega) = D_{\text{sub}}(q, \omega)$ and $g_{\text{top}} = K$. For a thin film of adsorbates on the 2D crystal, we can write $D_{\text{top}}(q, \omega) = 1/(\rho_{\text{top}}\omega^2)$ where $\rho_{\text{top}}$ is mass density of the adsorbates. In our simulations, we assume that the superstrate material is SiO$_2$ like the substrate and the interfacial spring constant per unit area for the top and
bottom interfaces of the 2D crystal are equal. Hence, like Eq. (14), the expression for the thermal boundary conductance is

\[
G(T) = \frac{4K^2}{(2\pi)^3} \int d^3 q \int_0^{\infty} d\omega \hbar \omega \frac{\partial N(\omega, T)}{\partial T} \times \frac{\text{Im}D_{\text{sub}}(q, \omega)\text{Im}D_{\text{2D}}(q, \omega)}{|1 - K[D_{\text{sub}}(q, \omega) + D_{\text{2D}}(q, \omega)]|^2}.
\]

(21)

III. ADDITIONAL DETAILS ON NUMERICAL CALCULATIONS

Although the details of our theory of heat transfer are described in Section II, there are two other important elements that are needed for the calculation of the thermal boundary conductance and warrant a more in-depth discussion before the theory can be made useful for numerical calculations. The first is the function form of the damping function for the flexural phonons while the second is the spring constant at the interface. The other material parameters such as the bending rigidity ($\kappa$) and the 2D crystal mass density ($\rho$) can be obtained from literature.

A. Damping function for flexural phonons

A key element of our theory is the form of the damping function $\gamma(\omega)$ that determines the rate at which the flexural (ZA) phonon dissipates energy internally to other intrinsic degrees of freedom and is necessary to produce a finite Kapitza resistance. First principles calculations of the room-temperature anharmonic phonon-phonon scattering rate for long-wavelength flexural phonons in single-layer graphene by Bonini et al. [29] suggest that $\gamma(\omega) \propto \omega$, i.e., the flexural phonon lifetime $\tau(\omega)$ is proportional to its period. The same linear relationship between the scattering rate and the frequency of the long-wavelength flexural phonons is also observed in Ref. [30]. In this work, we ignore the effects of direct electron-phonon coupling on flexural phonon scattering since the interaction is a second-order effect [31, 33] and the flexural phonon lifetimes in graphene can be satisfactorily explained [30, 34] without including the effects of flexural phonon scattering with electrons. Moreover, there is close agreement for the thermal conductivity in graphene between experimental data and theoretical estimates [30, 34] that are calculated using only anharmonic phonon coupling and without any electron-phonon interactions. Thus, the electron-phonon contribution to flexural phonon damping is small and can be neglected. Likewise, the thermal conductivity of MoS$_2$ can also be modeled without needing to consider the effects of electron-phonon scattering on the acoustic phonon lifetimes [35, 36].

Given that $\gamma(\omega) = 2/\tau(\omega)$ for a damped harmonic oscillator, we estimate from Ref. [29] that $\omega/\gamma(\omega) \approx 115$ in graphene at room temperature ($T_{RT} = 300$ K) although the ratio is slightly lower at $\sim 90$ in Ref. [30]. The quality factor in graphene nanoresonators has also been estimated to be around $\sim 100$ and to scale as $T^{-1}$ in molecular dynamics simulations [37]. Therefore, we propose a phenomenological expression for the temperature-dependent $\gamma(\omega)$ in graphene:

\[
\gamma(\omega, T) = \frac{\omega T}{\alpha T_{RT}}
\]

(22)

where $\alpha$ is equal to the ratio of the phonon lifetime to its period at room temperature. In our simulations, we set to $\alpha = 100$ for single-layer graphene and MoS$_2$. In the case of MoS$_2$, there is less certainty over the value of $\alpha$ as there is no readily available data on the relationship between flexural phonon lifetime and frequency although molecular dynamics simulations in Ref. [37] show that the quality factor for MoS$_2$ is about three times that for graphene, suggesting that $\alpha$ can be as high as $\sim 300$. We note that in spite of the high flexural phonon lifetimes in MoS$_2$, its thermal conductivity is much lower than that of graphene because of the low phonon group velocities in MoS$_2$ and the stronger anharmonicity for the in-plane longitudinal and transverse acoustic phonons [35, 36].

