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Functionalization effect on the thermal conductivity of graphene-polymer nanocomposites

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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 non-equilibrium molecular dynamics 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 of 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 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 \(3~6 Wm/K\) \[6-10\].](#)

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 composite. For graphene-polymer nanocomposites, Hu *et al.* [12] has 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 carbon nanotube (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 filler can reduce phonon scattering at graphene-polymer interface, leading to better coupling between the modes and 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 nano-sized structure, it is still a technical challenge to conduct experiment across the graphene polymer interface. Numerical simulation such as molecular dynamics (MD) modelling provides an alternative approach to study the interfacial thermal transport. In this study, we have conducted non-equilibrium 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 (CH₃-(CH₂-CH₂)₂₉-CH₃) 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 $30 \text{ \AA} \times 30 \text{ \AA} \times 77 \text{ \AA}$, 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 firstly, with dimensions of $25 \text{ \AA} \times 25 \text{ \AA} \times 200 \text{ \AA}$. 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 $\sigma=0.0032, 0.0064, 0.0096, 0.0144 \text{ \AA}^{-2}$ corresponds to 2, 4, 6, 9 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:

$$E_{total} = E_{bond} + E_{over} + E_{val} + E_{tors} + E_{vdW} + E_{Coulomb} \quad (1)$$

where E_{bond} , E_{over} , E_{val} , E_{tors} , E_{vdW} and $E_{Coulomb}$ 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].

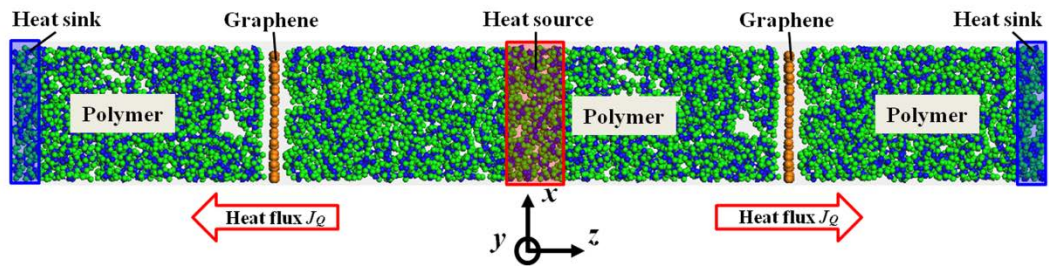


Figure 1. The model of graphene-polymer nanocomposite for non-equilibrium molecular dynamics simulations. The heat source is placed in the centre and heat sink placed in each end to generate the heat flux J_Q .

For all simulations, systems were firstly 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,

$$J_Q = -\kappa(\Delta T/\Delta z) \quad (2)$$

where J_Q is the heat flux; κ is the thermal conductivity; $\Delta T/\Delta z$ 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_κ is the [interfacial thermal conductance](#); ΔT 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 in constant volume and constant energy ensemble. According to Muller-Plathe algorithm [22], heat source and sink are placed on the center and each end of simulation cells to generate constant heat flux. When simulation systems reach steady state after 2.5 ns simulation, the heat flux can be calculated as $J_Q = \Delta E/2A\Delta t$, where ΔE is the energy added into heat source; A is the cross-sectional area of simulation cell; Δt is the time step.

