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Morphology and in-plane thermal conductivity of hybrid graphene sheets

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This paper investigates the morphology and in-plane thermal conductivity of hybrid graphene sheets (HGSs), which consist of un-hydrogenated and single-side or double-side hydrogenated strips, via molecular dynamics simulation. The study shows that the hydrogenation styles and hydrogen coverage significantly affect the morphology and thermal conductivity of HGSs. The thermal conductivity of HGSs decreases dramatically, compared to that of pure graphene sheets, and the magnitude falls in the range of 30%-75%. Such differences are explained by conducting the phonon spectra analysis. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4767388>]

Graphene (GE) is a single layer of graphite with all carbon atoms arranged in a honeycomb lattice (Fig. 1(a)). Since the mechanical extraction of GE from graphite,¹ extensive research has been conducted on its physical and mechanical properties.²⁻⁷ For example, GE has demonstrated an ultra-high thermal conductivity λ ,^{5,6,8,9} which makes it a promising material to be used in nanoelectronic devices for thermal transport and heat management. It has been found that the properties of GE can be tuned via various ways such as chemical functionalization^{10,11} and strain engineering.^{12,13} As one of chemical functionalization methods, hydrogenation can be used to open the bandgap of GE and transform GE from a conductor to a semiconductor or insulator.¹⁴⁻¹⁸ Furthermore, a semi-hydrogenation, i.e., a single-side hydrogenation on GE, induces magnetic moments and results in the change of the magnetic property from antiferromagnetic to ferromagnetic.⁴

Since the adsorption of hydrogen on GE sheets is reversible and can be applied controllably in different patterns,^{18,19} it is possible to construct “hybrid” graphene sheets (HGSs) that contain fully- and/or semi-hydrogenated GE strips. As a result, a pristine GE sheet can be divided into several sub-domains or sub-strips with different thermal,²⁰ electrical, and magnetic properties.^{19,21} This means that the insulating/antiferromagnetic and conducting/ferromagnetic properties can be integrated into a single GE sheet without the physical cutting and joining process. Thus, GE sheets can be tuned via different hydrogenation styles and hydrogen coverages to design or develop a wide range of nanoelectronic devices.

With increased interest in using HGSs in nano-devices, a fundamental understanding of the thermal conductivity behavior of HGSs is critical for better thermal management. It has been found that hydrogenation reduces λ of GE significantly even at a relatively low hydrogen coverage.²² The λ of HGSs depends on the hydrogenation pattern in terms of hydrogen coverage and the type and number of interfaces

between strips.^{20,23} However, the effect of hydrogenation on λ has not been fully understood. In particular, no study has been conducted on λ of semi-hydrogenated GE sheets or HGSs that contain semi-hydrogenated GE strips. On the other hand, external elastic strain applied to GE-based materials has been found to alter their thermal properties by changing their morphologies.^{13,24} Meanwhile, interfacial strain due to partial hydrogenation can affect the morphologies of HGSs.²⁵ It is predicted such interfacial strain would also have an effect on their thermal properties. Therefore, this study aims to understand the effect of the hydrogenation style and hydrogen coverage on the morphology and λ of HGSs via molecular dynamics (MD) simulations.

There are two typical styles of hydrogenation on GE reported till now. One style is to obtain graphane (GA), a fully double-side hydrogenated GE sheet with hydrogen atoms bonded to carbon atoms on both sides alternatively (Fig. 1(b)), where all the sp^2 bonds are transformed into sp^3 ones.^{14,26,27} The other style realizes graphone (GO), a single-side hydrogenated graphene sheet (Fig. 1(c)), by utilizing the reversibility of the hydrogenation process, i.e., removing all the hydrogen atoms at one side of GA, in which half of sp^3 bonds are transformed back into sp^2 bonds.^{4,18} Single- and double-side hydrogenation styles have been realized experimentally.^{14,28} In this study, another hydrogenation style is proposed in which the sp^3 bonds in the GO sheet are rearranged to be on both side (Fig. 1(d)). Since the hydrogenation of GE is reversible²⁹ and controllable,³⁰ this proposed style is possible to be realized experimentally. In the rearranged GO sheet, named RGO sheet thereafter, the hydrogen atoms within one zigzag chain are located on the same side of the sheet, while those within the neighboring chains are on the other side.

