Mechanisms of nonlocal effect on the vibration of nanoplates

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This letter presents a study of the mechanisms of nonlocal effect on the transverse vibration of two-dimensional (2D) nanoplates, e.g., monolayer layer graphene and boron-nitride sheets. It is found that such a nonlocal effect stems from a distributed transverse force due to (1) the curvature change in the nanoplates and (2) the surface stress due to the nonlocal atom-atom interaction. A single equivalent vibration wavelength is defined to measure the nonlocal effect on the vibration of 2D nanoplates. The critical equivalent wavelength of order 0.55 to 2.23 nm is obtained for significant nonlocal effect on monolayer graphene. © 2011 American Institute of Physics. [doi:10.1063/1.3579249]

Continuum mechanics theories play an indispensible role in characterizing mechanical responses of nanomaterials that are building blocks in nanotechnology. In extending the continuum theories into a nanoscale world one has to consider the distinct features that distinguish nanomaterials from their macroscopic counterparts. These include the interface van der Waals interaction[1,2] and the surface effect[3,4] on nanomaterials. In 1970s, nonlocal elasticity was proposed by Eringen[5,6] for small scale problems like dislocations and cracks in materials, where stresses at a reference point are functions of the strains at all points of the body. The theory is found to be in good agreement with lattice dynamics model in studying plane waves and the experiment on phonon dispersion.[6] In 2003, Sudak[7] applied the nonlocal theory to carbon nanotubes (CNTs) and identified its important role in nanomechanics. Subsequently, nonlocal effect has been studied extensively for the bucking, vibration and wave propagation of CNTs, monolayer graphene and microtubules in cells.[8–14]

In spite of its widespread use in nanomechanics, little has been discussed about its physical mechanisms and some fundamental issues in the nonlocal theory have not been clarified. For example, Eringen[5,6] suggested that the nonlocal effect should be determined by the quantity $\tau = e_0 a/l$, where e_0 is a constant appropriate to a material, a is the internal characteristic length (e.g., lattice parameter, granular distance) and l is an external characteristic length (e.g., crack length, wavelength). Recently this has been confirmed in numerical studies[8–14] but the physical implication of τ has not yet been explained. In addition, while deformation wavelength l can be easily found for one-dimensional nanobeams it is not clear how to define a single wavelength l for two-dimensional (2D) nanoplates, where deformation occurs along, e.g., the two sides of rectangular plates. Moreover nonlocal effect is due to the reduction in geometric size. It is thus of interest to find out the critical size for significant nonlocal effect on nanomaterials. In this letter, the aforementioned issues will be examined for the transverse vibration of rectangular nanoplates as shown in Fig. 1, where monolayer graphene is used as an example.

Recently elastic plate theory has been used to study monolayer graphene.[13,15–18] An agreement with molecular dynamics simulations has been achieved in predicting their responses under a central point load.[15,18] In particular, in Ref. 15, the linear plate model is found to be adequate for characterizing the small deflection vibrations[19] of these nanoplates. Thus, in this study, we incorporate the nonlocal theory into the linear plate model for the transverse vibration of 2D rectangular nanoplates. The obtained equation reads[13]

$$D\left(\frac{\partial^4 w}{\partial x^4} + 2\frac{\partial^4 w}{\partial x^2 \partial y^2} + \frac{\partial^4 w}{\partial y^4}\right) - (e_0 a)^2 m_0 \left(\frac{\partial^4 w}{\partial x^2 \partial t^2}\right.$$
$$\left. + \frac{\partial^4 w}{\partial y^2 \partial t^2}\right) + (e_0 a)^2 m_2 \left(\frac{\partial^6 w}{\partial x^4 \partial t^2} + 2\frac{\partial^6 w}{\partial x^2 \partial y^2 \partial t^2}\right.$$
$$\left. + \frac{\partial^6 w}{\partial y^4 \partial t^2}\right) + m_0 \frac{\partial^2 w}{\partial t^2} - m_2 \left(\frac{\partial^4 w}{\partial x^2 \partial t^2} + \frac{\partial^4 w}{\partial y^2 \partial t^2}\right) = 0,$$

