Electronic Supplementary Information

Interface thermal conductivities induced by van der Waals interactions

H. M. Dong,[1] H. P. Liang,[2] Z. H. Tao,[3] Y. F. Duan,[1] M.V. Milošević,[3*] and K. Chang[4*]*
[1)]School of Materials Science and Physics, China University of Mining and Technology, Xuzhou 221116, China
[2)]Beijing Computational Science Research Center, Beijing, 100193, China
[3)]Department of Physics and NANOlab Center of Excellence, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium
[4)] School of Physics, Zhejiang University, Hangzhou 310027, P. R. China
Corresponding authors: yifeng@cumt.edu.cn, milorad.milosevic@uantwerpen.be, and kchang@zju.edu.cn

S1. Phonon Transmission Coefficient

When an acoustic wave is projected from graphene into hBN through their vdWs interface, reflection and refraction phenomena occur at the interface plane, as illustrated in Fig. S1. The incident wave, reflected wave, and refracted wave propagate and transmit through the *ab* (*xy)* plane with the acoustic stress $\vec{p}$, the space coordinate $\vec{r}=(x,y,z)$, the acoustic velocity *v*, and mass density ρ in both layers, respectively. As a result, the following relationships are established, which are [1]

$$\vec{p}_1 = p_1 e^{i\omega\cdot r_1/v_1} = p_1^{\,i\omega\cdot(x\sin\theta_1 + z\cos\theta_1)/v_1}, \qquad (S1)$$

$$\vec{p}_1' = p_1' e^{i\omega\cdot r_1'/v_1} = p_1^{\,i\omega\cdot(x\sin\theta_1 - z\cos\theta_1)/v_1}, \qquad (S2)$$

$$\vec{p}_2 = p_2 e^{i\omega\cdot r_2/v_2} = p_2^{\,i\omega\cdot(x\sin\theta_2 + z\cos\theta_2)/v_2}, \qquad (S3)$$

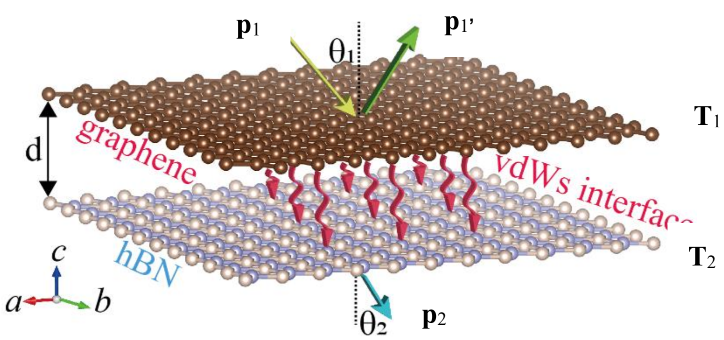

Fig. S1 The incident wave, reflected wave, and refracted wave at the vdWs interface.

Since the acoustic impedance $z_i = \rho_i v_i$ is the ratio of the acoustic stress $\vec{p}_i \cos\theta_i$ over an area to the volume velocity through that area [2], we can have

$$v_{1z} = \frac{p_1 \cos\theta_1}{\rho_1 v_1},\ v_{1z}' = \frac{p_1' \cos\theta_1}{\rho_1 v_1},\ and\ v_{2z} = \frac{p_2 \cos\theta_2}{\rho_2 v_2} \qquad (S4)$$

The interface for $z=0$ can be described using spring boundary conditions, taking into account the vdWs conditions [3], which are

$$\sigma_{zz}^2 = K_n(u_{1z} - u_{2z}),\ \sigma_{zx}^2 = K_t(u_{1x} - u_{2x}), \qquad (S5)$$

$$\sigma_{zz}^2 = \sigma_{zz}^1, \sigma_{zx}^2 = \sigma_{zx}^1, \qquad (S6)$$

where σ_{zz}, σ_{zx}, u_z, and u_x are normal and shear stresses and displacements at the interface. Parameters K_n and K_t, are the normal and transverse stiffnesses of a layer thickness, respectively. Moreover, $v_i = \partial u_i / \partial t = -i\omega u_i$, $K_n = K_A$, and $K_t = 0$ in this work.

