

Geometric Optimization and Mechanical Analysis of Multilayer Graphene Platelet Films: A Finite Element Approach

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Abstract

Monolayer graphene has been recognised for its superior strength and stiffness [1]. However, the scalability of producing flawless monolayer graphene films faces inherent challenges, primarily attributable to the manifestation of various imperfections, such as additional layers, wrinkles, or folds [2]. These imperfections significantly compromise the performance of monolayer graphene across diverse applications [3–4]. In contrast, the fabrication of large-size multilayer graphene platelet films (MGPFs) with commendable mechanical properties is comparatively more attainable and holds considerable promise for widespread applications in modern industries [5-7]. It is imperative to systematically investigate the dependences of the mechanical properties of multilayer graphene platelet films (MGPFs) on their geometric structures and to optimize the structural and geometric design of multilayer graphene platelet films. This optimization seeks to achieve a judicious combination of mechanical properties, thereby enhancing the functional efficacy of MGPFs in practical applications. To address these objectives, this paper employs finite element methods to construct a 3D macroscopic multilayer graphene RVE model with each layer being a 2D periodic random Voronoi graphene platelet structure [8]. The ensuing investigation aims to explore the influences of geometrical features [9], encompassing graphene platelet size, regularity degree, and area fraction, on the elastic modulus of MGPFs. The findings indicate a significant positive correlation between the elastic modulus of MGPFs and the size and area fraction of its graphene microplates, within a scale suitable for the study. This observation proves that the characteristic parameters of graphene platelets play a crucial role in influencing the macroscopic mechanical properties of the materials.

Key words: *Multilayer graphene platelet; Finite element; Elastic properties;*

References

- [1] Lee. C. et al., (2008). Measurement of the elastic properties and intrinsic strength of monolayer graphene, *Science*, 321, 385–388.
- [2] Wang. M. et al., (2021). Synthesis of large-area single-crystal graphene, *Trends Chem.*, 3, 15–33.
- [3] Wang. B. et al., (2018). Camphor-enabled transfer and mechanical testing of centimeter-scale ultrathin films. *Adv. Mater.*, 30, 1800888.
- [4] Zhu. W. et al., (2012). Structure and electronic transport in graphene wrinkles. *Nano Lett.*, 12, 3431–3436.
- [5] Peng. J. et al., (2017). High-performance nanocomposites inspired by nature, *Adv. Mater.*, V29, 1702959.
- [6] Wang. J. et al., (2012). Layered nanocomposites inspired by the structure and mechanical properties of nacre. *Chem. Soc. Rev.*, V41, 1111-1129.
- [7] Cheng. Q. et al., (2014). Bioinspired layered materials with superior mechanical performance, *Acc. Chem. Res.*, V47, 1256-1266.

- [8] Zhu. H.X. et al., (2001). Effects of cell irregularity on the elastic properties of 2D Voronoi honeycombs, *J. Mech. Phys. Solids*, V49, 857-870.
- [9] Zhu. H.X. et al., (2002). The geometrical properties of irregular two-dimensional Voronoi tessellations, *Philos. Mag.* A81, 2765- 2783.