ICCES, 2023, vol.27, no.1
DOI: 10.32604/icces.2023.09484

Tech Science Press

PROCEEDINGS

Uniaxial Compressive Mechanical Properties of Three-Dimensional Graphene: Theoretical Models and Molecular Dynamics Simulations

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ABSTRACT

As the first two-dimensional (2D) material discovered in experiments, graphene has attracted increasing attention from the scientific community [1]. And it possesses many superb mechanical, electronic and optical properties [2-4] due to its unique atomic structure. Its Young's modulus and failure strength are 1TPa and 130GPa [5], respectively. Thus, 2D graphene has been extensively used in nanosensors and nanocomposites [6-8], etc. In order to fabricate graphene-based devices which inherit outstanding properties of 2D graphene, materials scientists are trying to use 2D graphene as building blocks to construct three-dimensional (3D) carbon nanomaterials, such as 3D graphene networks [9-11]. Nowadays, these 3D carbon nanomaterials have become potential candidates which can be integrated into molecular sieves, supercapacitors and energy absorbing devices [12-14], etc. Therefore, it is important to investigate compressive mechanical properties and deformation mechanisms of 3D carbon nanomaterials.

Combining molecular dynamics (MD) simulations and continuum modeling, the uniaxial in-plane compressive properties and deformation mechanisms of honeycomb three-dimensional graphene, triangle-like 3D graphene and non-equilateral hexagon 3D graphene are investigated to elucidate configuration-property relationships, and the constitutive relations of three kinds of 3D graphene are derived to evaluate the compressive mechanical properties. Based on theoretical and MD simulation results, it is found that the compressive stress-strain responses of three types of 3D graphene can be divided into five stages. They are the linear elastic stage I, the stress plateau stage II, the van der Waals (vdW) hardening stage III, the initial crushing stage IV and the densification stage V, respectively. The compressive mechanical properties and deformation mechanisms of each stage are different.

In the linear elastic stage I, the stress increases linearly with increasing strain. Graphene sidewalls of 3D graphene undergo compressive deformation, bending deformation and rotation. In the stress plateau stage II, the plateau stress of 3D graphene is almost a constant with increasing the compressive strain. Graphene sidewalls undergo buckling deformation and rotation. In the vdW hardening stage III, the compressive stress gradually increases with the increase of strain. The distance between graphene sidewalls gradually decreases with the increase of compressive strain. And vdW repulsive interaction strength between two sidewalls gradually increases. In the initial crushing stage IV, as increasing the compressive strain, the stress increases exponentially. And the crushing region of graphene sidewalls gradually extends to the whole 3D graphene structure. In the densification stage V, the stress increases sharply with the increase of compressive strain. And 3D graphene is completely compacted.

Through analyzing energy absorption mechanisms and compression-unloading stress-strain curves for three types of 3D graphene, it is found that there are extraordinary compression-recovery properties and energy absorption capacities in 3D graphene. Besides, the Young's modulus, plateau stress and locking strain of 3D graphene gradually decrease with increasing graphene sidewall width.

KEYWORDS

Three-dimensional graphene; MD simulations; constitutive model; compression-recovery property

Funding Statement: This work was financially supported by the National Natural Science Foundation of China (Grant no. 11872268, 12172250). Grant Recipient: J. Guo. Sponsors' websites: https://www.nsfc.gov.cn/.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

References:

1. Novoselov, K. S., Geim, A. K., Morozov, S. V., Jiang, D., Zhang, Y. et al. (2004). Electric field effect in atomically thin carbon films. *Science, 306(5696),* 666-669.
2. Scaravonati, S., Sidoli, M., Magnani, G., Morenghi, A., Canova, M. et al. (2022). Combined capacitive and electrochemical charge storage mechanism in high-performance graphene-based lithium-ion batteries. *Materials Today Energy, 24,* 100928.
3. Dai, Z. B., Li, Z., He, Y. (2021). Local optical conductivity of bilayer graphene with kink potential. *Physical Review B, 103(12),* 125149.
4. Liu, X., Bie, Z., Wang, J., Sun, L., Tian, M. et al. (2019). Investigation on fracture of pre-cracked single-layer graphene sheets. *Computational Materials Science, 159,* 365-375.
5. Lee, C., Wei, X., Kysar, J. W., Hone, J. (2008). Measurement of the elastic properties and intrinsic strength of monolayer graphene. *Science, 321(5887),* 385-388.
6. Nag, A., Simorangkir, R. B. V. B., Gawade, D. R., Nuthalapati, S., Buckley, J. L. et al. (2022). Graphene-based wearable temperature sensors: A review. *Materials & Design, 221,* 110971.
7. Zhang, M., Fu, T., Fang, Z., Weng, S., Peng, X. (2022). Feature size coupling effect of nanolaminated graphene/copper composites. *International Journal of Mechanical Sciences, 227,* 107469.
8. Gangele, A., Pandey, A. K. (2018). Elastic and fracture characteristics of graphene-silicon nanosheet composites using nonlinear finite element method. *International Journal of Mechanical Sciences, 142-143,* 491-501.
9. Zhou, W., Xie, H., Wang, S., Wang, Q., Jena, P. (2020). A 3D porous honeycomb carbon as Na-ion battery anode material with high capacity, excellent rate performance, and robust stability. *Carbon, 168,* 163-168.
10. Wang, Y. C., Zhu, Y. B., Wu, H. A. (2021). Porous characteristics of three-dimensional disordered graphene networks. *Crystals, 11(2),* 127.
11. Guo, R., Zheng, Q., Wang, L., Fan, Y., Jiang, W. (2022). Porous N-doped Ni@ SiO2/graphene network: three-dimensional hierarchical architecture for strong and broad electromagnetic wave absorption. *Journal of Materials Science & Technology, 106,* 108-117.
12. Zhang, L., Zhang, F., Yang, X., Long, G., Wu, Y. et al. (2013). Porous 3D graphene-based bulk materials with exceptional high surface area and excellent conductivity for supercapacitors. *Scientific Reports, 3(1),* 1-9.
13. Wang, C., Pan, D., Chen, S. (2018). Energy dissipative mechanism of graphene foam materials. *Carbon, 132,* 641-650.
14. Gao, Y., Chen, Y., Zhong, C., Zhang, Z., Xie, Y. et al. (2016). Electron and phonon properties and gas storage in carbon honeycombs. *Nanoscale, 8(26),* 12863-12868.