



Structure-dependent mechanical properties of extended beta-graphyne



Jiaxing Qu^a, Hongwei Zhang^a, Jianxin Li^a, Shexu Zhao^a, Tienchong Chang^{a, b, *}

^a State Key Laboratory of Ocean Engineering, School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiao Tong University, Shanghai, 200240, China

^b Shanghai Institute of Applied Mathematics and Mechanics, Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai University, Shanghai, 200072, China

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ABSTRACT

Owing to their remarkable electronic and thermal properties, graphynes have been considered new promising carbon materials after graphene. However, our understanding of their structure-dependent mechanical properties is far from complete. In this paper an analytical molecular mechanics model is proposed to mathematically establish a relationship between the structure and the elastic properties of β -graphyne. Extensive molecular dynamics simulations are performed for comparison. We show that the elastic properties of β -graphyne exhibit a strong dependence on its structure. The in-plane stiffness, in-plane shear stiffness and layer modulus decrease with increasing percentage of the acetylenic linkages, while the Poisson's ratio increases. Further analysis demonstrates that this dependence of structure attributes to the change in bond density. Based on the concept of effective bond density, scaling laws are developed for the elastic properties of β -graphyne, which demonstrate a useful approach for linking mechanical properties of graphene allotropes to those of graphene.

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1. Introduction

Carbon exhibits versatile flexibility in forming different hybridization states (*i.e.*, sp , sp^2 , sp^3). Apart from some naturally existed ones, such as graphite (sp^2 -hybridize) and diamond (sp^3 -hybridize), many other carbon allotropes are possible to be constructed by altering the periodic binding motifs in the networks consisting of sp^3 -, sp^2 - and sp -hybridized carbon atoms [1–14].

In particular, graphene, a sp^2 -hybridized carbon allotrope, exhibits extraordinary electronic properties [15,16] such as the quantum Hall effect and giant carrier mobility, as well as excellent optical, thermal, and mechanical performance, making graphene an attractive building material for nano devices. This sp^2 -hybridized carbon allotrope inspired the combination of carbon allotropes with more hybridized states. With the introduction of sp constituents, Baughman et al. [17] postulated that graphynes can be alternative carbon planar forms constructed by partial or complete replacement of the aromatic bonds of graphene with the acetylenic

chains (single- and triple-bond) [18]. Based on different ratio of sp constituents, graphyne can have unlimited geometrical configurations, among which four typical structures, *i.e.*, α -graphyne, β -graphyne, γ -graphyne and 6, 6, 12-graphyne have attracted much attention recently [17–20].

Graphynes extend some novel properties beyond those of primitive graphene [21–30] and have been proposed to be used as energy storage [31], anode [32], gas separation [33], and water desalination materials [34]. Among graphyne family, β -graphyne (Fig. 1) exhibits outstanding properties. Malko et al. [25] predicted that Dirac cones and their associated electronic transport exist in β -graphyne, just like in graphene. Ouyang et al. [35] found that the zigzag β -graphyne nanoribbons possess superior thermoelectric performance with a thermoelectric figure of merit (ZT) of 0.5–1.5 at room temperature, at least one order higher than that of graphene. Despite these studies, the understanding of mechanical properties of β -graphyne is very limited.

The insertion of acetylenic linkages is detrimental to the mechanical properties of graphyne. For example, the elastic modulus of α -graphyne is at least one order lower than that of graphene [36]. The deterioration in mechanical properties (fracture strength and Young's modulus) of different graphynes is attributed to the lower atom density [37]. However, the structure dependent

* Corresponding author. Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, Shanghai, 200072, China.

E-mail address: tchang@staff.shu.edu.cn (T. Chang).

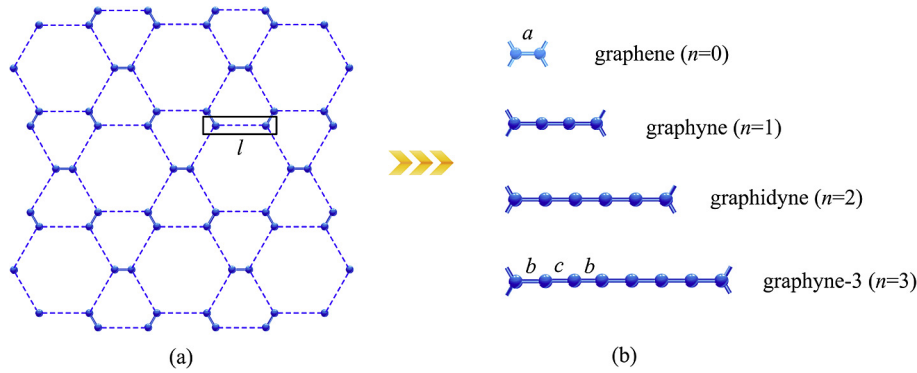


Fig. 1. (a) Schematic illustration of geometric structure of β -graphyne (b) Bond types in β -graphyne, where a , b and c are the lengths of aromatic, single and triple bonds, respectively. The length of carbyne chains is $l = [(n+1)b + nc]$, where n is the index number. (A colour version of this figure can be viewed online.)

mechanical property of β -graphyne is unexplored, especially the analytical relationship between the elastic properties and acetylene repeats (or bond density).

