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Inter-layer and intra-layer heat transfer in bilayer/monolayer graphene van der Waals heterostructure: Is there a Kapitza resistance analogous?

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Van der Waals heterostructures have exhibited interesting physical properties. In this paper, heat transfer in hybrid coplanar bilayer/monolayer (BL-ML) graphene, as a model layered van der Waals heterostructure, was studied using non-equilibrium molecular dynamics (MD) simulations. The temperature profile and inter- and intra-layer heat fluxes of the BL-ML graphene indicated that, there is no fully developed thermal equilibrium between layers and the drop in the average temperature profile at the step-like BL-ML interface is not attributable to the effect of Kapitza resistance. By increasing the length of the system up to 1 μm in the studied MD simulations, the thermally non-equilibrium region was reduced to a small area near the step-like interface. All MD results were compared to a continuum model and a good match was observed between the two approaches. Our results provide a useful understanding of heat transfer in nano- and micro-scale layered materials and van der Waals heterostructures. *Published by AIP Publishing.* <https://doi.org/10.1063/1.5025604>

Promising electrical, mechanical, and thermal characteristics of graphene and other layered materials will make them appropriate candidates for electronic, optomechanic, and thermal devices in the near future. Besides single-layer graphene, which has found a wide range of applications, its combination with other 2D or 3D materials in heterogeneous structures has found many other applications, making possible the manufacturing of nanoscale devices.¹ Depending on the structural characteristic of a graphene heterostructure, e.g., a step-like bilayer/monolayer (BL-ML) graphene interface, compared to covalent bonds, van der Waals interactions, can lead to special properties which are considerably different from those of pristine monolayer and even bilayer graphene sheets in some cases.²⁻⁵

In experimentally produced bilayer graphene or graphene flakes, it is often observed that the top-layer is interrupted suddenly while the bottom-layer still keeps going.^{6,7} Based on promising electronic properties of hybrid bilayer/monolayer graphene experimentally synthesized by epitaxial growth, investigating thermal properties of these structures is important in thermal management of electronic devices as well as thermoelectric applications.^{6,8-12} In such a hybrid layered nanostructure, the step-like configuration can be considered as an interface or intercept which imposes significant effects on the electrical properties. But from the phononic heat transfer point of view, the difference in properties between two sides of the interface may lead to major influences on heat carriers.¹³ It also brings all features of heat transfer at an interface, including phonon scattering and Kapitza resistance.^{14,15} One side of the interface consists of just covalent bonds, but the other side contains additional van der Waals interactions. This combination, especially when both sides of the system are connected to

different heat baths with different temperatures, may suggest a drop in the temperature profiles of the system at the interface, as it is widely known as Kapitza resistance.¹⁶⁻²¹ But in this kind of bilayer/monolayer hybrids (see Fig. 1), the step-like interface may not lead to a Kapitza resistance. The combination of intra-layer and inter-layer heat transfer makes the transfer phenomenon more complicated than that in non-layered media. For understanding the underlying physics, one should make it clear what is going on at the interface and what amount of heat is passing through within and between layers.

Although as the main research question, the thermal transport in a step-like bilayer/monolayer graphene interface in a van der Waals heterostructure is investigated, but the results can be generalized to any other layered medium with heterogeneous interactions. This combination makes the problem more interesting from fundamental and technological points of views. Due to the presence of strong intra-layer covalent bonds and weak inter-layer Lennard-Jones interaction, one should consider the effect of system size on inter-layer and intra-layer thermal transport. By increasing the system size and accumulation of intra-layer interactions, the cross-plane modes may become more important in bilayer region, leading to an interesting crossover in heat transfer; this is more evidently observed when one compares a small system with a macroscopic one. This could be addressed by atomistic simulations; however, in a very large system, we should compare the results with those obtained from continuum models. Thus, comparing continuum models with large scale atomistic simulations is important.

In this paper, temperature profile and heat flux variation are evaluated in a non-equilibrium thermal system consisting of a step-like bilayer/monolayer graphene interface. In spite of the similarities between preliminary results and Kapitza resistance feature, details of the temperature profile and

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FIG. 1. Schematic view of the atomistic structure of hybrid bilayer/monolayer graphene. The graphene half-layer and full-layer are marked in blue and red, respectively. Non-equilibrium heat transfer is generated by applying hot and cold baths at two ends of the structure at temperatures of T_h and T_c , respectively.

energy flux variation reveal there is no Kapitza resistance. The idea was supported by investigating the heat transfer in intra-layer (in-plane), inter-layer (cross-plane), and also through-interface. A continuum model is also provided and its results are compared with molecular dynamics (MD) results. To make valid comparisons, MD simulations are carried out in different length scales ranging from $0.1 \mu\text{m}$ to $1 \mu\text{m}$.