Furthermore, the intensity of acoustic wave I can be related to the acoustic stress p, namely $I = p^2 / 2\rho v$. $\sigma_{ik} = p\delta_{ik}$ and Snell's law $\sin\theta_1 / v_1 = \sin\theta_2 / v_2$ are included. As a result, the transmission coefficient of acoustic energy between the incident wave and the refracted wave is written as

$$\tau_\omega = \frac{I_2^{\ 2}}{I_1^{\ 2}} = \frac{4z_1 z_2 \cos\theta_1 \cos\theta_2}{(z_1 \cos\theta_2 + z_2 \cos\theta_1)^2 + \frac{\omega^2}{K_A^2}(z_1 z_2 \cos\theta_1 \cos\theta_2)^2} \qquad (S7)$$

S2. Net Heat Flux Density

The number of phonons of j mode incident on the area A at an incidence angle θ_1 in unit time at the angle frequency range $\omega \sim \omega + d\omega$ for the azimuthal angle $d\Omega = \sin\theta d\theta d\varphi$ in Fig. S1 is

$$n_{\omega,j} = \frac{N(\omega_j, T_i)}{\int d\Omega} v_{1,j} \cos\theta_1 d\Omega A, \qquad (S8)$$

with $N(\omega_j, T_i)$ being the density of phonon states and the temperature T_i. Thereby, the total number N_{total} of phonons per unit of time including all the modes and the frequencies can be obtained as,

$$N_{total} = \sum_j \int n_{\omega,j} d\omega_j\ . \qquad (S9)$$

As a result, we can calculate the heat flow flux J_1 by the acoustic phonons with energy $\hbar\omega_j$ transmitting from the material 1 to the material 2 per unit time, through the unit interface area, which reads [1]

$$J_1 = \sum_j \frac{N_{total}\hbar\omega_j\tau_\omega}{A}. \qquad (S10)$$

The heat flow flux J_2 from material 2 to material 1 can be estimated symmetrically. Finally, the net heat flux J is then calculated as,

$$\begin{aligned} J &= J_1 - J_2 \\ &= \frac{1}{2}\sum_J \int_0^{\omega_{j,c1}} \int_0^{\theta_{c1}} N(\omega_j, T_1)\hbar\omega_j v_{1,j}\tau_\omega \cos\theta_1 \sin\theta_1 d\theta_1 d\omega_j \qquad (S11) \\ &- \frac{1}{2}\sum_J \int_0^{\omega_{j,c2}} \int_0^{\theta_{c2}} N(\omega_j, T_2)\hbar\omega_j v_{2,j}\tau_\omega \cos\theta_2 \sin\theta_2 d\theta_2 d\omega_j. \end{aligned}$$

Here $\omega_{j,c}$ is the cut-off frequency for the j phonon mode. The critical angle $\theta_{j,c1} = \arcsin(v_{1,j}/v_{2,j})$ for $v_{1,j}/v_{2,j} < 1$, and $\theta_{j,c1} = \pi/2$ for $v_{1,j}/v_{2,j} \geq 1$.

S3. The DFT calculated data for the applied stress (strain)

	bond (Å)							
Graphene	1.42456							
hBN	1.4488							
strain	stress (*kB*)	stress (*N/m*)	*bond (Å)*	*r*₀ *(Å)*	*E*₀ *(eV/atom)*	σ *(eV/atom)*	ε *(Å)*	*K* *(eV/Å²)*
0.88	843.860	168.772	1.26319	3.2303	0.027049	0.02705	2.87784	0.18664
0.90	634.140	126.828	1.29190	3.2611	0.025229	0.02523	2.90533	0.17080
0.92	461.360	92.2720	1.32061	3.2876	0.023873	0.02387	2.92894	0.15903
0.94	320.500	64.1000	1.34932	3.3062	0.023446	0.02345	2.94550	0.15443
0.96	194.390	38.8780	1.37803	3.3103	0.023764	0.02376	2.94917	0.15614
0.98	87.270	17.4540	1.40674	3.3199	0.023446	0.02345	2.95769	0.15316
1.00	0.0335	0.006716	1.43544	3.3313	0.022644	0.02264	2.96785	0.14691
1.02	-70.980	-14.1960	1.46415	3.3502	0.021651	0.02165	2.98467	0.13889
1.04	-128.67	-25.7340	1.49286	3.3658	0.020637	0.02064	2.99860	0.13116

References

[1] J. Chen, X. F. Xu, J. Zhou, B. W. Li, Interfacial thermal resistance: Past, present, and future, Rev. Mod. Phys. 94, 025002 (2022).

[2] N. Hiremath, V. Kumar, N. Motahari, D. Shukla, An Overview of Acoustic Impedance Measurement Techniques and Future Prospects, Metrology 1, 17-38 (2021).

[3] S. I. Rokhlin and Y. J. Wang, Analysis of boundary conditions for elastic wave interaction with an interface between two solids, The Journal of the Acoustical Society of America 89, 503 (1991).