The functional form of Eq. (22) also means that flexural phonon damping increases linearly with temperature [38]. We stress that the functional form of Eq. (22) is approximate and that its frequency and temperature dependence can be in principle more precisely evaluated through DFT calculations and more sophisticated many-body techniques although this is beyond the scope of our current work. The damping is also expected to be higher when the graphene or MoS$_2$ has intrinsic defects such as grain boundaries or vacancies that can reduce the flexural phonon lifetimes through elastic scattering.
B. Density functional theory calculation-based estimate of spring constant at interface

Another important parameter needed for our numerical calculation is $K$, the spring constant per unit area for the interface. The numerical value of $K$ depends on the 2D crystal, the substrate and the surface atomistic structure of the substrate. We estimate the numerical values of $K$ from first principles calculations by computing the energy change when the 2D crystal is displaced from its equilibrium distance $d_0$ to the substrate surface. The change in energy per unit area for small displacements $d - d_0$ is thus

$$\frac{\Delta E}{A} = \frac{1}{2} K(d - d_0)^2,$$

where $\Delta E$ is the energy change for the interface, $A$ is the area of the interface and $d$ is the distance between the 2D crystal and the substrate surface.

We estimate $K$ for graphene and MoS$_2$ on H- and OH-terminated SiO$_2$ from density functional theory (DFT) calculations. The interlayer spacing-energy ($d - E$) profiles for the various heterostructures (graphene/SiO$_2$ and MoS$_2$/SiO$_2$) are calculated with the first-principles method within the framework of density functional theory by using the software package VASP [39]. The DFT-D2 method is adopted to simulate the van der Waals interactions across the interface. The Perdew-Burke-Ernzerhof functional is used as the exchange-correlation functional together with a cutoff energy of 400 eV. The slab models are constructed with the vacuum layer thicker than 10 Å. For the graphene/SiO$_2$ (MoS$_2$/SiO$_2$), the heterostructures are constructed based on a 4 × 4 (3 × 3) supercell for the graphene (MoS$_2$) and a 2 × 2 supercell for the SiO$_2$ (001) surface for better lattice match with lattice strains smaller than 2 percent. For simulating the SiO$_2$ (001) surface, a slab model with including seven Si layers is used and the atoms in the bottom O-Si-O atomic layers are saturated with hydrogen atoms and fixed during the structural optimization. Two types of surface of SiO$_2$ with OH-rich and H-rich chemical conditions are considered for both graphene/SiO$_2$ and MoS$_2$/SiO$_2$ heterostructures. We adopt a 3 × 3 × 1 Monkhorst-Pack (MP) grid for k-point sampling for the graphene/SiO$_2$ and graphene/MoS$_2$ structures. All the atomic models are fully relaxed until the forces are smaller than 0.005 eV/Å.

Figure 3 shows the supercell of the graphene/SiO$_2$ heterostructure used in our DFT calculations. The $K$ values for the graphene/SiO$_2$ interface can be estimated by fitting the parabola around the minimum of the $d - E$ curve. We also estimate the $K$ values for the MoS$_2$/SiO$_2$ interface using the same procedure. The extracted values ($K_{OH}$ and $K_H$) are given in Table I. We remark that the DFT-based estimated values of $K$ for the graphene/SiO$_2$ interface are an order of magnitude than the value estimated by Cullen et al. [40] from graphene adhesion to SiO$_2$ ($K \approx 9.0 \times 10^{18} \text{Nm}^{-3}$). Given the sensitivity of the TBC to the numerical value of $K$, the close agreement between our estimates of the graphene/SiO$_2$ TBC and experimental data (see Table II) suggests that the value of $K$ estimated in Ref. [40] is much too low.

|                | Graphene | MoS$_2$ |
|----------------|----------|---------|
| $K_{OH}$ (10^{19} \text{Nm}^{-3}) | 12.3 | 4.94 |
| $K_H$ (10^{19} \text{Nm}^{-3}) | 15.6 | 2.74 |
| $\kappa$ (eV) | 1.1 [41] | 9.6 [41] |
| $\rho$ (10^{-7} \text{kgm}^{-2}) | 7.6 | 31 |
| $\alpha$ | 100 | 100 |
| $\rho_{oh}$ (kgm^{-3}) | 2200 [41] |
| $c_L$ (ms^{-1}) | 5953 [41] |
| $c_T$ (ms^{-1}) | 3743 [41] |

Table I: Parameters in our numerical simulations. $K_{OH}$ and $K_H$ are the spring constants per unit area for the OH- and H-terminated SiO$_2$ interface, respectively, and also depend on the type of 2D crystal. $\kappa$ and $\rho$ are respectively the intrinsic bending rigidity and mass density per unit area of the 2D crystal used in Eq. [30].