The atomistic structure of hybrid bilayer/monolayer graphene is schematically shown in Fig. 1. The bilayer graphene is in the AB stacking mode which is more stable than the AA stacking mode. As it is shown in Fig. 1, the bilayer graphene was interrupted at its half-length from where it was extended as a monolayer graphene. Employing freezing atoms at two ends of the system, boundary conditions were fixed along the x-direction. The length of the structure was varied between $0.1 \mu\text{m}$ and $1 \mu\text{m}$ and periodic boundary conditions were applied in the y-direction. The width was set to 5 nm , which was large enough to avoid finite size effects in the y-direction. The inter-layer thickness in bilayer graphene was initially assumed to be $3.4 \text{ \AA}$. The Tersoff potential²² reparametrized for graphene by Lindsay and Broido²³ and the Lennard-Jones potential with parameters $\epsilon = 2.39 \text{ meV}$ and $\sigma = 0.34 \text{ nm}$ (Ref. 24) were used to describe the intra-layer and the inter-layer interactions, respectively. It has been recently shown that, Tersoff potential is suitable for studying phonon transport in graphene as it properly predicts the thermal conductivity of graphene, as compared to corresponding experimental data.^{25,26} Regarding these potential functions, Newton's second law of motion was integrated using the velocity Verlet algorithm with a time step of 1 fs . In order to investigate heat transfer in the BL-ML graphene, the system was firstly relaxed at 300 K for 1 ns using a Nosé-Hoover thermostat chain,^{27–29} which is a well-known and accurate method for temperature control. Using this thermostat, hot and cold baths were established at the two ends of the structure at temperatures of T_h and T_c , respectively. After 5 ns of being in the steady-state condition, data collection was started for calculating temperature distribution across the system. For this purpose, the structure was divided to several computational slices and the temperature profile (T) across each slice was calculated using $T = \frac{2}{3k_B N} \sum_{i=1}^N \frac{1}{2} m_i v_i^2$, where N is the number of atoms in each slice, k_B is the Boltzmann constant, m_i is the atomic mass, and v_i is velocity of each atom within the slice. The final temperature of each slice was calculated by time-averaging over 5 ns . All of the MD simulations were performed using the GPUMD (Graphics Processing Units Molecular Dynamics) code.³⁰

In the non-equilibrium molecular dynamics method, each computational slice is assumed to be locally in equilibrium. Considering the small size of a slice and long phonon mean free path, this assumption is challenging; however, the method has been widely used for predicting the thermal conductivity of materials.^{31–36} In the studied hybrid bilayer/monolayer graphene in the present research, two slicing methods were considered [methods (i) and (ii) in Fig. 2]. In method (i), the bilayer graphene was considered as an integrated structure with thermal equilibrium between its layers. In method (ii), however, no thermal equilibrium was assumed between the layers, i.e., each layer had its own temperature profile.

In order to investigate the accuracy of each slicing method, temperature profiles were calculated in a structure with the length of $L = 0.1 \mu\text{m}$, $T_h = 320 \text{ K}$, and $T_c = 280 \text{ K}$. The results of slicing methods (i) and (ii) are shown in Figs. 2(a) and 2(b), respectively. With method (i), there is a temperature drop at intercept which may be attributed to a Kapitza resistance between the two parts of the structure upon which no temperature difference is seen between the layers. In method (ii), temperature differences between layers of the bilayer part reveals that, thermal equilibrium between the layers has not been reached. The reason for such differences will be discussed in the next paragraph. Thus, the slicing method (i) does not lead to correct results as it returns non-existent Kapitza resistance at the intercept.

To better understand the heat transport in the BL-ML system, the temperature profiles of BL-ML, full monolayer, and full bilayer graphene samples are presented and compared in Fig. 3. As it can be seen, although the imposed temperature differences in all cases are the same ($T_h = 320 \text{ K}$ and $T_c = 280 \text{ K}$), the local temperature profiles, and correspondingly, the local heat fluxes in BL-ML differs from full mono- and bi-layer samples.

