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ADVANCED MANUFACTURING

The Research on Mechanical Properties and Compressive Behavior of Graphene Foam with Multi-scale Model

Computational simulation is an effective method to study the deformation mechanism and mechanical behaviour of graphene-based porous materials. However, due to limitations in computational methods and costs, existing research model deviate significantly from the real material in terms of the scale of structure. Therefore, building a highly accurate computational model and maintaining an appropriate cost is both necessary and challenging. This paper proposed a multi-scale modelling approach for finite element (FE) analysis based on the concept of structural hierarchy. The stochastic feature of the microstructure of porous materials are also considered. The simulation results of the regular structure model and the Voronoi tessellation model are compared to investigate the effect of regularity on the material properties. Despite some shortcomings, other microstructural features of porous graphene materials can be gradually introduced to improve the material model step by step. Thus the developed multiscale model has great potential to simulate the properties of materials with mesoscopic size structure such as graphene foam (GF).

Keywords:
Computational simulation, graphene-based, porous materials, fulti-scale, finite element.

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INTRODUCTION

Graphene foam (GF) is a promising multifunctional material for military, energy, and aerospace industry. The materials have excellent mechanical, thermal, and electrical properties due to the combination of the two-dimensional characteristics of graphene with the three-dimensional (3D) structural features of porous materials. However, the conflicting demands of different properties on structural parameters, such as varying requirements of mechanical and electrical properties for material density, result in multifunctional applications of GF remaining a challenge. In the past few years, several molecular dynamics (MD) models have been developed to investigate the relationship between the meso-structural characteristics of graphene porous materials and their mechanical properties.

Qin et al. [1] constructed an all-atom molecular dynamics (AAMD) GF model by mimicking the process of GF synthesis by CVD. Based on the model, they calculated the basic mechanical properties of GF, such as young's modulus, buckling modulus, tensile strength, and compressive strength, under different density. To explore relationship between the density and tensile response of GF, Patil et al. [2] investigated the deformation behaviour of GF under uniaxial tension by using a MD model. They proposed a power law dependence on the density for the tensile strength of this material. To expand the simulation domain of the MD method, the coarse-grained molecular dynamics (CGMD) method has also been developed by some scientists. Wang et al. [3] developed a CGMD model based on the CG model of graphene in the work of Cranford and Buehler [4]. Using their MD model, Wang's team studied the elastic deformation behaviour of GF by observing the evolution of microstructure of the material under uniaxial compression. In another two works, they also discussed the energy dissipative mechanism [5]and the characteristics of high elasticity of GF[6]. Their works are useful for understanding GF elasticity behaviour.

Similarly, Pan et al. [7] used the CGMD model to analyse the compression and recovery behaviour of GF with hole wall under large strain. The mesoscopic evolution of structure and the deformation trends of the graphene walls in GF were also studied. They revealed that the multilevel residual deformation is distributed to the mechanical interlocking behaviour among the hole-flakes. It should be noted, however, that due to the modelling mechanism and approach of MD models, even the CGMD models differ in scale from the real GF material by two to four orders of magnitude. Hence, the simulation results do not match the real material properties, which makes it difficult to provide effective guidance for the study of macroscopic materials properties.

The mechanical properties of graphene foams (GF) are intricately linked to both the microstructure and the macrostructural design of the material. On a microscopic scale, GF exhibits a multitude of irregular unit cells, and the non-uniformity in their structure significantly impacts the material's properties. However, it's worth noting that the individual unit cells tend to have nearly tetrahedral shapes, and the size distribution of these cells remains relatively constrained. Consequently, the morphological disparities and microstructural heterogeneity among GF cells exert only a minimal influence on the material's macroscopic behaviour. Building upon insights and research from prior studies, this paper introduces a cell model that closely mimics the microstructure of GF. This model is constructed and simulated using the finite element method. Furthermore, by applying periodic boundary conditions, the cell model is scaled up to represent a structure with macroscopic dimensions. This approach allows for the modelling and analysis of GF's multi-scale structure. The impact of cell regularity is also investigated using various cell models. Through these models, it becomes possible to effectively predict and calculate the properties of macroscopic-scale materials structured in the manner of graphene foam. This research facilitates a deeper understanding of the mechanical behaviour of GF and contributes to the ability to make accurate predictions and assessments of graphene foam-structured materials on a macroscopic level.

