Modelling the mechanical properties of multilayer graphene platelet films

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Abstract

Although perfect monolayer graphene sheet has been well known to have superior mechanical properties [1], it is very difficult to fabricate large-sized perfect graphene sheets due to unavoidable imperfections, e.g. additional layers, wrinkles, or folds [2]. In engineering applications, multilayer graphene platelet films (MGPFs) are more widely used because the fabrication of MGPFs is comparatively more attainable, and moreover, MGPFs could have mechanical properties comparable to those of large-sized perfect multilayer graphene films [3-5]. The elastic properties [6, 7] and the bending performance [8] of MGPFs have been found to significantly depend on their geometrical parameters, however, the in-depth understanding about how the different geometrical parameters affect the elastic properties and the bending performance remains to be very poor. Thus, to achieve optimal design of MGPFs still remains challenging.

In this work, we aim to quantify the effects of the different geometrical parameters on all the five independent elastic constants and the bending performance of MGPFs, to find out the dominant deformation mechanisms, and to optimise the design and maximise the mechanical properties/performance of MGPFs. Realistic 3D periodic multilayer random irregular representative volume element (RVE) models for MGPFs are constructed, with each layer being a 2D periodic random Voronoi polygon structure [9,10] and each polygon representing a graphene platelet. The individual graphene platelets in a MGPF are held together by van der Waals interaction forces between the staggered graphene platelets. We use the commercial finite element software ABAQUS to simulate the mechanical properties and the bending performance of MGPFs. The graphene platelets are represented by S4R shell elements and the van der Waals interactions between any two staggered graphene platelets are modelled by a single layer of solid elements with the equivalent isotropic elastic properties. We have developed thousands of random RVE models to investigate the effects of the different geometrical parameters on the five independent elastic properties and the bending stiffness of MGPFs, and the normalised/dimensionless results of five independent properties and bending

stiffness of MGPFs are obtained and compared with those of the relevant experimental measurements and computational simulation results in literature. In addition, we have studied the effects of defects (e.g. missing graphene platelets) on these properties. The results obtained in this work can not only help to maximise the mechanical properties and performance of MGPFs, but also apply to other materials such as nacre and seashells.

Key words: *Multilayer graphene platelet films; Elastic properties; Bending stiffness, Deformation mechanisms, Finite element simulation.*

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