The HGS that contains both GE and GA strips is called GA-HGS, and so are GO-HGS and RGO-HGS. Figure 2 illustrates the model configuration of an HGS with the length $L_0 = 20$ nm and width $W_0 = 5$ nm. A GA/GO/RGO strip is embedded in between two GE strips of which the length is along the heat flux direction. The width of the GA/GO/RGO

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FIG. 1. Schematic of various sheets: (a) GE, (b) GA, (c) GO, and (d) RGO.

strip is denoted by W , and the area fraction of the strip to the whole sheet is given by their width ratio $f = W/W_0$. Thus, the hydrogen coverage of the HGSs can be expressed by f .

The classical non-equilibrium MD method is applied to study the thermal properties using the AIREBO potential,³¹ which is embedded in the LAMMPS package.³² The initial configuration is constructed based on structural optimization of an HGS sheet, which will be explained in detail later. The periodic boundary condition is applied along both the width and length directions. At first, the initial configuration is equilibrated at 300 K for 50 ps with the time step $\Delta t = 0.5$ fs. Upon realization of the equilibrium state, a constant heat flux J is then imposed into the system at each time step by adding a small amount of heat $\Delta\zeta$ into the heat source (with a thickness of 2δ) in the middle and meanwhile reducing $\Delta\zeta/2$ from heat sinks (with a thickness of δ) at both ends. After enough simulation time, a stable temperature gradient ∇T is established along the heat flux direction. As a result, the thermal conductivity λ can be obtained based on Fourier's law $J = -\lambda \nabla T$ in which J is given by $J = \Delta\zeta/(2A\Delta t)$ with A denoting the cross-section area, i.e., $\lambda = -\Delta\zeta/(2A\Delta t \nabla T)$. In the area calculation, the HGSs are set to have the same thickness of 0.34 nm, which is the interlayer distance of graphite.

During the modeling, structural optimization is used to get a suitable configuration for thermal conductivity calculation, and realized based on the investigation of the morphologies of HGSs. Their primal configurations are constructed using the lattice parameter of GE and then relaxed at 300 K. The simulation results show that all the HGSs deviate from the primal planar morphology and exhibit prominent flexures (Fig. 3). It is found that large periodic ripples are formed in all the HGSs upon relaxation. For the same width ratio, GA- and RGO-HGSs exhibit small wavelength periodic ripples due to the hydrogen distribution on both sides of the sheet, whereas GO-HGSs exhibit large wave length periodic ripples as well as buckling and kinks due to the hydrogen presence on single side of the sheet. The wave length and magnitude of the ripples strongly depend on the hydrogen coverage.

The deformation in terms of ripples, kinks, and buckling in these HGSs is mainly caused by the lattice mismatch

between GA (GO/RGO) and GE strips. Due to hydrogenation, it is found that the lattice parameter of the GA, GO, and RGO sheets is increased by around 5%, which is in good agreement with previous studies.^{25,33} Hence, the hydrogenation induces interfacial strain between GA (GO/RGO) and GE strips, leading to the warping of the HGSs, a phenomenon similar to the warping of pure GE sheets induced by their compressive edge stress.^{34–36}

Mechanical and physical properties of a GE sheet strongly depend on its structure, particularly its morphology.³⁷ In practical applications, GE sheets are generally used in their flat form, which can be realized by subjecting them to external in-plane tensile loads. This study considers the thermal properties of HGSs only when they exhibit flat morphology. Therefore, before imposing the heat flux J to the HGSs, structural optimization is conducted to reduce or minimize the ripples or buckling by applying an equal biaxial stretching on their initial configurations which is constructed using the lattice parameter of GE. The critical stretching ratios at which all these HGSs at 300 K begin to exhibit flat morphology are obtained to avoid excessive stretching effect. The study shows that almost all these HGSs with different width fractions f can become flat when the biaxial stretching ratio R increases to around 1.05, a value that matches the lattice parameter increase in the GA (GO/RGO) sheets. Moreover, these HGSs stretched at this ratio are found to remain flat after the heat flux is imposed.

The thermal conductivities λ of GE, GA, GO, and RGO sheets are calculated, as listed in Table I. The results of GE and GA sheets demonstrate consistency with those reported in the literature with minor deviations.²⁰ The minor difference may be caused by the deviations in calculating λ from the number of sample data collected, the number of iterations and the length of simulation time. It has been pointed out

FIG. 2. Schematic of an HGS. The GA/GO/RGO strip (red color) is embedded in between GE strips (grey color).