IV. RESULTS AND DISCUSSION

We use our theory to calculate the Kapitza resistance for single-layer graphene and MoS$_2$ on solid SiO$_2$. The parameters in our simulations are given in Table II. We evaluate the two-dimensional integral in Eq. (16) numerically with a rectangular grid in $q$ and $\omega$. We set a frequency cutoff of 65 meV which approximates the max-
mum flexural phonon energy at the Brillouin zone edge in most 2D materials. At low and room temperature, the numerical value of $G$ is relatively insensitive to the cutoff.

We note here that the following simulated TBC values are for an idealized flat interface at which the 2D crystal has full adhesion to the substrate or the superstrate in the case of the encased 2D crystal. The effective TBC values may be lower under most experimental conditions where some surface roughness is present, resulting in the reduction of the effective adhesion and contact area between the 2D crystal and the substrate\cite{15 22 12 43}. Thus, the simulated TBC values can be interpreted as the upper bounds for the TBC of real interfaces.

A. Sensitivity of numerical results to damping friction

We calculate the room temperature (300 K) thermal boundary conductance for bare graphene and MoS$_2$ on OH-terminated SiO$_2$ at different values of $\alpha$ using Eq. (14) and the parameters from Table I except $\alpha$. Therefore, the TBC decreases and converges numerically to zero. The effect is more pronounced for graphene. This indicates that without any damping friction, the use of Eq. (14) yields an infinite Kapitza resistance. Physically, this means that damping friction in single-layer 2D crystals is necessary to produce a reasonable finite Kapitza resistance. It also confirms our earlier analysis of the weak-coupling approximation in Ref.\cite{15} which gives a TBC of $\sim 300$ MWK$^{-1}$m$^{-2}$, an order of magnitude larger than experimental data. In contrast, our default value of $\alpha = 100$ gives us a room-temperature TBC of $G = 34.6$ MWK$^{-1}$m$^{-2}$ which is in very good agreement with published experimental data of bare single-layer graphene\cite{12 15} ($\sim 25$ MWK$^{-1}$m$^{-2}$) considering the uncertainty in the input parameters. We also observe that the TBC for MoS$_2$ is considerably less sensitive to the numerical value of $\alpha$ compared to graphene. When $\alpha$ is quadrupled from 100 to 400, the TBC decreases from $G = 3.1$ MWK$^{-1}$m$^{-2}$ to 2.2 MWK$^{-1}$m$^{-2}$. This considerably weaker $\alpha$-dependence in MoS$_2$ implies that our choice of $\alpha = 100$ will not affect our TBC estimates for MoS$_2$ significantly.

B. Bare single-layer graphene and MoS$_2$

We calculate the TBC for bare single-layer graphene and MoS$_2$ on OH- and H-terminated SiO$_2$ surface in the temperature range of 5-400 K using Eq. (14) and the parameters from Table I. The computed results are shown in Fig. 5 along with the room-temperature experimental data for bare graphene and MoS$_2$ from Refs.\cite{15} and \cite{19}. At room temperature, the TBC values for graphene are relatively close regardless of the surface termination type (H or OH) although the H-terminated surface gives slightly higher TBC values. In contrast, the TBC values for MoS$_2$ vary significantly at all temperature. At 300 K, we have $G = 1.05$ and 3.10 MWK$^{-1}$m$^{-2}$ for H- and OH-terminated SiO$_2$ surfaces, respectively, indicating that bare MoS$_2$ dissipates heat much more efficiently to the OH-terminated SiO$_2$ surface than to the H-terminated surface. This is not surprising considering that $K_{OH}$ is significantly higher than $K_{H}$ for MoS$_2$ (see Table II) because of the stronger coupling between MoS$_2$ and OH-terminated SiO$_2$. The simulated room-temperature TBC values are summarized in Table III. At temperatures below 100 K, the TBC scales approximately as $G \propto T^4$, assuming the temperature dependence of $\gamma(\omega) \propto T$ given in Eq. (22).

