Journal Name

ARTICLE TYPE

Cite this: DOI: 00.0000/xxxxxxxxxx

Exploration of mechanical, thermal conduction and electromechanical properties of graphene nanoribbon springs

Brahmanandam Javvaji,[a] Bohayra Mortazavi,[a] Timon Rabczuk[b,c] and Xiaoying Zhuang*[a,d,e]

Received Date
Accepted Date

DOI: 00.0000/xxxxxxxxxx

1 Comparison with AIREBO potential

The closeness between the semi-circular segments of GNRH when $h_\theta > 30^\circ$ lead to high deflections due to the strong repulsions. However, there exist weak van der Walls interactions between these segments, which are not counted through the Tersoff potential. In order to check the effect of weak interactions on the mechanical and thermal properties of GNRH, we repeat the simulations for $2.5-1.6-45^\circ$ GNRH system with adaptive intermolecular reactive empirical bond order (AIREBO) potential[1]. Tensile response from both the potentials is nearly same upto a strain of 1.5 (Fig. 1(a)). Thereafter, an early rise in stress and early failure is observed with the AIREBO potential. Finally, we observe an underestimation for the failure strain and tensile strength. This may be due to the reactive nature of the potential avoids the re-bonding between carbon atoms and resulting the failure. Earlier reports[2] further suggest that AIREBO potential underestimates the mechanical properties of carbon nanostrucures.

Fig. 1(b) shows the convergence of thermal conductivity for $2.5-1.6-45^\circ$ GNRH with Tersoff and AIREBO potentials. The AIREBO potential underestimated the thermal conductivity due to incorrectness in estimating high frequency phonon modes[3]. Therefore, the predictions from Tersoff potential for the present spring systems are more reliable.

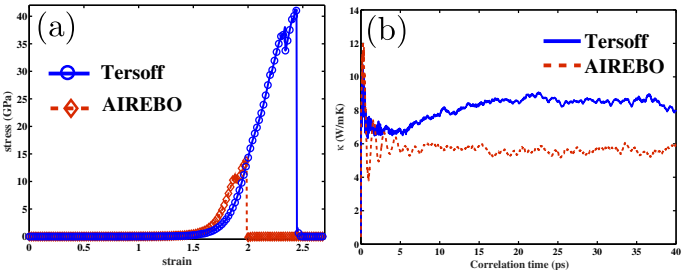

Fig. 1 (a) Stress-strain and (b) thermal conduction response with Tersoff and AIREBO interatomic potentials for $2.5-1.6-45^\circ$ GNRH.

2 Comparison with armchair configuration

In order to check the dependence of chirality on the properties of spring systems, we perform simulations with zigzag configuration for $9-1.6-2.5$ GNRS.

Fig. 2(a) shows the initial atomic arrangement for zigzag GNRS and armchair GNRS. The tensile response in Fig. 2(b) of zigzag and armchair configurations is identical upto the first drop in stress. The tensile strength of armchair configuration is slightly higher than the zigzag configuration. This difference is due to the different initiation of bond failure. Noticeable increase in the thermal conductivity of armchair GNRS over zigzag GNRS in Fig. 2(c) corresponds to the changes in edge localized phonon modes. Such changes help in transporting the thermal energy more in armchair configuration and increased the thermal conductivity[4].

The results of bending induced polarization for armchair GNRS in Fig. 2(d) is closely match with the zigzag GNRS response. The bending deformation induce a out-of-plane polarization by the changes in pyramidalization angle, which is almost equal for both zigzag and armchair GNRS.

This comparative study confirms that the predicted results vary slightly with the chirality or edge state of the GNR spring system.

