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Mingchao Wang\textsuperscript{a}, Dilini Galpaya\textsuperscript{a}, Zheng Bo Lai\textsuperscript{a}, Yanan Xu\textsuperscript{a} & Cheng Yan\textsuperscript{a}

\textsuperscript{a} School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, QLD 4001, Australia

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Surface functionalization on the thermal conductivity of graphene–polymer nanocomposites

Mingchao Wang, Dilini Galpaya, Zheng Bo Lai, Yanan Xu and Cheng Yan*

School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, QLD 4001, Australia

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Exploring thermal transport in graphene–polymer nanocomposite is significant to its applications with better thermal properties. Interfacial thermal conductance between graphene and polymer matrix plays a critical role in the improvement of thermal conductivity of graphene–polymer nanocomposite. Unfortunately, it is still challenging to understand the interfacial thermal transport between graphene nanofiller and polymer matrix at small material length scale. To this end, using nonequilibrium molecular dynamics (NEMD) simulations, we investigate the interfacial thermal conductance of graphene–polyethylene (PE) nanocomposite. The influence of functionalization with hydrocarbon chains on the interfacial thermal conductance of graphene–polymer nanocomposites was studied, taking into account the effects of model size and thermal conductivity of graphene. An analytical model is also used to calculate the thermal conductivity of nanocomposite. The results are considered to contribute to the development of new graphene–polymer nanocomposites with tailored thermal properties.

Keywords: graphene; functionalization; nanocomposite; interface; thermal transport

1. Introduction

Graphene possesses exceptional electrical, mechanical, and thermal properties [1–3], which make it an ideal candidate as filler for making composite materials. For instance, the reported value of thermal conductivity of graphene is about 3000 W/mK [3–5], while most of the polymers have thermal conductivity less than 0.5 W/mK. Adding a small percentage of graphene to the polymer matrix can greatly enhance its thermal conductivity. Recent studies have indicated that significant improvements in thermal conductivity have been achieved in these nanocomposite systems (3–6 W/mK) [6–10].

It has been found that interfacial thermal conductance between fillers and polymer matrix is crucial to the thermal transport in composites. Recently, Huxtable et al. [11] reported that the exceptionally small interfacial thermal conductance (~12 MW/m²K) restricts the heat transport in a carbon nanotube (CNT) composite. For graphene–polymer nanocomposites, Hu et al. [12] have reported an effective interfacial thermal conductance of 30 MW/m²K between graphene and phenolic resin. Chemical functionalization serves as an effective routine to enhance the thermal conductivity of CNT/graphene–polymer nanocomposites [13–15]. Theoretical analysis [16] reported that chemical functionalization of CNT can surprisingly increase by two orders of composite conductivity. Since
Vibrations are the primary mode of thermal transport in polymers, covalent bond between the matrix and the filler can reduce phonon scattering at graphene–polymer interface, leading to better coupling between the modes, which increases the conductance [16,17]. However, the influence of chemical functionalization on interfacial thermal conductance in graphene–polymer nanocomposites has not been well understood. Due to the nanosized structure, it is still a technical challenge to conduct experiments across the graphene–polymer interface. Numerical simulation such as molecular dynamics (MD) modeling provides an alternative approach to study the interfacial thermal transport. In this study, we have conducted nonequilibrium molecular dynamics (NEMD) simulations to study the thermal transport across graphene–polymer interface. The effect of functionalization, i.e., grafting hydrocarbon chains to graphene layer with covalent bonds, on the interfacial thermal conductance was also investigated. The effect of model size and thermal conductivity of graphene was taken into account. We then predicted the thermal conductivity of nanocomposite based on a theoretical model.

2. Model and methodology

Due to structural simplicity, polyethylene (PE) was selected in the simulation, whose molecule \((\text{CH}_3-(\text{CH}_2-\text{CH}_2)_{29}-\text{CH}_3)\) is composed of 30 monomers. Two models were built using Material Studio (Accelrys Inc) to simulate PE and graphene–PE nanocomposite. The PE model was prepared with the dimensions of \(30 \times 30 \times 77\) Å, with an initial density of 0.8 g/cc. To build the graphene–PE nanocomposite model, a sandwich structure with graphene placed in the middle of PE matrix was prepared first, with dimensions of \(25 \times 25 \times 200\) Å. Then, the model was duplicated along the stacking direction for later simulations, as shown in Figure 1. Graphene layers grafted with short linear hydrocarbon chains \((-\text{C}_n\text{H}_{2n+1}, n = 15)\) were established in order to explore the effect of functionalization on interfacial thermal conductance (Figure 2). Such covalent end-grafting with a range of grafting densities \(\sigma = 0.0032, 0.0064, 0.0096, \) and \(0.0144\) Å\(^{-2}\) corresponds to two, four, six, and nine, respectively, linear hydrocarbon chains grafted on graphene layers. The interatomic interactions were described by an \(ab\) initio force field (polymer consistent force field (PCFF)) [18]. All MD simulations were performed with the large-scale atomic/molecular massively parallel simulator (LAMMPS) package [19]. In general, the total potential energy of a simulation system contains the following terms:

\[
E_{\text{total}} = E_{\text{bond}} + E_{\text{over}} + E_{\text{val}} + E_{\text{tors}} + E_{\text{vdW}} + E_{\text{Coulomb}}
\]  

(1)

Figure 1. The model of graphene–polymer nanocomposite for nonequilibrium molecular dynamics simulations. The heat source is placed at the center and heat sink is placed at each end of the simulation cells to generate the heat flux \(J_Q\).
where $E_{\text{bond}}, E_{\text{over}}, E_{\text{val}}, E_{\text{tors}}, E_{\text{vdW}},$ and $E_{\text{Coulomb}}$ are the energies corresponding to bond, over-coordination, angle, torsion, van der Waals (vdW), and Coulomb interactions, respectively. The detailed expression for each component of the total potential energy can be found anywhere else [20,21].

For all simulations, systems were first equilibrated at constant volume and constant temperature of 300 K for 0.25 ns with a time step of 0.25 fs. Then, they were equilibrated at constant temperature of 300 K and constant pressure of 1 atm for 0.5 ns with the same time step. The thermal conductivity is calculated on the basis of Fourier’s law,

$$J_Q = -\kappa \left( \frac{\Delta T}{\Delta z} \right) \quad (2)$$

where $J_Q$ is the heat flux, $\kappa$ is the thermal conductivity, and $\Delta T/\Delta z$ is the temperature gradient. As for the interfacial thermal conductance, it is calculated using the expression

$$J_Q = -G_{\kappa} \Delta T \quad (3)$$

where $J_Q$ is the heat flux across the interface, $G_{\kappa}$ is the interfacial thermal conductance, and $\Delta T$ is the temperature variation across the interface. To calculate thermal conductivity of pure PE and interfacial thermal conductance of nanocomposite, NEMD method is applied to both models of pure PE and graphene–PE nanocomposite at constant volume and constant energy ensemble. According to Müller-Plathe algorithm [22], heat source and heat sink are placed at the center and at each end of simulation cells, respectively, to generate a constant heat flux. When the simulation systems reach steady state after 2.5 ns of simulation, the heat flux can be calculated as $J_Q = \Delta E/2A\Delta t$, where $\Delta E$ is the energy added into heat source, $A$ is the cross-sectional area of simulation cell, and $\Delta t$ is the time step.
3. Results and discussion

3.1. Model validation

In order to validate the PCFF potential for thermal transport simulation in graphene–PE nanocomposite, the thermal conductivity of the PE was calculated using NEMD method. Figure 3 shows the heat flux and the temperature profile. The temperature gradient is linear, indicating the regime of linear response in heat source/sink simulation. The thermal conductivity of the PE model is calculated as $\kappa_{\text{PE}} = 0.3599 \text{ W/mK}$. This value is in agreement with the previous simulations [23,24], which validates the model and methodology used in this work.

3.2. Effect of length and functionalization on the thermal conductivity of graphene

In NEMD simulations, the model size is finite and can influence the calculated interfacial thermal conductance. Recent research has demonstrated that there is no obvious dependence of matrix thickness (block size $L$ along the stacking direction) on the interfacial thermal conductivity of graphene–polymer nanocomposite [24]. Therefore, only one value of matrix thickness ($L = 35 \text{ Å}$) is chosen in this work [24]. Such matrix-size independence might be owing to the fact that the propagating vibration modes in polymer matrix have the propagation lengths on the order of a few bond lengths, and the block size of 35 Å is large enough to involve all the significant vibration modes in PE matrix. However, the length of graphene is crucial to its thermal conductivity. Small model size can omit some significant modes of long wavelengths. We thus discuss the effect of the length and functionalization on the thermal conductivity of graphene. As shown in Figure 4(a), the thermal conductivity of monolayer graphene $\kappa$ is deteriorated by functionalization with grafted hydrocarbon chains. Functionalization at a very small grafting density of 0.0032 Å$^{-2}$ surprisingly leads to the drop of $\kappa$ around 69%. With the increase of grafting density, the drop of $\kappa$ becomes slower and gets saturated at a value of 80%. The reduction trend of $\kappa$ caused by hydrocarbon chains is similar to that caused by methyl and phenyl groups [25]. The falling thermal conductivity of graphene lies in the formation of sp$^3$ bonds between graphene and hydrocarbon chains, which can soften the high-frequency phonon modes and weaken the in-plane energy transfer. Moreover, $\kappa$ also enhances with the increase of simulation cell in Figure 4(b). This can be attributed to the ballistic nature of thermal transport, which is also observed in pure graphene.