We compare our simulated TBC values with those measured from experiments on bare graphene or MoS$_2$ on SiO$_2$ at room temperature. By using an ultrafast optical pump pulse and monitoring the transient reflectivity on the picosecond time scale, Mak et al.\cite{15} obtained $\sim 25$ MWK$^{-1}$m$^{-2}$ for the room-temperature TBC of bare graphene on SiO$_2$. A similar value is estimated by Freitag et al. in Ref.\cite{15}. Ni et al.\cite{20} obtained a value of $\sim 30$ MWK$^{-1}$m$^{-2}$ from their molecular dynamics (MD) simulations of single-layer graphene on amorphous SiO$_2$ while Ong and Pop\cite{44} obtained $\sim 58$ MWK$^{-1}$m$^{-2}$ from the MD simulation of a single-walled carbon nanotube on SiO$_2$. These experimental and MD simulation values compare favorably with our estimate of 34.6 MWK$^{-1}$m$^{-2}$ for graphene on OH-terminated SiO$_2$. For bare MoS$_2$ on SiO$_2$, a TBC value of $G \geq 3.2$ MWK$^{-1}$m$^{-2}$ is estimated from Ref.\cite{19} using $G \geq (R_{tot} - R_{ox})^{-1}$,
Experimental H-SiO $\sim 10^5$ value for bare graphene. Like with our simulated TBC in Ref. [14], and much larger than the corresponding TBC values for OH-terminated SiO$_2$ surfaces, respectively, indicating that encased MoS$_2$ dissipates heat much more efficiently to the OH-terminated SiO$_2$ surface than to the H-terminated surface like in bare MoS$_2$. The temperature dependence of the TBC also varies with the 2D crystal. At temperatures below 100 K, the TBC scales approximately as $G \propto T^3$ for graphene and $G \propto T^{0.7}$ for MoS$_2$.

**Table II:** Computed values of the room temperature (300 K) thermal boundary conductance (TBC) values in MWK$^{-1}$m$^{-2}$ for bare and SiO$_2$-encased single-layer graphene and MoS$_2$ with OH- and H-terminated SiO$_2$ interfaces. The experimentally estimated TBC values for bare and encased graphene and bare MoS$_2$ on SiO$_2$ are also shown for comparison.

|          | OH-SiO$_2$ | H-SiO$_2$ | Experimental |
|----------|------------|-----------|--------------|
| Bare Gr  | 34.6       | 42.1      | $\sim 25$ [15, 18] |
| Encased Gr | 105       | 144       | $\sim 83$ [14] |
| Bare MoS$_2$ | 3.10  | 1.05      | $\geq 3.2$ [19] |
| Encased MoS$_2$ | 5.07 | 1.70      | $\sim$ |

Figure 5: Temperature dependence of the thermal boundary conductance (TBC) for bare single-layer graphene (Gr) and MoS$_2$ on OH- and H-terminated SiO$_2$ surface. The data point for bare graphene from Mak et al. [15] is represented by the open circle while the data point for bare MoS$_2$ from Taube et al. [19] is represented by the open triangle.

where $R_{\text{ex}} = 1.96 \times 10^{-7}$ m$^2$KW$^{-1}$ is the thermal resistance of 275 nm of amorphous SiO$_2$, with a thermal conductivity [14] of 1.4 MWK$^{-1}$m$^{-1}$, and $R_{\text{tot}} = 5.08 \times 10^{-7}$ m$^2$KW$^{-1}$ is the total interfacial thermal resistance measured using an optothermal method based on Raman spectroscopy [19]. This estimate is remarkably close to our calculated value of 3.10 MWK$^{-1}$m$^{-2}$ for bare MoS$_2$ on OH-terminated SiO$_2$. For both graphene and MoS$_2$, given the good agreement between the simulated TBC values for OH-terminated SiO$_2$ and experimental TBC data, this indirectly suggests that the spring constant per unit area $K_{\text{OH}}$ for the OH-terminated surface is more representative of real SiO$_2$ surface in experimental systems.

