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MOLECULAR AND CONTINUUM MECHANICS MODELING OF GRAPHENE DEFORMATION

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Abstract. The elastic response of a circular single graphene sheet with a diameter of 65.32 Å under a transverse central load is studied using molecular dynamics (MD), closed-form elasticity solution (EL), and finite element method (FEM). Results showed that the mismatch in deformation profiles between MD calculations and continuum mechanics methods is about 8~9% at a central deflection of one graphene layer thickness. The mismatch reduces to less than 5% when the central deflection increased to a 10-layer thickness. The mismatch rooted from mechanics: MD predicts predominant bond stretching mode while continuum mechanics predict a bending to stretching transition process under increasing deflection. Results suggest that continuum mechanics can yield predictions close to molecular mechanics under large deformation for certain loading configurations when modes of deformation are similar.

1. INTRODUCTION

Current interests in building nano structures and devices raise the question of what design tools to use, for instance, to describe the mechanical behavior of nano-sized components. Simulations using molecular dynamics (MD) methods have been adopted to study the mechanical behavior of nano wires, for instance, their bending, torsion, and compression behavior [1-4]. Recently, large-scale molecular dynamics simulations have been performed to study the properties and processes of nanoelectronic structures [5]. However, MD simulation for large and complex nano structures usually requires expensive computational facilities as well as intensive computation. On the other hand, continuum mechanics, which has been used conventionally by engineers to compute mechanical behavior of solid bodies ranging from ultra-thin films to large structures, can yield results efficiently in a short time span. For more complicated structures when closed-form solution is difficult to obtain, numerical methods such as finite element method (FEM) have been used extensively. Indeed, continuum mechanics has been applied to study the mechanical properties of fullerenes [6]. The elastic strain energy derived based on elasticity theory showed good agreement with results from using *ab initio* method. However, the question of how well the elastic response of nano structures predicted by molecular mechanics and continuum mechanics compared to each other reminds unclear, especially at large deformations.

In this work, we study the elastic response of a simple system, namely, a single-layered graphene sheet under a central load. Study of single-layered graphene sheet is fundamental in nano-scale because fullerenes and carbon nano tubes are viewed as deformed graphite sheets [6,7]. Besides, the mechanical properties of single crystal graphite are well understood [8], and the elastic properties are two dimensionally isotropic due to the hexagonal symmetry of a graphite sheet. Comparisons between results from MD, EL, and FEM are presented to shed light on whether continuum mechanics can be used to describe the behavior of nano-sized structures.

2. THEORY AND METHOD

A 1392-atom, single layered circular graphene sheet is constructed by using Hyperchem®, a MD code. The central hexagonal-carbon ring is displaced perpendicularly with reference to the circular circumference of the film. To achieve an equilibrium blistering profile of the sheet, the total internal energy is mini-

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Fig. 1. Deformation of a graphene sheet under a central displacement of 10*h.*

mized using a general purpose empirical force field method, MM+ (denoted as MD/MM+ hereafter), which works very well for carbon-based systems. The accuracy of a molecular mechanics method depends on the database used to parameterize the method. Frequently, these methods give the best results for a limited class of molecules or phenomena because it can calculate values that are closer to experiment than lower level *ab initio* techniques. The diameters of the hexagonal ring and the graphene sheet are 2.84 and 65.32 Å, respectively, and the thickness of the sheet is taken as 1.4 Å. A deformed graphene sheet with a central deflection 10 times the carbon atom diameter is shown in Fig. 1.

Closed-form EL solution for a thin circular film undergoing large central deformation was obtained previously [9]. When a thin film with radius, *a*, thickness, *h*, elastic modulus, *E*, Poisson ratio, ν, and flexural rigidity, $D = Eh^3/12(1-\nu^2)$, is under an external central load, *P*, applied via a cylindrical flat punch of radius, *c*, an average membrane stress, *N*, arises and the sheet profile, *w*(*r*), can be shown to be

$$= \frac{\varphi}{\beta^2}\{C_1\beta[I_0(\beta\xi) - I_0(\beta)] - C_2\beta[K_0(\beta\xi) - K_0(\beta)] - \log\xi\} \quad (1)$$

with

$$\xi = \frac{r}{a},\ \zeta = \frac{c}{a},\ W = \frac{w}{h},$$

$$\beta = \left(\frac{Na^2}{D}\right)^{1/2},\ \varphi = \frac{Pa^2}{2\pi Dh},$$

$$C_1 = \frac{1}{\beta^2}\left[\frac{K_1(\beta\zeta) - K_1(\beta)/\zeta}{I_1(\beta)K_1(\beta\zeta) - I_1(\beta\zeta)K_1(\beta)}\right]$$

and

$$C_2 = \frac{1}{\beta^2}\left[\frac{I_1(\beta\zeta) - I_1(\beta)/\zeta}{K_1(\beta)I_1(\beta\zeta) - K_1(\beta\zeta)I_1(\beta)}\right],$$

where $I_i(x)$ and $K_i(x)$ are the i^{th} order of the modified Bessel functions of the first and second kind, respectively. Note that W_0 is a monotonic increasing function of the normalized membrane stress β. A large W_0 suppresses the bending component, and therefore stretching becomes the dominant deformation mode.