To examine the effect of the length of the system, the temperature profiles for BL-ML with dimensions of $L = 0.5$ and $1 \mu\text{m}$ are shown in Fig. 4. It should be noted that, at the vicinity of the heat baths, there are nonlinear effects (artefacts of heat baths in MD simulations) that were removed in order MD results to be comparable with the continuum model. As it can be seen, the layers of the bilayer part differed in temperature, especially for smaller length of the system. This was due to low thermal conductivity between layers of the bilayer graphene (cross-plane thermal conductivity) described by weak van der Waals atomic interactions compared to high in-plane thermal conductivity of graphene layers which could be addressed by strong intra-layer covalent interactions.³⁷ Since the top layer of the bilayer graphene was only connected to

FIG. 2. Temperature profiles in the BL-ML graphene extracted from two slicing methods (i) and (ii). Method (i) leads to appearance of a non-existent Kapitza resistance, where, half-layer graphene is disconnected as it is shown in (a) while method (ii) reveals that there is no thermal equilibrium between the half-layer and full-layer, as depicted in (b).

the hot bath, the heat current must go through the layers of the bilayer graphene with low inter-layer thermal conductivity, developing some temperature differences between different graphene layers. In order to better understand the heat transfer in the BL-ML graphene, heat flux distribution across the structure was calculated. For this purpose, inter-layer and intra-layer heat fluxes are shown in Fig. 5. Intra-layer heat flux from a computational slice (e.g., A) to another slice (e.g., B) in each layer was calculated using microscopic definition of heat flux as follows:³⁸

$$q_{A \rightarrow B} = -\frac{1}{2} \sum_{i \in A} \sum_{j \in B} \left\langle \left(\frac{\partial \sum_{k \neq i} U_{ik}}{\partial \vec{r}_{ij}} \cdot \vec{v}_j - \frac{\partial \sum_{k \neq j} U_{jk}}{\partial \vec{r}_{ji}} \cdot \vec{v}_i \right) \right\rangle, \quad (1)$$

FIG. 3. Temperature profiles for the BL-ML, full monolayer (ML) and full bilayer (BL) graphene samples with $L = 0.5 \mu m$.

FIG. 4. Temperature profile in the BL-ML graphene for $L = 0.5$ and $1 \mu m$. The discrete points refer to MD results and the continuous black lines correspond to continuum results.

where $\vec{r}_{ij} \equiv \vec{r}_j - \vec{r}_i$ is the difference in the position between atom i and atom j , $\vec{v}$ is the atomic velocity, and U_{ik} is the bond energy between atoms i and k . Inter-layer heat flux could be calculated from the difference in intra-layer heat flux between two adjacent slices according to the energy conservation law. As shown in Fig. 5, the inter-layer heat flux between two layers of the bilayer graphene increases with length; this is due to decreased heat flux along the top layer (half-layer). So, the heat flux through layers reaches its maximum value at the end of the half-layer graphene, where the maximum temperature difference between the top and bottom layers takes place. The heat flux in the bottom graphene layer (full-layer) also increases along the length, reaching a maximum value at $x = L/2$ and remaining constant for $x > L/2$.

In order to see what happens when the system length is very large, a continuum model was considered for solving the heat conduction equation in the BL-ML graphene structure. The layers were considered to be continuous with the in-plane thermal conductivity of κ_{ip} . In order to model cross-plane thermal conductivity, a thin layer with the thermal conductivity of κ_{cp} was considered in between the plates. The κ_{ip} and κ_{cp} were extracted from MD simulations based on the linear portion of temperature gradient in the monolayer graphene and temperature differences between layers of the bilayer graphene, respectively, and considered as inputs into the continuum model. As a length-dependent parameter, κ_{ip} was calculated to be 1546 W/mK and 1950 W/mK for $L = 0.5 \mu\text{m}$ and $1 \mu\text{m}$, respectively, which are in good agreements with previous reports on the thermal conductivity of graphene.^{25,26} The value of κ_{cp} was found to be 0.015 W/mK, i.e., clearly much lower than κ_{ip} . The thickness of each layer was set to $t = 3.4 \text{ \AA}$. In this way, the heat conduction equation across the structure for calculating the temperature