FIG. 3. Periodic ripples form in GA-, GO-, and RGO-HGSs with different width fractions f upon relaxation. Particularly, kinking and buckling are found in GO-HGSs.

TABLE I. Thermal conductivities λ (W/mK) of pure GE, GA, GO, and RGO sheets.

	Present results	Reported results ²⁰	λ/λ_0
GE	77.3	89.6	1.0
GA	33.2	28.8	0.43
GO	30.7	...	0.40
RGO	19.6	...	0.25

that the application of different heat fluxes would also lead to minor deviation in λ .³⁸ It is also necessary to note that the λ of GE sheets with dimensions of a few microns was experimentally measured to be in the range of 2500–5000 W/mK.^{5,6} The GE sheets in the present model and reported models^{13,20} have dimensions no more than 20 nm and demonstrate about the same value of λ , which, however, is much smaller than 2500–5000 W/mK due to the size effect at the nanoscale.^{9,13,20} The phonon mean free path of GE that affects λ is about 1 μ m, which means that the phonon paths in these modeled GE sheets would be cut off, thus resulting in a much lower λ .

For convenience, λ of a GE sheet is denoted by λ_0 . The λ of the GA sheet is found to be 43% of λ_0 . Such a decrease is caused by the transformation of all the sp^2 bonds in GE sheet to the sp^3 bonds in GA sheet, because the thermal transport ability of the sp^3 bonds is lower than that of the sp^2 bonds.^{20,22} In contrast, the λ of the GO sheet is found to be 40% of λ_0 , which is slightly lower than that of the GA sheet, though only one half of the sp^2 bonds in GE sheet are transformed into the sp^3 bonds in the GO sheet and these bonds are isolated by each other. In the RGO sheet, the numbers of sp^2 and sp^3 bonds equal to those of the GO sheet. However, the λ of the RGO sheet is 40% smaller than that of the GO sheet (refer to Table I).

Previous studies have demonstrated that the thermal conductivity λ of nanostructures can also be affected by their internal strain.^{12,13,24} In this study, the λ of GA-, GO-, and RGO-HGSs would also be affected by their internal strain due to the biaxial stretching applied to make them in the flat form. Nevertheless, since all the HGSs are under the same stretching ratio, the effect of the internal strain on λ is not quantitatively analyzed here. This study focuses on the effect of the hydrogenation style and hydrogen coverage on λ .

Fig. 4 illustrates the effect of the hydrogen coverage f on λ of flat HGSs. The values of the λ in this figure are normalized with respect to λ_0 . The ratio λ/λ_0 of these sheets for

FIG. 4. Dependence of λ of GA-HGSs, GO-HGSs and RGO-HGSs on f .

$f=0$ is around 0.7 rather than 1, which is due to the 5% biaxial stretching applied. In the presence of hydrogenated strip in GE sheets, the λ further drops significantly in all these HGSs. There is a sharp decrease in the λ when $f < 0.2$, and there onwards slight reduction observed for $0.2 < f < 0.8$. However, a slight increasing trend is observed when $0.8 < f$. The dramatic reduction can be attributed to the introduction of sp^3 bonds into the sheets with pure sp^2 bonds, which induces interfacial phonon scattering between the GE and the GA/GO/RGO strips, while the increasing trend is due to the disappearance of these interfaces as well as approaching to uniform distribution of sp^3 (in GA-HGSs) or combination of sp^2 and sp^3 bonds (in GO-/RGO-HGSs) as f approaches 1.0. Moreover, RGO-HGSs always have the lowest value of λ among the three HGSs for any given f . A similar sharp decay in λ has been reported for randomly hydrogenated GE.²⁰ This sharp decay can be explained by the fact that the structural effect around each hydrogenated site reduces λ and when the hydrogenation coverage reaches up to 10%, the entire structure would be disturbed, resulting in a drastic reduction in λ and leaving less room for further reeducation in λ . For GA-HGSs, a gradual decay in λ , a trend slightly different from the result here, was reported.²⁰ The difference is because the present study considers the interfacial strain effect. This highlights the importance of considering the interfacial strain effect as well as the interfacial phonon scattering effect for patterned configurations with interfaces. Because of these two types of interface effects, the rule of mixture cannot be used for calculating λ of HGSs. In general, the interface effect will make the rule of mixture not applicable for calculating the physical properties of the combination of different structures.