In this paper, based on a molecular mechanics model, we obtain a set of close-form expressions for the elastic properties of β -graphyne, which perfectly match results from molecular dynamics simulations. We show that the in-plane stiffness, in-plane shear stiffness and layer modulus are decreasing functions while Poisson's ratio is an increasing function of the number of acetylenic linkages.

2. Analytical model

According to molecular mechanics theory, the force field depends on the relative position of individual atoms. When a structure is deformed, the energy stored in the structure is a sum of several individual energy sources. In the molecular force field, the total potential energy of system, E_t , can be expressed as

$$E_t = U_\rho + U_\theta + U_\omega + U_\tau + U_{vdw} + U_{es} \quad (1)$$

where U_ρ , U_θ , U_ω and U_τ refer to energies associated with bond stretching, angle variation, inversion and torsion, respectively; U_{vdw} , U_{es} are energies associated with van der Waals and electrostatic interactions.

In case of different materials and loading conditions, various functional forms may be used for these energy terms, and some secondary energy terms are neglected to obtain the analytical results more directly. In this work, for β -graphyne subjected to in-plane loadings at small strains, the energy terms associated with torsion, inversion, van de Waals and electrostatic interactions are negligible [36,38–43], and only those with bond stretching and angle variation are predominant in the total potential energy. We use harmonic potentials to characterize the interactions between atoms, which had been proved to be efficient and accurate enough at small strains.

Just like other carbon allotropes [36,38–44], the structure of β -graphyne (Fig. 1) can be treated as a stick-spiral system, and a stick-spiral model can be used to obtain the explicit expressions of its elastic properties. In the stick-spiral model [39], an elastic stick with an axial stiffness of K is used to model the stretching force of the carbon-carbon bond and a spiral spring with a stiffness of C to model the moment arising from the variation of the angle. Furthermore, the bending stiffness of stick is assumed to be infinite because the chemical bonds will always remain straight regardless of the applied load. The total potential energy of the system can thus be expressed as a function of the bond elongation and the

bond angle variance

$$E_t = U_\rho + U_\theta = \frac{1}{2} \sum_i K_i (dr_i)^2 + \frac{1}{2} \sum_j C_j (d\theta_j)^2 \quad (2)$$

where dr_i is the elongation of bond i and $d\theta_j$ is the variance of bond angle j .

Elastic properties of 2D isotropic materials can be described by Young's modulus, Y , and Poisson's ratio, ν . Owing to the ambiguous definition of the thickness of monolayer 2D materials, we use the in-plane stiffness, Y_s , instead of Y in the following discussion. The elastic properties of β -graphyne can be obtained directly by analyzing the force-deformation response of its unit cell (Fig. 2a) in the stick-spiral model, similar to the procedure presented by Hou et al. [36,43] for deriving the analytical expressions for the elastic properties of α -graphyne and γ -graphyne. We consider a β -graphyne sheet under axial loads along the armchair direction as shown in Fig. 2a. Force equilibrium analysis of local structures (Fig. 2b) in a unit cell (with a length of U_A and U_Z in the armchair and zigzag directions, respectively) leads to the following governing equations.

$$2f_2 = K_a da_A \quad (3)$$

$$f_2 \cos \alpha = -K_n [(n+1)db_Z + ndc_Z] = -K_n lz \quad (4)$$

$$\left(\frac{b_Z}{2} + \frac{n}{2}(b_Z + c_Z) \right) f_2 \sin \alpha + m = (C_{aa} + C_{ab})d\alpha + C_{ab}d\beta = (2C_{aa} + C_{ab})d\alpha \quad (5)$$

and

$$f_1 = K_n [(n+1)db_A + ndc_A] \quad (6)$$

$$\frac{a_Z}{2} (f_1 - f_2) \sin \beta = C_{ab} (d\alpha + 2d\beta) \quad (7)$$

$$(f_1 - f_2) \cos \beta = -K_a da_Z \quad (8)$$

$$\left(\left(1 - (-1)^i \right) \frac{c_Z}{4} + \left(1 + (-1)^i \right) \frac{b_Z}{4} + (n-i) \left(\frac{b_Z}{2} + \frac{c_Z}{2} \right) \right) f_2 \sin \alpha = C_{bc} d\varphi_i, 1 \leq i \leq n \quad (9)$$

In the above equations, K_a is the stick stiffness of aromatic bonds (the subscripts A and Z represent the armchair and zigzag

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