distribution across the half-layer (T_{hl}) and the full-layer (T_{fl}) can be written as follows:

$$\begin{aligned} \frac{d^2 T_{hl}}{dx^2} - P(T_{hl} - T_{fl}) &= 0, & 0 \leq x \leq L/2, \\ \frac{d^2 T_{fl}}{dx^2} + P(T_{hl} - T_{fl}) &= 0, & 0 \leq x \leq L/2, \\ \frac{d^2 T_{fl}}{dx^2} &= 0, & L/2 \leq x \leq L \end{aligned} \quad (2)$$

with the boundary conditions as

$$\begin{aligned} \text{At } x = 0 : \quad T_{hl} &= T_{fl} = T_H, \\ \text{At } x = L/2 : \quad \frac{dT_{hl}}{dx} &= 0, \quad \frac{dT_{fl}}{dx} \quad \text{and} \\ T_{fl} &\text{ are continuous functions,} \\ \text{At } x = L : \quad T_{fl} &= T_C, \end{aligned} \quad (3)$$

where T_H and T_C are the hot and cold bath temperatures, respectively, and $P = \frac{\kappa_{cp}}{\kappa_{ip} t^2}$. The two above-mentioned equations are coupled, so that those must be solved simultaneously. By algebraic summation of equations and analytically solving them, temperature profiles across the layers were obtained as follows:

$$\begin{aligned} T_{hl}(x) &= T_H - A \left(\frac{x}{2} - \frac{\sinh(\sqrt{2Px})}{2\sqrt{2P} \cosh(\sqrt{P/2L})} \right), & 0 \leq x \leq L/2, \\ T_{fl}(x) &= T_H - A \left(\frac{x}{2} + \frac{\sinh(\sqrt{2Px})}{2\sqrt{2P} \cosh(\sqrt{P/2L})} \right), & 0 \leq x \leq L/2, \\ T_{fl}(x) &= T_H - \frac{T_H - T_C}{L} x, & L/2 \leq x \leq L \end{aligned} \quad (4)$$

where

$$A = \left(\frac{T_H - T_C}{L/2} \right) / \left(\frac{3}{2} + \frac{\tanh(\sqrt{P/2L})}{L\sqrt{2P}} \right). \quad (5)$$

The temperature profiles obtained from the analytical solution of energy equations are shown in Fig. 4 (continuous black lines). It should be noted that the hot and cold temperature values in the continuum model were set to corresponding values in MD simulation after removing artefacts in temperature profiles. Accordingly, a good agreement was found between MD results and continuum model results. The temperature jump at the intercept could be calculated from the continuum model in terms of the structure length and applied temperature difference to the thermal baths, as follows:

$$\Delta T|_{x=L/2} = (T_{hl} - T_{fl})|_{x=L/2} = \frac{2(T_H - T_C) \tanh(\sqrt{P/2L})}{3L\sqrt{P/2} + \tanh(\sqrt{P/2L})}. \quad (6)$$

The heat flux calculated from the continuum simulation is also shown in Fig. 5 (continuous lines). According to the

FIG. 5. Intra-layer and inter-layer heat flux distributions calculated via MD simulation (points) and continuum modelling (lines) for the BL-ML graphene with $L = 0.5 \mu\text{m}$. The heat flux in the full-layer increases with x , reaching to its maximum value at $x = L/2$, while it follows a decreasing trend with increasing x in the half-layer. Based on the energy conservation law, the difference of $q''_{full-layer}$ and $q''_{half-layer}$ at each x equals to $q''_{inter-layer}$.

continuum results, the same trend to MD results was followed by heat flux in the BL-ML graphene.

In summary, the temperature distribution and inter-layer and intra-layer heat fluxes were calculated in a hybrid bilayer/monolayer graphene system at the non-equilibrium steady state using molecular dynamics simulations and continuum heat conduction modelling. Accordingly, it was revealed that, in systems of shorter length, a temperature drop is seen between the layers, not only at the step-like interface, but also in a considerable part of the bilayer graphene. Thus, defining a Kapitza resistance at the planar intercept is an unrealistic practice. It was also shown that, the temperature drop will gradually vanish when the system increases in size. All MD results were compared to the continuum model and a good match was observed between the two approaches. Our findings can provide useful understanding concerning heat transfer not only in bilayer/monolayer graphene, but also in other layered 2D materials and van der Waals heterostructures.

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