Institute for Research in Fundamental Sciences

مقاله نامه ی بیست و ششمین کنفرانس بهاره فیزیک- ۲۲-۲۳ خرداد ماه ۱۳۹۸

شماره(۳۴)

Effect of torsional deformation on the thermal conductivity of 2D nanomaterials: A molecular dynamics study

Saeed Arabha[1], Ali Rajabpour[1,2]

[1] *Advanced Simulation and Computing Laboratory (ASCL), Imam Khomeini International University, Qazvin, Iran*

[2]*School of Nano-Science, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran*.

Abstract

The thermal conductivity of nanoscale materials is largely dependent on the applied strain and deformations. In this paper, the effect of torsional deformation and consequent wrinkles on the thermal conductivity of graphene, hexagonal boron nitride (h-BN) and molybdenum disulfide (MoS2) nanostructures have been investigated by performing non-equilibrium molecular dynamics simulation. It is found that the wrinkles caused by applying the torsion result in reducing the thermal conductivity of nanostructures. Although the effect of created distortions is tangible, these wrinkles have the most influence on the thermal conductivity of MoS2 and the least on the thermal conductivity of h-BN. The results of this study can be beneficial for estimating the values of applied torsion and wrinkle amplitude by measuring the thermal conductivity variations.

Due to the low thickness and slight bending strength of two-dimensional structures, some wrinkles are formed in these materials [1]. Although the most significant factor in forming wrinkles is inherent properties but heating and cooling operations, mechanical strains, and boundary conditions are among the factors that affect the accumulation and amplitude of these wrinkles. It has been shown that multiplicity of chemical carbon-carbon bonds leads to unintentional ripples in graphene plate that appear due to thermal fluctuations [2]. In addition to thermal fluctuations, interatomic forces between the nanostructures and substrate can also contribute to generation and amplification of ripples [3]. In recent years, some studies have been evolved on the created pattern as a result of the growth of a thin elastic layer in macro scale [4].

Previous studies have shown that the formation of wrinkles in graphene increases the phonon dispersion and consequently decreases the thermal conductivity of graphene [5]. According to studies on the thermal properties of graphene, the behavior prediction of other two dimensional nanostructures such as MoS2 and h-BN in the presence of wrinkles is also a challenging subject.

In this paper, we use non-equilibrium molecular dynamics (MD) simulations to study the effect of torsional deformation and its resulting wrinkles on the thermal conductivities of graphene, h-BN, and MoS2 nanostructures. The thermal conductivities are calculated at different torsional angles up to the failure points for each structure. The relation between the thermal conductivity reduction and the wrinkle amplitude is also discussed.

Schematic view of the atomistic model is shown in figure 1a. After applying the temperature boundary conditions, the internal boundary is rotated to reach the desired torsional deformation level. To calculate the temperature gradient, the simulation box is apportioned into 20 slabs along the radial direction and the temperature at each part is determined separately. As it is shown in figure 1b, a logarithmic temperature distribution appeared in the middle of the specimen (figure 1b). In this method, the heat flux q can be calculated from the energy exchange between cold and hot boundaries. The effective thermal conductivity coefficient is then calculated by Fourier's law.

$$\kappa = -q'' \left(\frac{\partial T}{\partial r}\right)^{-1} \quad (1)$$

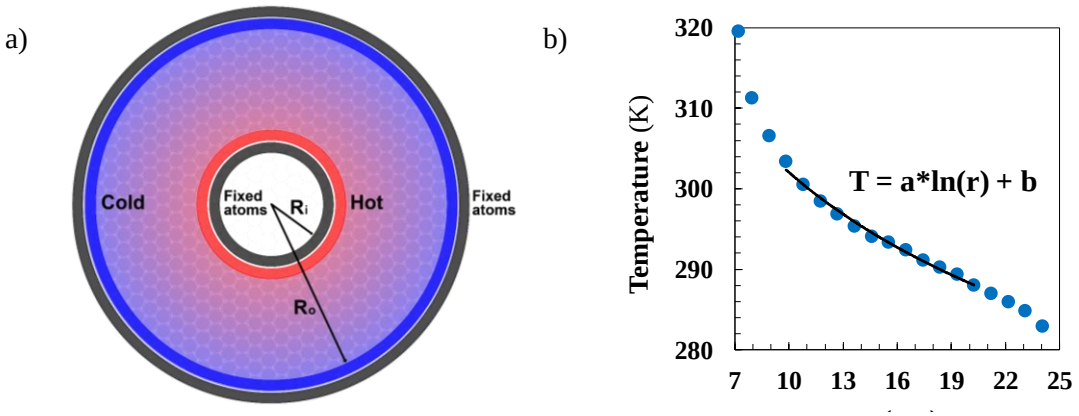

Figure 1: (a) MD simulation setup for thermal conductivity prediction of graphene, MoS2, and h-BN under torsional deformation (θ). (b) Temperature gradient obtained from NEMD simulation to calculate $\frac{\partial T}{\partial r}$.

