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The morphology of graphene on an elastic graded substrate

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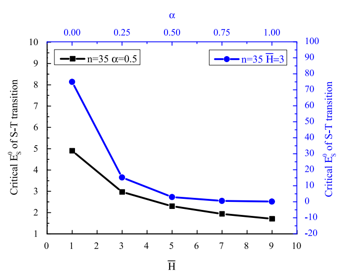
HIGHLIGHTS

- The effects of substrate thickness and surface graded parameter on graphene morphology are investigated.
- The effects of substrate thickness and surface graded parameter on snap-through transition of graphene are discussed.
- Substrate Poisson's ratio effect on graphene morphology is studied.

GRAPHICAL ABSTRACT

The results indicate that the graded parameter α is proved to be a dominated factor to control the morphology and S-T transition of graphene. With the increase of the substrate thickness, the graphene is more likely to remain flat on the substrate surface.



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ABSTRACT

We study snap-through transition and morphology of multilayer graphene on an elastic substrate, which has power-law grading modulus. It is indicated that both the inhomogeneous thickness and graded parameter of substrate have effects on corrugation and snap-through transition of graphene. The increase of graded parameter of substrate results in less corrugation of graphene. The snap-through transition of graphene is more likely to happen for larger graded parameter or thickness of substrate. This work provides theoretical guidance to control graphene morphology by changing the substrate thickness and grade in certain case.

1. Introduction

Recently, morphological characteristics of graphene on various substrate have attracted great interest of considerable researchers due to its excellent mechanical [1,2] and electronic [3–6] properties. Since the properties of graphene are closely related to the graphene morphology [7–9], it is essential to understand morphological properties of graphene to promote the number of potential applications, such as device fabrication [9–12], transparent conductors [13] and composite materials [14,15]. Morphologies of graphene on substrate have three types: conform to substrate, partly conform to substrate and remain flat on substrate. A sudden morphological transition of graphene from conform to the substrate to become flat on the substrate is called snap-through transition (S-T transition), which is demonstrated through experimental and theoretical researches [8,16–19]. Scharfenberg et al. [16,17] revealed that the thickness of graphene was the factor that related to the S-T transition of graphene on microscale corrugated elastic and metallic surfaces. Li and Zhang [18,19] demonstrated that the morphology of graphene can be controlled by the patterned corrugations substrate. Aitken and Huang [20], Gao and Huang [21] and Xiong and Gao [22] studied the surface roughness effect on morphology and snap-through instability of graphene. In the previous study, graphene was assumed to rest on substrate which has a constant stiffness. However, many practical systems which have elastic substrate with inhomogeneous

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stiffness are often encountered in various natural and artificial materials and devices [23]. To our best knowledge, there are few works focused on substrate grading effect on graphene morphology and S-T transition.

In this study, we propose a model based on classical plate theory to show how the graphene thickness, substrate reference stiffness, substrate thickness, substrate graded parameter and the Poisson's ratio of substrate influence the morphology and S-T transition of graphene. This work could offer a theoretical guidance for controlling graphene morphology by changing the relevant parameters of the substrate in certain cases.

2. Theoretical foundation

In our study, we consider the multilayer graphene on a compliant substrate, which lies on a rigid substrate in turn. Assuming that the compliant substrate has constant Poisson's ratio and follows power-law grading modulus along the depth direction z as the following form [23]:

$$E_s(z) = E_s^0 \cdot z^{\alpha} \tag{1}$$

where E_s^0 is the reference material constant, α is the graded parameter of substrate, which ranges from 0 to 1.

Fig. 1 shows the schematic diagram of multilayer graphene on compliant substrate with power-law grading modulus (Fig. 1a) and the three types of graphene morphologies (Fig. 1b, Fig. 1c and Fig. 1d), respectively. The transition of the graphene morphology changing sharply from Fig. 1c or Fig. 1d to Fig. 1b is S-T transition. $h_n = 0.335n$ nm is the thickness of graphene, n represents the number of graphene layers and the thickness of the compliant substrate is denoted as H.

The substrate surface and graphene morphology are described by

$$w_s = A_s \cos(2\pi x/L), \; w_g = A_g \cos(2\pi x/L) \tag{2}$$

respectively, where L is the wavelength, A_s and A_g are the amplitudes of substrate and multilayer graphene, respectively.