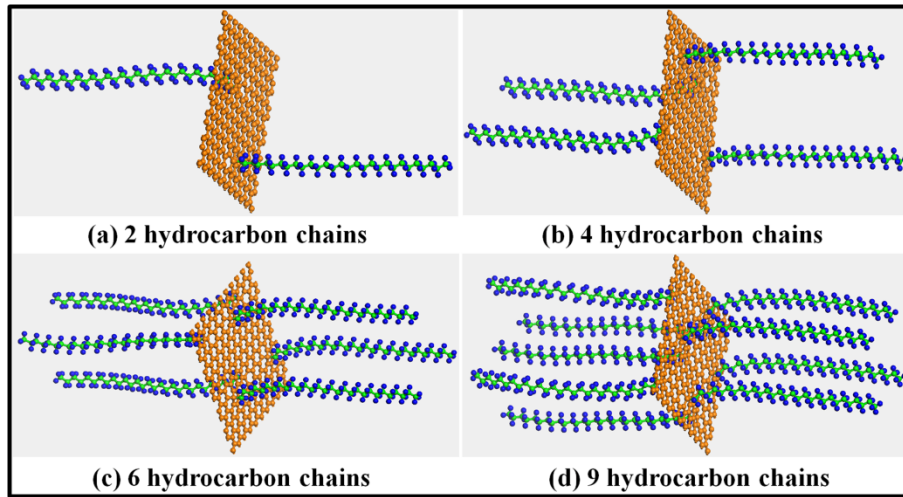


Figure 2. Monolayer graphene grafted with (a) 2, (b) 4, (c) 6 and (d) 9 linear hydrocarbon chains.

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 $\kappa_{PE}=0.3599$ W/mK. This value is in agreement with the previous simulations [23, 24], validated the model and methodology used in this work.

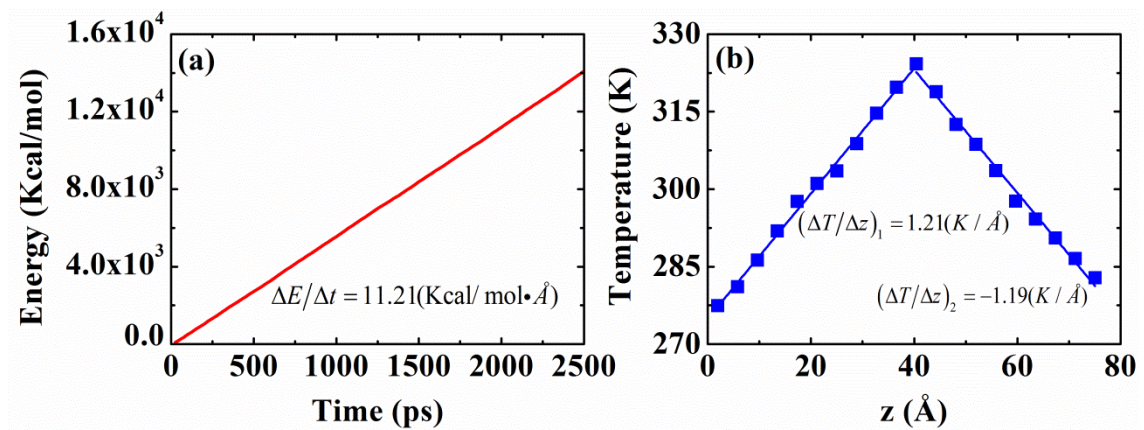


Figure 3. (a) Heat energy in PE system versus time. (b) Steady-state temperature profile along the entire length of the PE model.

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 ($L=35 \text{ \AA}$) 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 \AA 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 κ is deteriorated by functionalization with grafted hydrocarbon chains. Functionalization at a very small grafting density of 0.0032 surprisingly leads to the drop of κ around 69%. With the increase of grafting density, the drop of κ becomes slower and gets saturated at a value of 80%. The reduction trend of κ 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, κ 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.