C. Effect of top SiO$_2$ layer on thermal boundary conductance

We calculate the TBC for SiO$_2$-encased single-layer graphene and MoS$_2$ on OH- and H-terminated SiO$_2$ surface in the temperature range of 5-400 K using Eq. (21) and the parameters from Table I. The computed results are shown in Fig. 6 along with the temperature-dependent experimental data for encased graphene from Refs. [14] and the simulated room-temperature TBC values are given in Table II. The TBC values are significantly higher for encased graphene and MoS$_2$ than for the bare 2D crystals at all temperatures. In particular, the room-temperature TBC calculated for graphene on OH-terminated SiO$_2$ is 105 MWK$^{-1}$m$^{-2}$, in good agreement with the experimental values of $\sim 83$ MWK$^{-1}$m$^{-2}$ in Ref. [14], and much larger than the corresponding TBC value for bare graphene. Like with our simulated TBC values for bare graphene, the computed values for the OH-terminated SiO$_2$ interface is closer to experimental values. However, the TBC data from Ref. [14] does not decrease as much with temperature as does our simulated data. This weaker temperature dependence may be due to the functional form of $\gamma(\omega)$ we assumed in Eq. (22). It is possible that a more accurate calculation of the temperature-dependent flexural phonon lifetime similar to what is done in DFT-based calculations of the thermal conductivity [29, 30] will yield a TBC temperature dependence closer to experiments. In addition, the $\gamma(\omega) \propto T$ scaling may not hold at lower temperatures where defect scattering of the flexural phonons may be the limiting factor instead of anharmonic phonon interaction in real graphene. We also find that the TBC values for MoS$_2$ vary significantly at all temperature with the surface termination type. At 300 K, we have $G = 5.07$ and $1.70$ MWK$^{-1}$m$^{-2}$ for H- and OH-terminated SiO$_2$ surfaces, respectively, indicating that encased MoS$_2$ dissipates heat much more efficiently to the OH-terminated SiO$_2$ surface than to the H-terminated surface like in bare MoS$_2$. The temperature dependence of the TBC also varies with the 2D crystal. At temperatures below 100 K, the TBC scales approximately as $G \propto T^3$ for graphene and $G \propto T^{0.7}$ for MoS$_2$.

D. Transmission analysis of bare and encased graphene

The question the arises as to why the thermal boundary conductance is much higher for encased 2D crystals than for their bare counterparts. The transmission function in Eqs. (14) and (21) is given by

$$\Xi(q, \omega) = \frac{4K^2\Im[D_{\text{sub}}(q, \omega)]\Im[D_{2D}(q, \omega)]}{\left|1 - K[D_{\text{sub}}(q, \omega) + D_{2D}(q, \omega)]\right|^2};$$

and its spectrum helps us to identify the dominant channels in heat dissipation. For an encased 2D crystal, we use $\Xi_{2D}(q, \omega)$ instead of $D_{2D}(q, \omega)$ in $\Xi(q, \omega)$. To illustrate the effect of the superstrate on heat dissipation, we plot the transmission spectra for bare and encased...
suggests that the TBC becomes strongly size-dependent when its interface area is comparable to or smaller than $l_c^2$.

In contrast, Fig. 7(b) shows a very substantial low-frequency contribution in the transmission spectrum of encased graphene, which also can be seen in Fig. 7(c) where we plot the total transmission per unit area $(2\pi)^{-2} \int d^2q \Xi(q, \omega)$. This is because the coupling of the 2D crystal to the superstrate results in the hybridization of the 2D crystal flexural modes with the superstrate Rayleigh modes. These hybrid modes can be scattered more easily into the substrate. The enhanced transmission of these low-frequency hybrid modes results in a significantly higher TBC for encased graphene. This difference in the low-frequency phonon contribution in the TBC of encased graphene also explains why the low-temperature scaling of $G$ is different in Figs. 4 and 5. At low frequencies, the total transmission per unit area scales as $\omega^{3.2}$ and $\omega^2$ in bare and encased graphene, respectively. The considerably weaker contribution of the low-frequency modes in bare graphene means that at lower temperatures, the higher-frequency modes do not contribute to interfacial heat transfer and the TBC decreases more rapidly as the temperature is reduced.