Figure 3. (a) Heat energy in PE system versus time. (b) Steady-state temperature profile along the entire length of the PE model.
3.3. **Interfacial thermal conductance of graphene–PE nanocomposite**

Both heat flux and temperature profile in graphene–polymer nanocomposite are determined using NEMD method. Then, the corresponding interfacial thermal conductance can be calculated in terms of Equation (3). Figure 5(a) shows obvious temperature drop at graphene–PE interface, which dominates the overall temperature across the whole model. This temperature drop leads to the value of interfacial thermal conductance to be \( G_\kappa = 76.5 \text{ MW/m}^2\text{K} \), which is close to the value obtained in previous work [24]. Figure 5(b) shows a plot of \( G_\kappa \) as a function of grafting density for linear hydrocarbon chains. It is observed that after grafting linear hydrocarbon chains to monolayer graphene, the interfacial thermal conductance are surprisingly enhanced. Grafting only two chains (\( \sigma = 0.0032 \text{ Å}^{-2} \)) on each side of graphene raises \( G_\kappa \) by 33.3%. When grafting up to six chains (\( \sigma = 0.0096 \text{ Å}^{-2} \)), \( G_\kappa \) is remarkably enhanced by 196%, which is higher than the enhancement caused by increasing the layer number of graphene. At higher grafting density, the increase of \( G_\kappa \) becomes much smaller, showing a saturation trend of interfacial thermal conductance. We then refer to the effect of chain length on \( G_\kappa \). At \( \sigma = 0.0096 \text{ Å}^{-2} \), \( G_\kappa \) gets enlarged with the increase of chain length. According to Chen’s work, thermal conductivity of single PE chain enhances with the chain length until 1 \( \mu \text{m} \). Therefore, the larger thermal conductivity of longer chains enables the larger interfacial thermal conductance at graphene–PE interfaces. As for the influence of graphene length on \( G_\kappa \), previous work [24] indicated that increasing graphene length can...
enhance \( G_\kappa \). However, such enhancement will be saturated when graphene size is larger than about 79 Å.

In order to explore the underlying mechanism of improvement of \( G_\kappa \), Hu et al. [26] demonstrated that the heat transport between graphene and polymer matrix is dominated by their low-frequency vibration modes. Grafted hydrocarbon chains can widen the overlap in low-frequency vibration modes and consequently enhance the interfacial thermal conductance. Our results are also consistent with the previous study of interfacial thermal conductance of CNT–polymer nanocomposite [27]. Therefore, functionalization of graphene by grafting hydrocarbon chains is an effective approach to improve the interfacial thermal conductance of graphene–polymer nanocomposite.

3.4. Thermal conductivity of graphene–PE nanocomposite

Using the interfacial thermal conductance \( G_\kappa \) evaluated by NEMD simulations, we can evaluate the thermal conductivity of graphene–PE nanocomposite. Generally, graphene fillers are randomly oriented in the polymer matrix. The thermal conductivity of the nanocomposite with randomly oriented fillers can be calculated by an analytical formula based on the effective medium approach [28]. In this theoretical model, the condition of well-dispersed fillers in matrix is assumed. Hence, the effects of exfoliation and aggregation of fillers are not considered in this work. According to Nan’s work, the analytical formula can be written as follows:

\[
K^* = K_m \frac{3 + f[2\beta_{11}(1 - L_{11}) + \beta_{33}(1 - L_{33})]}{3 - f[2\beta_{11}L_{11} + \beta_{33}L_{33}]}
\]  

(4)

with

\[
\beta_{11} = \frac{K_{11}^C - K_m}{K_m + L_{11}(K_{11}^C - K_m)}, \quad \beta_{33} = \frac{K_{33}^C - K_m}{K_m + L_{33}(K_{33}^C - K_m)}
\]  

(5)

\[
K_{11}^C = K_p/(1 + \gamma L_{11}K_p/K_m), \quad K_{33}^C = K_p/(1 + \gamma L_{33}K_p/K_m)
\]  