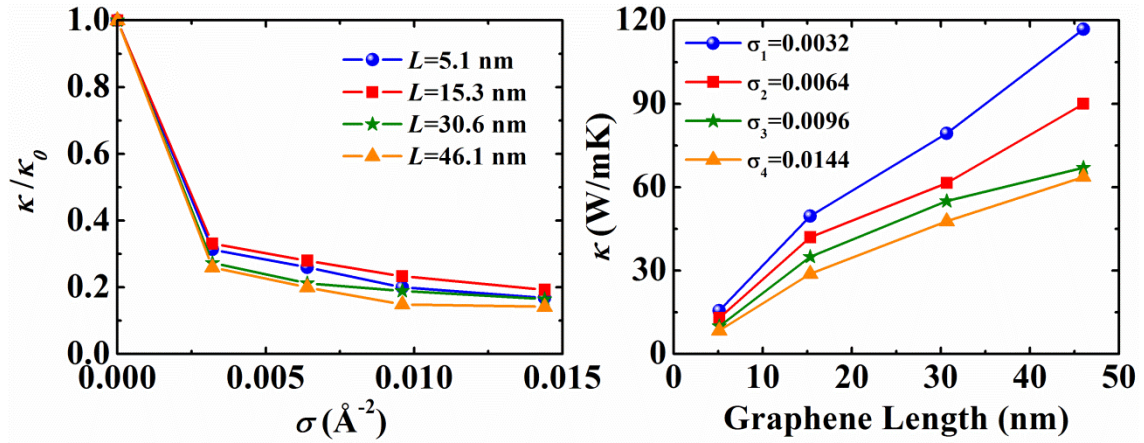


Figure 4. (a) Normalized thermal conductivity of functionalized graphene κ/κ_0 versus grafting density σ . κ_0 represents the thermal conductivity of pure graphene. (b) Thermal conductivity of functionalized graphene versus graphene length L .

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 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_κ 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 ($\sigma=0.0032 \text{ \AA}^{-2}$) on each side of graphene raises G_κ by 33.3%. When grafting up to 6 chains ($\sigma=0.0096 \text{ \AA}^{-2}$), G_κ is remarkably enhanced by 196%, which is higher than the enhancement by increasing layer number of graphene. At higher grafting density, the increase of G_κ becomes much smaller, showing a saturation trend of **interfacial thermal conductance**. We then refer to the effect of chain length on

G_{κ} . At $\sigma=0.0096 \text{ \AA}^{-2}$, G_{κ} 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_{κ} , previous work [24] indicated that increasing graphene length can enhance G_{κ} . However, such enhancement will be saturated when graphene size is larger than about 79 \AA .

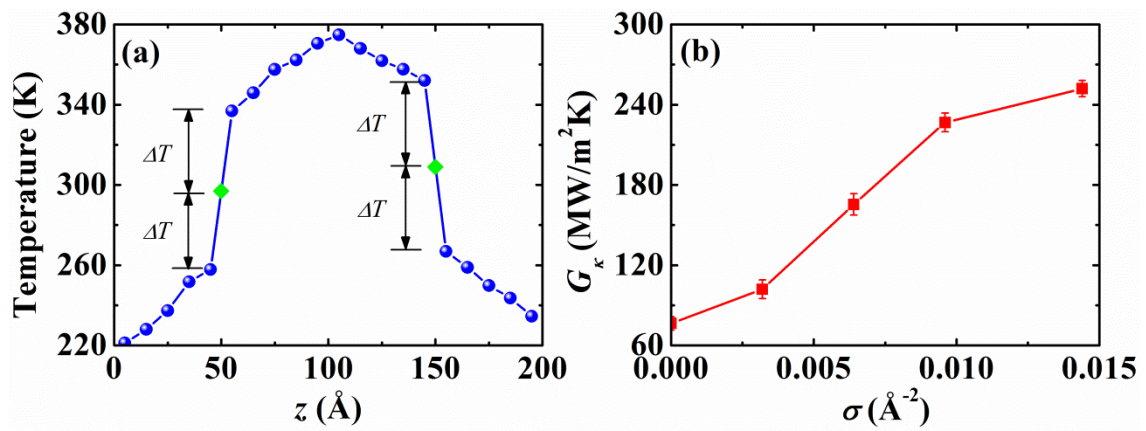


Figure 5. (a) Steady-state temperature profile in the case of monolayer graphene without functionalization. (b) Interfacial thermal conductance G_{κ} versus grafting density σ .