METHODOLOGY

The key aspect of this study is the modelling of the geometrical features (GF), with a particular focus on the cell model. In this paper, the Kelvin cell structure, which is the most used regular cell structure in porous modelling, is introduced to create a fully regular finite element model. The Kelvin cell structure, recognized for its typical Body-Centred Cubic (BCC) configuration, is composed of a four-open decahedron consisting of eight hexagonal and six square faces.

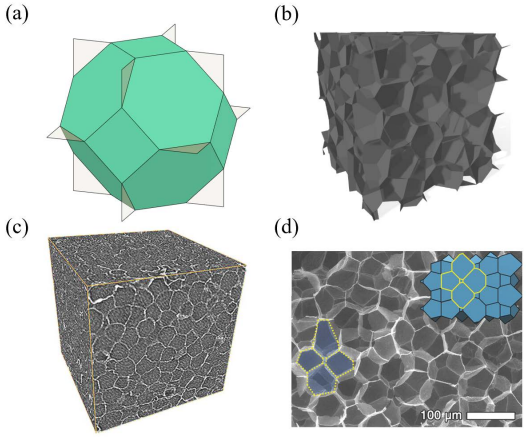

Fig. 1. (a) The schematic of Voronoi foam model and (b) inclusion packaging code; (c) 3D reconstructed X-ray microtomography image; (c)SEM image of GF [8].

Additionally, 12 triangular plates are included in the model to create a cell model with a periodic boundary structure. This structure is widely adopted as a simplified regular structure for foams due to its excellent resemblance to actual foam shapes.

Periodic boundary conditions are imposed on the unitary model according to the methodology given in a previous paper[9]. Here, the relative density is used as a parameter to calculate the elastic properties of the models with different structural dimensions. The relative density ρ can be obtained according to the following equation:

$$\rho = 1.185\frac{t}{L} - 0.4622\left(\frac{t}{L}\right)^2 \quad (1)$$

Where t is the thickness of wall of model, L is the edge length of Kelvin model.

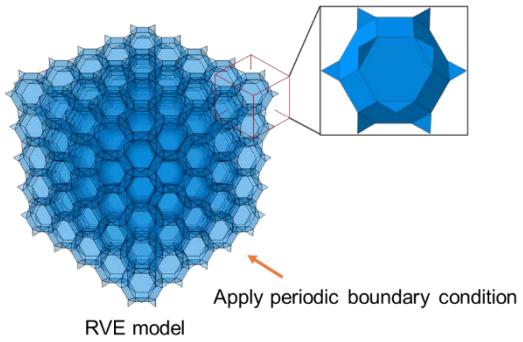

Fig.2. The schematic of GF multiscale model.

Furthermore, the study explores the possibility of constructing an irregular 3D foam structure model based on the Voronoi tessellation algorithm. This algorithm divides the simulation domain around each randomly generated seed into regions closest to the respective seed. The model generated through this algorithm is more in line with the way real foams naturally form and exhibits a desirable level of randomness. To construct the irregular cell model using the Voronoi tessellation algorithm, a minimum allowable distance denoted as δ is introduced to regulate the separation between the points used as seeds for the tessellation process. The value of δ can be employed to control the extent of irregularity in the resulting foam structure. For the creation of a regular lattice containing n identical tetrakaidekahedral cells within the volume V_0 a minimum distance denoted as d_0 between any two adjacent points is determined using equation below [10]:

$$d_0 = \frac{\sqrt{6}}{2}\left(\frac{V_0}{n\sqrt{2}}\right)^{1/3} \tag{2}$$

This minimum distance calculation likely ensures that the tessellation process yields a structured and consistent irregular foam model. To obtain n cells by tessellating a space of volume V_0 with Voronoi tessellation, the maximum δ should be less than d_0; otherwise, it will result in a lack of cells. In this cubic RVE case, to construct a random Voronoi tessellation with n cells in an $L \times L \times L$ cubic RVE space, the maximum δ should be:

$$\delta_{max} = \frac{\sqrt{6}}{2}\frac{L}{2^{1/6}n^{1/3}} \tag{3}$$

When δ is equal to 1, the three-dimensional Voronoi lattice is completely regular and is a cubic lattice with closed-hole Kelvin cells. Here four unitary models with different degrees of regularity (0.2,0.4,0.6,0.8) are constructed to compare with the fully regular model.