Physically, heat is exchanged between the SiO$_2$ substrate and bare graphene when an incoming substrate bulk phonon scatters inelastically off the graphene/SiO$_2$ interface and dissipates part of its energy within the graphene through the intrinsic flexural phonon damping, as represented schematically in the inset of Fig. 7(a). This scattering process efficiently dissipates energy from the substrate to the graphene when the substrate bulk phonon has a frequency (and hence energy) approximately equal to the corresponding graphene flexural phonon for the same $q$. On the other hand, in encased graphene, the incoming substrate bulk phonon also scatters inelastically off the graphene/SiO$_2$ interface and the energy is dissipated into the graphene. Part of the energy is absorbed by the intrinsic flexural phonon damping while part of it is absorbed by the flexural damping component from coupling to the superstrate. The latter can be interpreted as the partial transmission of energy into the bulk of the superstrate, as schematically represented in the inset of Fig. 7(b).

**E. Heat dissipation pathways**

Our calculations of the thermal boundary conductance for bare and encased single-layer 2D crystals show that the presence of a superstrate on the 2D crystals can substantially increase the TBC between the 2D crystal and its substrate. In the bare 2D crystal, the energy from the intrinsic degrees of freedom (nonflexural phonons and electrons) are dissipated to the substrate via anharmonic or electron-phonon coupling to the flex-

Figure 6: Temperature dependence of the thermal boundary conductance (TBC) for SiO$_2$-encased graphene (Gr) and MoS$_2$ on OH- and H-terminated SiO$_2$ interfaces. The open circles correspond to temperature-dependent TBC data for single-layer encased graphene taken from Chen et al. [14].

graphene on OH-terminated SiO$_2$ in Fig. 7. Given that $0 \leq \Xi(q, \omega) < 1$, the transmission spectrum for bare graphene [see Fig. 7(a)] is zero almost everywhere although the transmission peak is close to unity along the dispersion curve for the flexural phonons for $\omega \gtrsim 19$ meV, indicating the greater contribution from high-frequency modes. At lower frequencies ($\omega < 19$ meV), the transmission of individual low-frequency modes becomes rapidly more smeared out. In addition, the transmission is zero for $\omega < c_T q$ since there are no substrate bulk acoustic phonon modes satisfying this condition, i.e., $\text{Im}D_{\text{sub}}(q, \omega) = 0$ for $\omega < c_T q$. Physically, this means that heat dissipation can only take place when there is coupling to the substrate bulk acoustic phonons. Remarkably, the contribution of the low-frequency modes to interfacial heat transfer is relatively small for bare graphene. The crossover at $\omega = 19$ meV is determined by the point where the graphene flexural phonon dispersion curve intersects the substrate transverse acoustic phonon dispersion curve, as can be seen in Fig. 7 and is given by $\omega = \sqrt{\rho / k c_T^2}$. Below the crossover frequency, the substrate transverse acoustic phonons with the same wave vector $q$ have higher energy than the corresponding graphene flexural phonons. This reduces the probability of the flexural mode coupling with the continuum of substrate bulk phonons, which acts as a dissipative bath, and transferring energy into the substrate [21].

Another way to understand this cutoff is that the region $\omega > c_T q$ corresponds to substrate phonons with a transverse momentum component of $q$ and a frequency of $\omega$, and these phonons scatter with graphene flexural phonons with the same $q$ and $\omega$. We can also associate a characteristic length scale with the crossover point, given by $l_c \sim 2\pi / q_c = 0.8$ nm where $q_c = \sqrt{\rho / k c_T}$. This suggests that the TBC becomes strongly size-dependent...
data, suggesting that the electron-phonon contribution with only dissipation from anharmonic phonon coupling densities [46]. Nevertheless, our estimates of the TBC may be significant at high electron temperatures and densities [31–33] and is expected to be small although the weak-coupling approximation is not numerically valid. The mechanical attachment of a superstrate results in additional resonant channels for energy to be absorbed by the flexural phonons and then transferred to the substrate, leading to a higher thermal boundary conductance.