In order to explore the underlying mechanism of improvement of G_{κ} , 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 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_κ 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

$$K^* = K_m \frac{3 + f [2\beta_{11}(1 - L_{11}) + \beta_{33}(1 - L_{33})]}{3 - f [2\beta_{11}L_{11} + \beta_{33}L_{33}]} \quad (4)$$

with

$$\beta_{11} = \frac{K_{11}^C - K_m}{K_m + L_{11}(K_{11}^C - K_m)}, \quad \beta_{33} = \frac{K_{33}^C - K_m}{K_m + L_{33}(K_{33}^C - K_m)} \quad (5)$$

$$K_{11}^C = K_p / (1 + \gamma L_{11} K_p / K_m), \quad K_{33}^C = K_p / (1 + \gamma L_{33} K_p / K_m) \quad (6)$$

$$L_{11} = \frac{p^2}{2(p^2 - 1)} + \frac{p}{2(1 - p^2)^{3/2}} \cos^{-1} p, \quad L_{33} = 1 - 2L_{11} \quad (7)$$

where K^* is isotropic thermal conductivity of nanocomposite; K_m is the thermal conductivity of the matrix; f is filler volume fraction and equal 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; $\gamma = (1 + 2p)\alpha$, where $\alpha = a_\kappa/a_3$ and $a_\kappa = K_m/G_\kappa$; G_κ is the [interfacial thermal conductance](#).

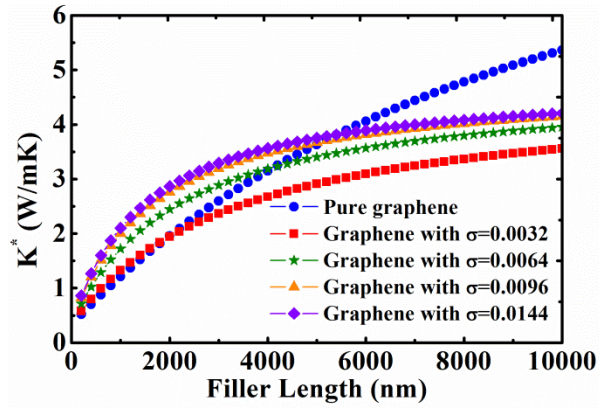


Figure 6. Thermal conductivity of nanocomposite K^* with different types of graphene fillers ($\sigma=0.0032\sim 0.0144 \text{ \AA}^{-2}$) as a function of filler length L .

According to Equation (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 $G_k=76.5 \text{ MW/m}^2\text{K}$ for nanocomposite with pure graphene, and $K_p=400 \text{ W/mK}$ and $G_k=102\sim 252 \text{ MW/m}^2\text{K}$ for nanocomposite with functionalized graphene. Figure 6 shows K^* of graphene-polymer nanocomposite as a function of filler length. When filler length L below 5000 nm, K^* in all cases rise 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 ($\sigma \geq 0.0096 \text{ \AA}^{-2}$). 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 nanocomposite all the time.

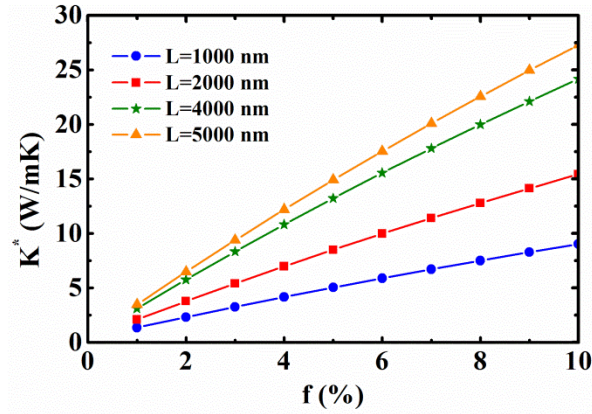


Figure 7. Thermal conductivity of nanocomposite K^* with different nanofiller volume fractions f and filler length L .

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 $L=5000 \text{ nm}$, 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 M/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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