[a] *Institute of Continuum Mechanics, Leibniz Universität Hannover, Applestr. 11, 30167 Hannover, Germany.*
[b] *Institute of Structural Mechanics, Bauhaus University Weimar, Marienstrasse 15, 99423 Weimar, Germany.*
[c] *College of Civil Engineering, Department of Geotechnical Engineering, Tongji University, Shanghai, China.*
[d] *Division of Computational Mechanics, Ton Duc Thang University, Ho Chi Minh City, Vietnam.*
[e] *Faculty of Civil Engineering, Ton Duc Thang University, Ho Chi Minh City, Vietnam, Email: xiaoying.zhuang@tdtu.edu.vn*

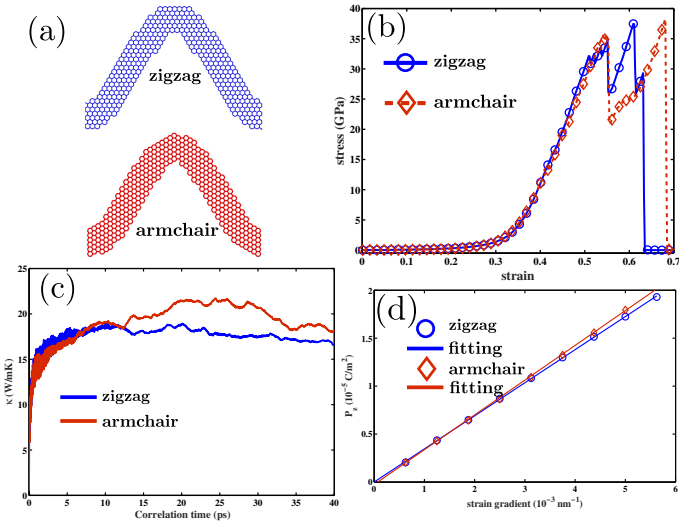

Fig. 2 (a) Schematic of zigzag and armchair unitcell of GNRS. (b) Stress-strain and (c) thermal conduction response and (d) bending induced polarization response for $9-1.6-2.5$ GNRS.

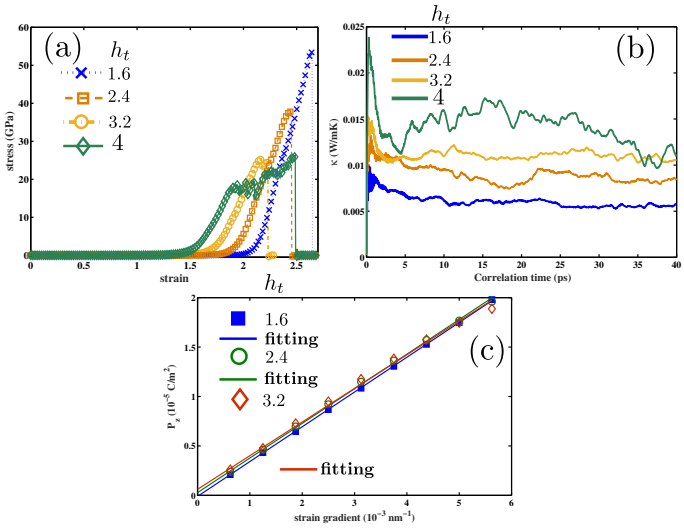

Fig. 3 (a) Stress-strain, (b) thermal conduction and (c) bending induced polarization response at different GNRH width h_t when h_θ is 45°. h_r is 5 nm for (a) and (b) and 2.5 nm for (c).

3 Effect of width

Notes and references

1 S. J. Stuart, A. B. Tutein and J. A. Harrison, *The Journal of Chemical Physics*, 2000, **112**, 6472–6486.

2 I. V. Lebedeva, A. S. Minkin, A. M. Popov and A. A. Knizhnik, *Physica E: Low-dimensional Systems and Nanostructures*, 2019, **108**, 326–338.

3 C. Si, X.-D. Wang, Z. Fan, Z.-H. Feng and B.-Y. Cao, *International Journal of Heat and Mass Transfer*, 2017, **107**, 450–460.

4 Y. Chu, T. Ragab and C. Basaran, *Computational Materials Science*, 2014, **81**, 269–274.