Figure 7: Plot of the transmission spectrum \( \Xi(q, \omega) \) [see Eq. (10)] for (a) bare and (b) encased graphene on OH-terminated SiO\(_2\) at \( T = 300 \) K. The dashed and dotted lines correspond to the graphene flexural (\( \omega = \sqrt{\kappa/\rho} \)) and substrate transverse acoustic (\( \omega = cT/\rho \)) phonon dispersion curves, respectively. The insets show a schematic representation of the bulk substrate phonon scattering with the graphene flexural phonon. (c) Comparison of the total transmission per unit area spectrum \( (2\pi)^{-2} \int d^2q \Xi(q, \omega) \) for bare (solid red line) and encased graphene (dashed blue line) on OH-terminated SiO\(_2\) at \( T = 300 \) K. The inset shows the same spectra but with a logarithmic scale. The small fuzzy peaks are an artifact of the numerical integration in \( q \).

Figure 8: Schematic representation of the physical model of heat dissipation in bare and covered single-layer 2D crystals. The flexural phonons in the bare 2D crystal absorb energy from the nonflexural phonons and electrons via anharmonic and direct electron-phonon coupling, and dissipate it into the substrate. The mechanical attachment of a superstrate results in additional resonant channels for energy to be absorbed by the flexural phonons and then transferred to the substrate, leading to a higher thermal boundary conductance.

Figure 8: Schematic representation of the physical model of heat dissipation in bare and covered single-layer 2D crystals. The flexural phonons in the bare 2D crystal absorb energy from the nonflexural phonons and electrons via anharmonic and direct electron-phonon coupling, and dissipate it into the substrate. The mechanical attachment of a superstrate results in additional resonant channels for energy to be absorbed by the flexural phonons and then transferred to the substrate, leading to a higher thermal boundary conductance.

V. SUMMARY AND CONCLUSIONS

We have modified the theory by Persson, Volokitin and Ueba [13] and recast it in the Landauer form to study the Kapitza resistance of graphene and other single-layer 2D crystals on a solid substrate. We have shown that the weak-coupling approximation is not numerically valid and that the inclusion of a damping function for the flexural phonons is necessary to produce dissipation within the graphene and yield a finite Kapitza resistance. The phenomenological form of the damping function is de-
duced from published first-principles results. We have also shown how our theory can be modified to accommodate the effects of a superstrate. We have used DFT calculations to estimate the spring constant per unit area for the different interfaces. Our computed thermal boundary conductance values for bare single-layer graphene and MoS$_2$ are in good agreement with published experimental data. The theory also suggests that there is no significant contribution to interfacial heat transfer by low-frequency phonon modes in bare single-layer 2D crystals.

We also find that the encasement of the 2D crystal by a SiO$_2$ superstrate results in a $\sim 3\times$ increase in the thermal boundary conductance for graphene. This explains why the Kapitza resistance measured in experiments for SiO$_2$-encased graphene is substantially lower than for bare graphene. This resistance reduction is also predicted to be true for single-layer MoS$_2$. Our analysis shows that the increase in the thermal boundary conductance is due to the additional low-frequency transmission channels from coupling with the superstrate. We also find in bare 2D crystals that there is a crossover frequency below which phonons do not contribute significantly to cross-plane heat dissipation to the substrate. Our calculations suggest that the termination of the SiO$_2$ surface has a much stronger influence on the Kapitza resistance for MoS$_2$ than for graphene. The theoretical framework described in this work provides the basis for understanding how the modification of interfaces and 2D crystals at the nanoscale can be utilized to reduce the Kapitza resistance to improve interfacial heat dissipation, an important issue in the thermal management of nanoscale devices using 2D materials.

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Appendix A: Numerical bounds for transmission function $\Xi(q, \omega)$

Let us write $KD_{\text{sub}}(q, \omega) = x_1 + iy_1$ and $KD_{\text{2D}}(q, \omega) = x_2 + iy_2$ where $x_i$ and $y_i$ are real numbers for $i = 1, 2$. Thus, the transmission function in Eq. (10) can be written as

$$\Xi(q, \omega) = \frac{4y_1y_2}{(1 - x_1 - x_2)^2 + (y_1 + y_2)^2} \leq \frac{4y_1y_2}{(y_1 + y_2)^2}.$$ 

Given that $y_1, y_2 \geq 0$, this means that

$$\frac{4y_1y_2}{(y_1 + y_2)^2} \leq 1$$

and therefore, we have $0 \leq \Xi(q, \omega) \leq 1$. 

* Electronic address: ongzy@ihpc.a-star.edu.sg

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