Based on these cell models, representative volume element (RVE) models with different microstructures are constructed. Simulation analysis of the macroscopic model of the GF can be achieved by imposing periodic boundary conditions on the RVE model. The focus here is to calculate the elastic properties of the GF multiscale model through six loading cases (three pure shear cases and three uniaxial compression cases), as shown in Fig 3.

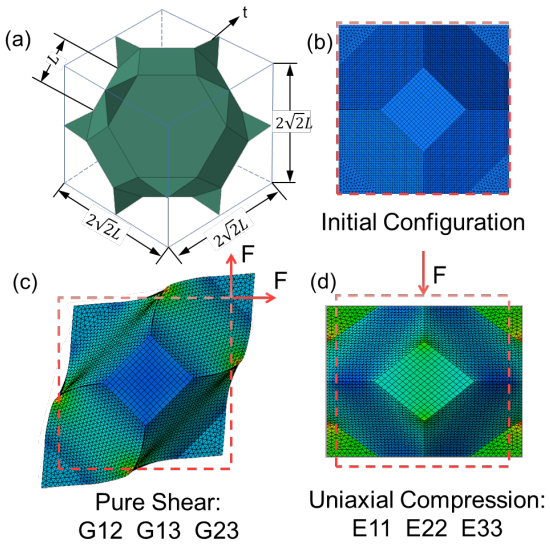

Fig. 3. The schematic of configuration and load case of GF model.

RESULTS AND DISCUSSION

As the BCC cell model is symmetrical about three orthogonal planes, material properties based on this model can be obtained directly from the simulation results of the individual cell model.

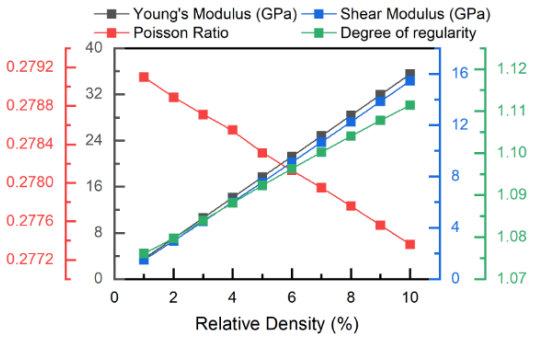

Fig. 4. Elastic properties of GF model with different relative densities.

In ABAQUS, the elastic parameters of the perfect RVE model are calculated under 6 loading conditions (3 uniaxial compression and 3 pure shear conditions). The elastic properties of GA are calculated to be approximately linearly related to the relative density of the material. The fitting polynomial functions of the elastic properties are shown as below :

$$\frac{E_{GA}}{E_g} = 0.3435\left(\frac{\rho_{GA}}{\rho_g}\right) + 0.1803\left(\frac{\rho_{GA}}{\rho_g}\right)^2 \tag{4}$$

$$\frac{G_{GA}}{G_g} = 0.1438\left(\frac{\rho_{GA}}{\rho_g}\right) + 0.1308\left(\frac{\rho_{GA}}{\rho_g}\right)^2 \tag{5}$$

$E_{GA}, \rho_{GA}, G_{GA}(E_g, \rho_g, G_g)$ is elastic modulus, density, and shear modulus of GF (graphene materials), respectively.

For irregular models, models with different degrees of regularity were constructed as shown in the following Fig 5.