To elucidate the underlying mechanism of the above phenomenon, a detailed analysis of the phonon spectra is conducted by using the Fix-Phonon code.^{39,40} The total spectra of GE, GO, RGO, and GA sheets are presented in Fig. 5(a). It shows that hydrogenation in GO, RGO, and GA sheets remarkably softens the G-band of the phonon spectra, which means the softening of the system and the reduction of the Debye temperature, thereby decreasing λ .

In addition to the G-band softening, the enhanced coupling effect between the in-plane and out-of-plane phonon modes of the hydrogenated GE sheets provides another explanation to their dramatic reduction in λ . In Fig. 5(b), the overlap of the in-plane and out-of-plane components of the power spectra, denoted by $S_{\text{in-out}}$, is calculated as^{22,41} $S = \int P_1(\omega)P_2(\omega)d\omega / (\int P_1(\omega)d\omega \int P_2(\omega)d\omega)$, where $P_1(\omega)$ and $P_2(\omega)$ are the powers of the in-plane and out-of-plane phonon spectra, respectively. It is found that after hydrogenation, $S_{\text{in-out}}$ increases significantly from 0.1 to 0.5, which indicates that the two phonon modes are strongly coupled. Hence, the phonon scattering effect between them is greatly enhanced and reduces the thermal conductivity.⁴² Further study shows that the $S_{\text{in-out}}$ is closely related to the out-of-plane displacement of the carbon atoms. For the GE, GO, RGO, and GA sheets, the averaged out-of-plane displacements of carbon atoms are found to be 0.09, 0.22, 0.31, and 0.80 Å, respectively, corresponding to their $S_{\text{in-out}}$ values of 0.11, 0.43, 0.44, and 0.49, which means the larger the out-of-plane displacement, the larger the $S_{\text{in-out}}$ would be.

FIG. 5. (a) Total phonon spectra of pure GE, GO, RGO, and GA sheets, and (b) their in-plane (dash line) and out-of-plane (solid line) spectrum components, with $S_{\text{in-out}}$ denoting the overlap.

To explain why the thermal conductivity of RGO sheets is much lower than that of GO and GA sheets, the phonon spectra of the hydrogenated (sp^3 bonds) and unhydrogenated (sp^2 bonds) carbon atoms are calculated for both the GO and the RGO sheets (Fig. 6) and the overlap between these spectra, denoted by $S_{\text{CC-CH}}$, is also calculated, but with $P_1(\omega)$ and $P_2(\omega)$ denoting the powers of phonon spectra of the unhydrogenated and hydrogenated carbon atoms, respectively. The fact that RGO sheets have much smaller $S_{\text{CC-CH}}$ value than GO sheets indicates the scattering effect between the phonon modes of sp^3 and sp^2 bonds are more intensive in the RGO sheets, which further lowered their thermal conductivity, as compared to that of the GO and GA sheets. Moreover, same phenomenon is found by analyzing the phonon spectra of GO and RGO strips inside the GO- and RGO-HGSs. Since the phonon spectra of GE strips in different HGSs are found to be almost the same, it is reasonable to attribute the lower thermal conductivity of RGO-HGSs to the more intensive phonon scattering effect between the sp^2 and sp^3 bonds in the RGO strip. The phonon spectra analysis reveals that the combined effect of the G-band softening, $S_{\text{in-out}}$ and $S_{\text{CC-CH}}$ reduces the thermal conductivity of GE significantly in the presence of hydrogenation.

FIG. 6. The phonon spectra of the carbon atoms with sp^2 (black solid line) and sp^3 bonds (red dot line) in GO and RGO sheets, with $S_{\text{CC-CH}}$ denoting the overlap.

In conclusion, MD simulations are conducted to study the thermal conductivity of GA-HGSs, GO-HGSs, and RGO-HGSs. The effect of hydrogenation styles and hydrogen coverage f on their morphology and thermal conductivity is investigated. It shows that hydrogenation can induce periodic ripples in these HGSs and even buckling in GO-HGSs. Simulation results reveal that the λ of the HGSs with flat morphology is 30% to 75% less than that of the pure GE sheets and such decrease depends on f . Moreover, among these HGSs, RGO-HGSs always have the lowest λ . Such phenomena are explained by conducting the phonon spectra analysis. It is found that the coupling effect of the in-plane and out-of-plane phonon modes in GE sheets is significantly enhanced by hydrogenation. The intensive phonon scattering effect between hydrogenated and unhydrogenated carbon atoms inside the RGO-HGSs is responsible for their low λ as compared to those of the GO-HGSs.

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