In this study, we investigate the thermal conductivity of three types of 2D nanostructures under twisting at the internal boundary. We first define shear strain (γ) parameter with respect to the torsional deformation (θ) as follows:

$$\gamma = \left(R_i / (R_o - R_i)\right) * \theta \qquad (2)$$

Figure 2 shows that by increasing the strain (torsional deformation), the thermal conductivity of all 2D nanostructures decreases. By applying torsional strain, elongation and compression happen within the atomic bonds of two-dimensional nanostructures. This change in the bond's length causes minor variations in the vibrational patterns and thus reduces thermal conductivity [6]. Moreover, the wrinkles increase the phonon scattering rates in a deformed 2D nanostructure that leads to a decrease in the thermal conductivity [7].

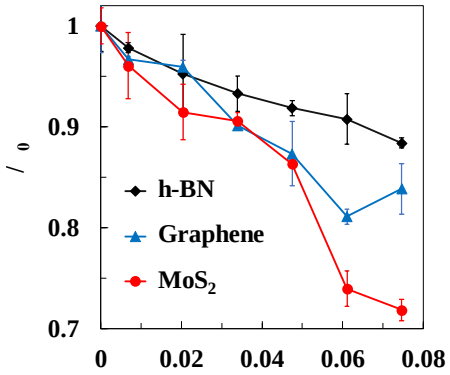

Figure 2: Normalized in-plane thermal conductivities of graphene, h-BN and MoS2 under torsional deformations with respect to the applied strain (γ).

To investigate the relation between the wrinkle's amplitudes and the reduction of the thermal conductivity of a 2D material, we present the thermal conductivity in terms of wrinkle amplitude of graphene nanostructure under different values of the torsional deformation (from θ=0° to the failure point) in figure 3. It is found that as the wrinkle amplitude increases, the thermal conductivity will be further reduced. Figure 3b shows that the thermal conductivity reduction is linearly proportional to square of the wrinkle amplitude.

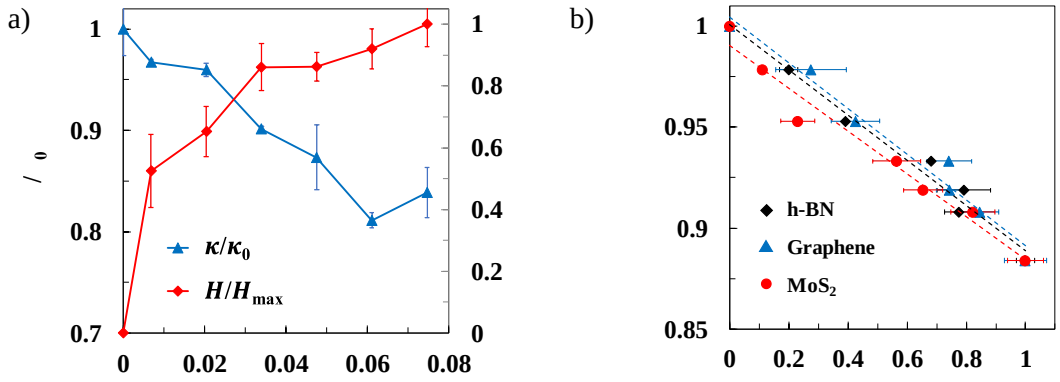

Figure 3: (a) Normalized in-plane thermal conductivity (κ) and the wrinkle amplitude (H) of graphene under torsional deformations with respect to the applied strain level (γ). (b) The thermal conductivity reduction versus of the square wrinkle amplitude $(H/H_{max})^2$.

Summary

In summary, utilizing non-equilibrium molecular dynamics method, it has been shown that wrinkles play an important role in the thermal conductivity of 2D nanostructures. The thermal conductivity of three types of 2D nanostructures (graphene, h-BN and MoS2) were examined under torsional deformation. It was found that applying the torsional deformation up to the failure point results in a reduction of 20 to 30 percent in the thermal conductivity of these nanostructures. The reduction was the highest for MoS2 nanostructure and the lowest for h-BN nanostructure. It was also revealed that the amplitude of wrinkles has a direct effect on the thermal conductivity of a 2D nanostructure, so that as the wrinkles amplitude (H) increases, the thermal conductivity (k) will be further reduced ($k \sim H^2$). These results have important implications for understanding heat transfer mechanisms in 2D materials and also for engineering of thermal transport in electronic devices.

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