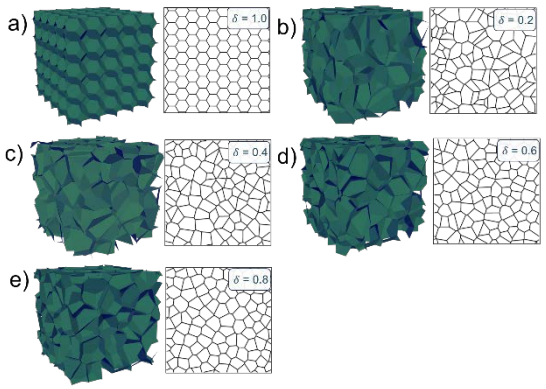

Fig. 5. RVE GF model with different regularity δ. a) δ=1; b) δ=0.2; c) δ=0.4; d) δ=0.6; e) δ=0.8.

The properties of the GF models with respect to the degree of regularity are shown in Fig 6. It can be seen that, the kelvin cell model, on the other hand, has an overall higher performance than the irregular model due to the regular symmetry of the structure. Whereas, influenced by the degree of irregularity, there is some fluctuation in the material properties of the irregular model when evaluating the calculated properties, but the deviation is generally around 5%.

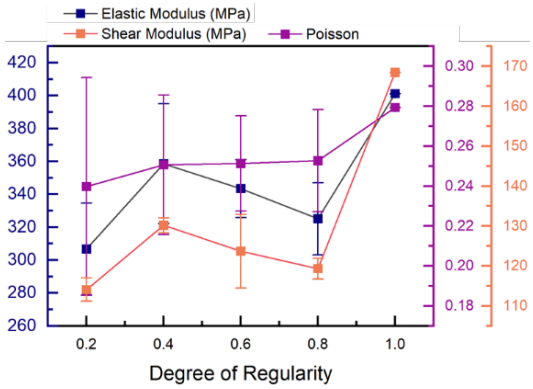

Fig. 6. Comparison of elastic properties of GFs with different regularities.

Here, the degree of anisotropy of different model with various regularity are discussed as shown in Fig 7. The degree of anisotropy (DOA) is obtained by the following formula [11].

$$\mathrm{DOA} = \frac{2 * (S_{11} - S_{12})}{S_{44}} = \frac{2 * (1 + v) * \mathrm{G}}{E} \tag{6}$$

Where S_ij is elastic constants; E is elastic modulus; v is the Poisson ratio; G is the shear modulus.

The degree of anisotropy will be higher than several other irregularity models when a regularity model close to 0.6 is used.

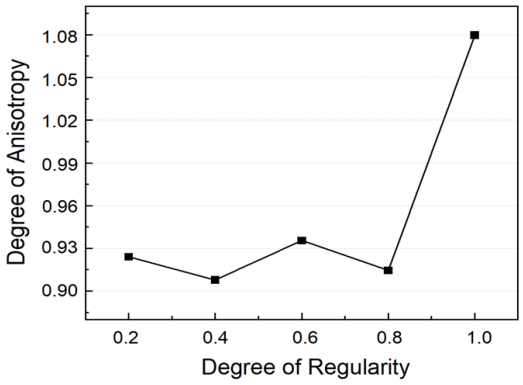

Fig. 7. Degree of anisotropy of GFs with different regularities.

CONCLUSION

This modelling approach allows the deformation of the RVE model to be used to analyse the influence of the microstructure on the material properties, while the periodic boundary method is used to predict the mechanical properties of the calculated macro size material. The construction of a suitable cell model is therefore the key to this approach. There are some differences between the BCC model and the real material structure, but these differences are reduced when the number of RVE cells in the macroscopic model of the material is sufficiently large. When the size of the macroscopic model is large enough, the effect of inhomogeneities in the microstructure of the material on the mechanical properties of the material is greatly diminished. However, this model can overestimate the mechanical properties of the material due to the relatively perfect structure. The anisotropic graphene foam model based on Voronoi lattice is closer to the real microstructure in terms of topology (distribution of faces, edges, and vertices). However, considering the actual computational workload, the prediction accuracy of the model constructed by this algorithm is not significantly better than that of the model constructed by BCC.

Both cell structure modelling methods still have a great potential for development, such as introducing defects and inhomogeneous material distribution present in real materials to bring the RVE model closer to the microstructure of the material. In addition, as the main constituent material of the material wall, the graphene sheet is also affected by the thickness and inhomogeneity of the material, etc., and its elastic property parameters need to be further considered.

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Conflicts of interest
The authors declare no conflict of interest.

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