(1)

where x and y are Cartesian coordinates, w is the transverse displacement, t is time, m_0 and m_2 are mass density per unit area and inertia mass, and D is the bending rigidity of the nanoplates. Consider simply supported boundaries the solution of Eq. (1) reads $w = W \sin[(m\pi/L_x)x]\sin[(n\pi/L_y)y]e^{-i\omega t}$, where W is the vibration amplitude, L_x and L_y are the lengths of the nanoplate (Fig. 1), and m and n are half wave numbers of the vibration in x and y directions. In addition, ω is angu-
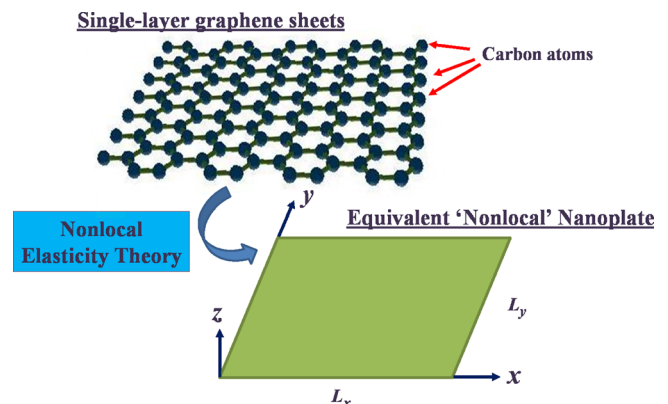

FIG. 1. (Color online) Molecular representation of a graphene sheet and its equivalent nonlocal nanoplate.

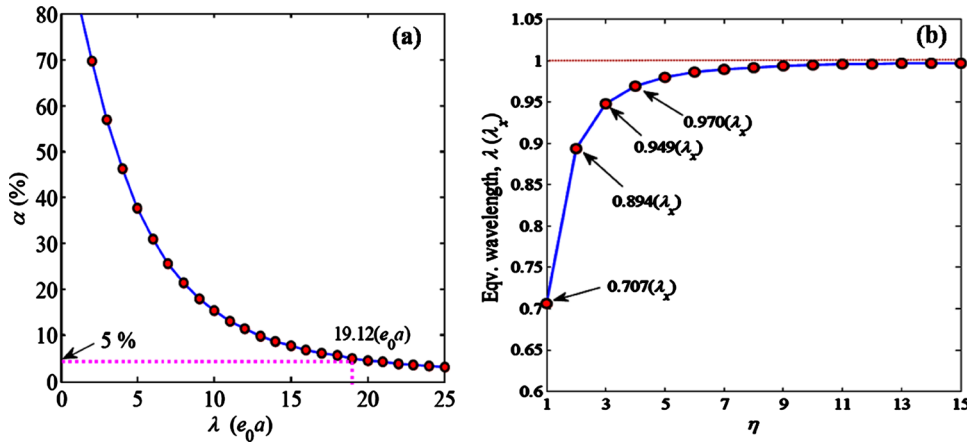a)Author to whom correspondence should be addressed. Electronic mail: chengyuan.wang@swansea.ac.uk.

FIG. 2. (Color online) (a) The relative change in frequency α as a function of the equivalent wavelength λ. Here, the unit used for λ is $(e_0 a)$, and (b) the dependence of the equivalent wavelength λ on ratio η.