The strain components are given by

$$\varepsilon_{xx} = \frac{1}{2}\left(\frac{\partial w_g}{\partial x}\right)^2, \; \varepsilon_{xy} = \frac{1}{2}\frac{\partial w_g}{\partial x}\frac{\partial w_g}{\partial y}, \; \varepsilon_{yy} = \frac{1}{2}\left(\frac{\partial w_g}{\partial y}\right)^2 \tag{3}$$

The in-plane strain energy of the multilayer graphene is given by

$$\begin{aligned} U_g^m &= \iint \frac{C_n}{2}[(\varepsilon_{xx}+\varepsilon_{yy})^2 + 2(1-\nu)(\varepsilon_{xy}^2 - \varepsilon_{xx}\varepsilon_{yy})]dxdy \\ &= \iint \frac{C_n}{8}\left[\left(\frac{\partial w_g}{\partial x}\right)^4 + 2\left(\frac{\partial w_g}{\partial x}\right)^2\left(\frac{\partial w_g}{\partial y}\right)^2 + \left(\frac{\partial w_g}{\partial y}\right)^4\right]dxdy \end{aligned} \tag{4}$$

where C_n is the in-plane elastic modulus. $\nu = 0.33$ represents the Poisson's ratio of graphene [24].

The bending energy of the multilayer graphene is given by

$$U_g^b = \iint \frac{D_n}{2}\left[\left(\frac{\partial^2 w_g}{\partial x^2} + \frac{\partial^2 w_g}{\partial y^2}\right)^2 + \frac{1}{2}(1-\nu)\left[\left(\frac{\partial^2 w_g}{\partial x \partial y}\right)^2 - \frac{\partial^2 w_g}{\partial x^2}\frac{\partial^2 w_g}{\partial y^2}\right]\right]dxdy \tag{5}$$

where D_n is the bending rigidity of the graphene.

The strain energy of the multilayer graphene is

$$U_g = U_g^b + U_g^m \tag{6}$$

The substrate is compliant and elastic. We ignore the shear stress on the graphene/compliant substrate. The resulting strain energy of the substrate is equivalent to the work done by the graphene-substrate normal stress T_3 on the graphene/compliant substrate interface [25,26]. And the strain energy of compliant substrate is given by

$$U_{sub} = \iint \frac{1}{2} T_3(x,y)(w_g - w_s)\, dxdy \tag{7}$$

The normal stress between the graphene and compliant substrate is obtained by solving the boundary value problem [25,26]

$$T_3 = g\overline{E}_s^0\left(\frac{2\pi}{L}\right)w \tag{8}$$

with $g = g((2\pi/L)H, \; \nu_s)$, $\overline{E}_s^0 = E_s^0/(1-\nu_s^2)$.

In our work, we assume two limiting cases of graphene on substrate. The first one is that the graphene is allowed to slide freely on the substrate surface. In this case, the contribution of the in-plane stretching on strain energy can be ignored ($U_g^m = 0$) and [25]

$$g = \frac{\sqrt{2}}{2}\coth\left(\sqrt{2}\frac{2\pi}{L}H\right) + \frac{2\pi}{L}H\text{csch}^2\left(\sqrt{2}\frac{2\pi}{L}H\right) \tag{9}$$

We can see that g is independent of the Poisson's ratio ν_s and is a function of $(2\pi/L)H$.

The second limiting case is assuming that there is no relative slide between the graphene and the substrate and g can be written as [25]

$$g = \frac{4((2\pi/L)H)^2 + (3-4\nu_S)\coth\left(2\sqrt{2}(2\pi/L)H\right) - 4(3-2\nu_s)\nu_s + 5}{\sqrt{2}(3-4\nu_S)\sinh(2\sqrt{2}(2\pi/L)H) - 4(2\pi/L)H} \tag{10}$$

Thus, the total strain energy of the system can be written as

$$U = U_g^b + U_g^m + U_{sub} \tag{11}$$

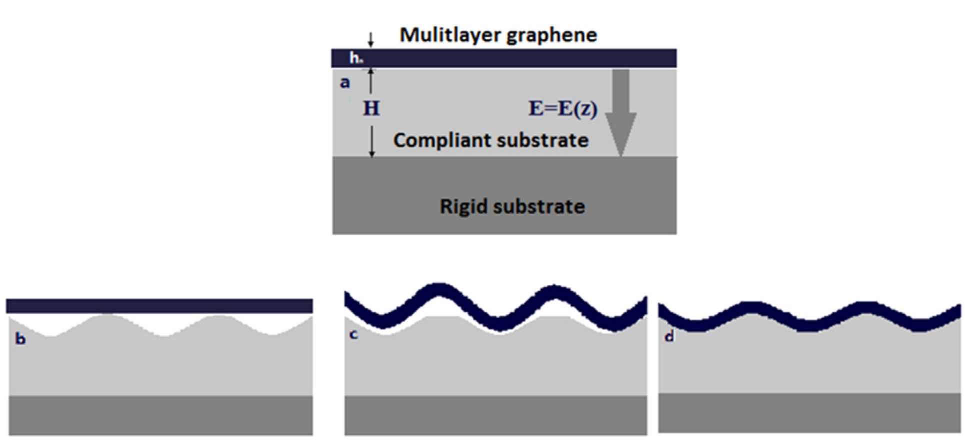

Fig. 1. (a): Schematic diagram of substrate with power-law grading modulus and three types of the graphene morphologies on substrate (b): remain flat on the substrate, (c): partly conform to the substrate and (d): conform to the substrate, respectively.