(6)

\[
L_{11} = \frac{p^2}{2(p^2 - 1)} + \frac{p}{2(1 - p^2)^{3/2}} \cos^{-1}p, \quad L_{33} = 1 - 2L_{11}
\]  

(7)

where \( K^* \) is isotropic thermal conductivity of nanocomposite; \( K_m \) is the thermal conductivity of the matrix; \( K_p \) is the thermal conductivity of the filler; \( K_{ii}^C (i = 1,3) \) are the equivalent thermal conductivities of nanocomposite along x and z axes; \( f \) is filler volume fraction and equals to 0.017 for our models; \( p = a_3/a_1 \) is the aspect ratio of graphene given by the ratio of shortest to longest radii of the filler; \( \gamma = (1 + 2p)a \), where \( a = a_\kappa/a_3 \) and \( a_\kappa = K_m/G_\kappa \); and \( G_\kappa \) is the interfacial thermal conductance.

According to Equations (4)–(7), we can calculate the thermal conductivity of nanocomposites with different length and grafting densities of graphene nanofiller. We use material parameters \( K_p = 1000 \text{ W/mK} \) and \( G_\kappa = 76.5 \text{ MW/m}^2\text{K} \) for nanocomposite with pure graphene, and \( K_p = 400 \text{ W/mK} \) and \( G_\kappa = 102–252 \text{ MW/m}^2\text{K} \) for nanocomposite with functionalized graphene. Figure 6 shows \( K^* \) of graphene–polymer nanocomposite as a
function of filler length. When filler length $L$ is below 5000 nm, $K^*$ in all cases rises rapidly with increasing filler length $L$. Grafting linear hydrocarbon chains to monolayer graphene enhances $K^*$ of nanocomposite. Within such range of $L$, larger grafting density contributes to higher interfacial thermal conductance and leads to higher $K^*$ than pure graphene. However, there is no obvious enhancement of $K^*$ induced by further increase of grafting density ($\sigma \geq 0.0096 \text{ Å}^{-2}$). When $L$ is larger than 5000 nm, $K^*$ reaches a value of plateau, except in the case of pure graphene. This is in that $K^*$ for pure graphene has larger limit value than that for functionalized graphene. Hence, $K^*$ for pure graphene becomes larger than that for functionalized graphene within this range. Such failure of $K^*$ enhancement can be attributed to the decrease of thermal conductivity of functionalized graphene. Therefore, increase of interfacial thermal conductance cannot enhance the overall thermal conductivity of nanocomposites all the time.

We then focus on the effect of nanofiller volume fraction $f$ on the overall thermal conductivity of nanocomposites. $G_\kappa = 252 \text{ MW/m}^2\text{K}$ is considered and $f$ varies from 1% to 10%. As shown in Figure 7, $K^*$ gets surprisingly enhanced with increasing $f$. Moreover, larger filler length contributes to higher enhancement of $K^*$. For instance, at $L = 5000$ nm,
\( K^* \) at \( f = 10\% \) is 800\% higher than that at \( f = 1\% \). Such increase by filler volume fraction is much larger than filler length, which acts as a more efficient parameter improving thermal conductivity of nanocomposites. The theoretical analysis results here are also in agreement with recent experimental results, such as Shahil and Balandin’s work [6], which reported that nanocomposites with graphene \( f = 10\% \) has a thermal conductivity of 23 W/mK. However, experimental results reported by Song et al. [29] are much lower than our simulation results. This may be attributed to some possible factors, such as aggregation of nanofillers, wrinkles, and bad graphene–polymer interfaces.

4. Conclusions

In this work, we have conducted MD simulations to investigate the thermal transport in graphene–polymer nanocomposite. The effects of functionalization on both thermal conductivity of graphene and interfacial thermal conductance of graphene–polymer nanocomposite were systematically investigated. Our simulation results indicate that functionalization with grafted hydrocarbon chains can reduce the thermal conductivity of graphene. On the other hand, it can strengthen the coupling between graphene and polymer and increase the corresponding interfacial thermal conductance. An analytical model was also utilized to predict the thermal conductivity of nanocomposite. It was found that there is a critical value of filler length, beyond which functionalization fails to enhance the overall thermal conductivity of nanocomposite. Furthermore, filler volume fraction of graphene fillers plays a governing role in dictating the overall thermal conductivity of graphene–polymer nanocomposites. Our studies provide an effective approach to enhance the thermal transport in graphene–polymer nanocomposite.

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