lar frequency and $i=\sqrt{-1}$. Putting the solution into Eq. (1) leads to an equation $f(\omega^2) \times W = 0$. The condition for nonzero W is $f(\omega^2) = 0$ which gives

$$\omega^2 = \frac{\omega_0^2}{1 + 4\pi^2[(e_0 a/\lambda_x)^2 + (e_0 a/\lambda_y)^2]}$$

$$= \frac{\omega_0^2}{1 + 4\pi^2(e_0 a/\lambda)^2} \quad \text{and} \quad \lambda = \lambda_x\left(\frac{\eta}{\sqrt{\eta^2 + 1}}\right), \qquad (2)$$

where ω_0 is the angular frequency given by classical plate theory, $\lambda_x = 2L_x/m$ and $\lambda_y = 2L_y/n$ are the wavelength in x and y directions, and $\eta = \lambda_y/\lambda_x \geq 1$. It is easy to see in Eq. (2) that $(e_0 a/\lambda)^2 = (e_0 a/\lambda_x)^2 + (e_0 a/\lambda_y)^2$ which naturally defines a single equivalent wavelength λ for 2D nanoplates, and shows that the nonlocal effect on the vibration of 2D nanoplates is indeed controlled by the single parameter τ $(=e_0 a/l$ where $l=\lambda)$ defined by Eringen.[5,6]

Here, the nonlocal effect can also be measured by the relative change in frequency $\alpha = (\omega_0 - \omega)/\omega_0 = 1 - 1/\sqrt{1 + 4\pi^2(e_0 a/\lambda)^2}$. As shown in Fig. 2(a), α declines with increasing λ and becomes less than 5% at $\lambda > 19.12$ $(e_0 a)$. Thus, assume that at $\alpha < 5\%$ the nonlocal effect is small enough to be neglected, 19.12 $(e_0 a)$ nm can be considered as the critical equivalent wavelength for significant nonlocal effect on the nanoplate vibration.

For monolayer graphene the length of C–C bond (0.142 nm) can be used as internal characteristic length a (Ref. 7) and e_0 is of the order 0.2 to 0.82.[10–12] Thus, the critical wavelength λ_{cr} for the transverse vibration of monolayer graphene is of order of magnitude 0.55 to 2.23 nm, which is in accordance with 0.9 to 2.35 nm obtained for the wave propagation in CNTs.[12]

As shown above, the equivalent wavelength λ is essential for the nonlocal effect on the vibration of nanoplates. Based on Eq. (2) Fig. 2(b) shows that λ grows with rising η $(=\lambda_y/\lambda_x \geq 1)$ and approaches an asymptotic value λ_x, when η is sufficiently large. To evaluate the influence of λ_y and λ_x on λ, we consider following two cases.

Case (1) $1 \leq \eta < 4$: in this case, λ_y rises from λ_x to $4\lambda_x$ and λ increases from $0.707\lambda_x$ to $0.970\lambda_x$. Here, both λ_x and λ_y affect λ significantly and lead to $\lambda < \lambda_x \leq \lambda_y$. Accordingly $e_o a/\lambda > e_o a/\lambda_x \geq e_o a/\lambda_y$ indicating that the nonlocal effect of 2D nanoplates is generally stronger than that obtained in x or y direction. The minimum λ is achieved when $\lambda_x = \lambda_y$.

Case (2) $\eta \geq 4$: in this case, $\lambda_y \geq 4\lambda_x$ and λ falls in the range of $(0.97\lambda_x$ and $\lambda_x)$. Thus, λ or the overall nonlocal

effect characterized by $e_o a/\lambda$ is predominantly determined by the shorter wavelength λ_x whereas the influence of longer one λ_y is negligible.

It is well known that, at small displacement w, $(\partial^2 w/\partial x^2) + (\partial^2 w/\partial y^2)$ represents the curvature change in nanoplates. For simply supported nanoplates they can be expressed as $4\pi^2[(1/\lambda_x)^2 + (1/\lambda_y)^2]W = 4\pi^2(1/\lambda)^2 W$. Thus Eq. (2) suggests that smaller λ results in stronger nonlocal effect as it corresponds to a larger curvature change on nanoplates. Further, Eringen[6] pointed out that "nonlocal theory accounts for surface physics, an important asset not included in classical theories" as the effect of surface tension or compression is included in the nonlocal theory. For 2D plates, only the stresses in the surface are considered in continuum mechanics whereas those normal to the surface are assumed to be zero.[16] This assumption reflects the unique features of single-atom layer nanoplates, e.g., graphene and boron-nitride sheets. It follows that the nonlocal effect of 2D nanoplates originates from the surface stresses due to the nonlocal interaction between the atom at reference point and all other atoms in the single-atom thick surface. This provides an insight to the present understanding, i.e., different from 3D nanowires where the surface effects and nonlocal interactions are considered as independent mechanisms,[20] for 2D nanoplates surface effect is a result of nonlocal atom-atom interactions.

Similar to the effect of surface stress on 1D nanowires,[3,4] the curvature change in nanoplates results in a normal component of the surface stress σ, which leads to a distributed transverse force $q = \sigma(\partial^2 w/\partial x^2 + \partial^2 w/\partial y) = 4\pi^2\sigma(1/\lambda)^2 W$ on the nanoplates [Fig. 3(a)]. This force q alters the equivalent bending rigidity and finally changes the vibration frequency of nanoplates. Based on this theory, the indicator $(e_0 a/\lambda)^2$ measures the transverse force $q = 4\pi^2\sigma(1/\lambda)^2 W$, where $(1/\lambda)^2$ reflects the curvature change and $(e_0 a)$ is related to the surface stresses.

Moreover, the frequency of nonlocal nanoplates is lower than that of classical plates [Eq. (2)], which implies that the surface stress should be compression. Such a compressive surface stress has been observed for monolayer graphene in a recent experiment.[21] To show the significance of the mechanisms behind the nonlocal effect, we plotted in Fig. 3(b) the normalized frequency ω/ω_0 against $(e_0 a/\lambda)^2$ which reflects the effect of the transverse force q.

In conclusion, we show that the nonlocal effect on one-atom layer nanoplates originates from the surface compres-
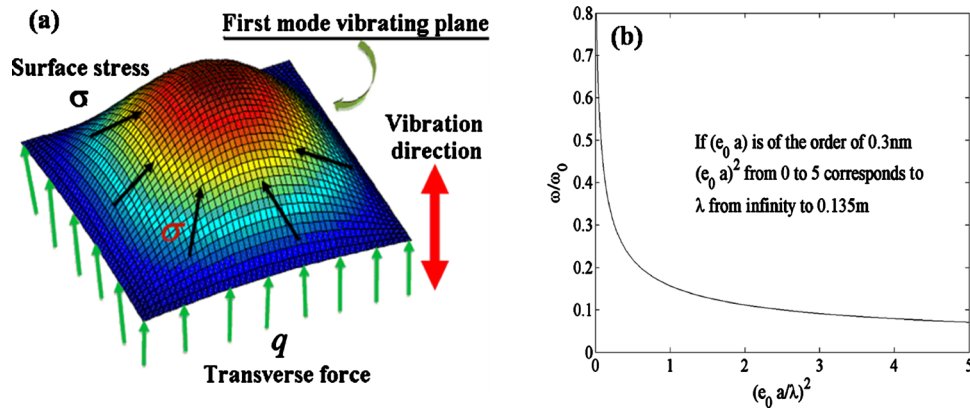
FIG. 3. (Color online) (a) Transverse force q on a vibrating nanoplate due to the curvature change and surface stress σ. (b) The dependence of ω/ω_0 on $(e_0 a/\lambda)^2$.

sion due to the nonlocal atom-atom interaction on the 2D surfaces. Such surface compression and curvature change results in a distributed transverse load on the nanoplates, which reduces their equivalent structural rigidity and downshifts their vibration frequency. The nonlocal effect can thus be quantified by the dimensionless parameter $(e_0 a/\lambda)$ where $(e_0 a)$ is related to the surface stress and the equivalent wavelength λ reflects the curvature change. λ for the 2D nanoplates is defined in Eq. (2) and $19.12(e_0 a)$ is identified as the critical value of λ for significant nonlocal effect on the transverse vibration of nanoplates.

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