FEM of a graphene sheet is constructed using ANSYS®. The elastic modulus of the graphene sheet is taken to be 1020 GPa, the in-plane elastic modulus of graphite, and the Poisson's ratio is taken to be 0.163 [4]. The FE mesh consists of 100 axisymmetrical shell elements and 101 nodes. A uniform pressure is applied in a central region with radius of 1.42 Å such that a central deflection of 1*h*, 3*h*, 5*h*, and 10*h* are achieved. The accuracy of FEM solution is examined by two ways. First, the solutions of the initial meshed model and the finer meshed model are compared. If the two meshes give nearly the same results, then the mesh is probably adequate. If the two meshes yield substantially different results, then further mesh refinement might be required. The model is refined until nearly identical results are obtained. Second, nonlinear FEM solution used is for handling large deformations.

3. RESULTS AND DISCUSSION

Normalized deformation profiles obtained by MD, EL, and FEM are shown in Figs. 2 and 3. For clarity of presentation only deformation profiles of 1*h* and 10*h* are shown. It is seen that a better resemblance of the deformation profile is found between MD and EL results, as compared to MD vs. FEM. Inconsistency of the deformation profiles around the loading point is noticeable, particularly between FEM and MD. This could be attributed to the effect of bending of the graphene "plate" caused by uniform pressure at the center in the FEM model. For EL, however, deformation at the center is negligible, and hence the discrepancy is less obvious. The average mismatch of the deformation profile, Δ*W*, between the any two models can be quantified by putting

$$\Delta W = \frac{\sum_{i=1}^{m}|W_{i-MM} - W_i|}{mW_0}, \quad (2)$$

where $W_{i\text{-}MM}$ is the displacement from MD/MM+, W_i the displacement from either EL or FEM calculations, and *m* the number of points taken evenly along the profile (here *m* = 17). Table 1 shows Δ*W* between any two of the three models studied. In

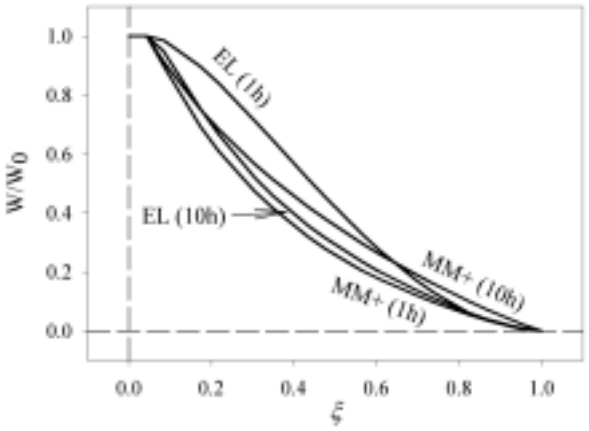

Fig. 2. Graphene deformation profiles obtained by MM+ and EL.

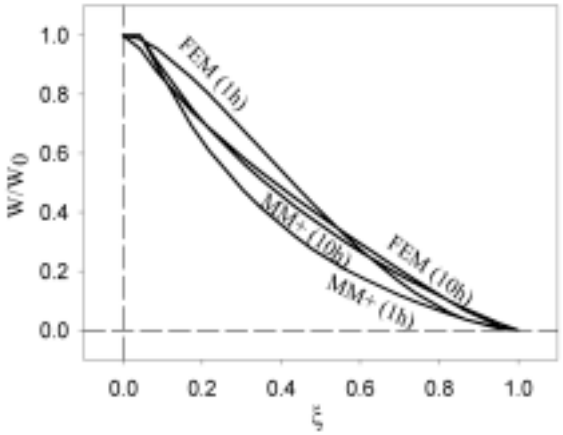

Fig. 3. Graphene deformation profiles obtained by MM+ and FEM.

general, the mismatch is large at small W_0 and gradually decreases as W_0 increases. For MD method, the flexibility of all bonds in terms of both stretching and shearing at all W_0 gives rise to a "pseudo-stretching" nature. Since the bending component is virtually suppressed and stretching prevails in MD, the inconsistency with the other two models, where bending is significant, is relatively large at small W_0 but decreases as W_0 increases. At large W_0, bending subsides and stretching dominates in both EL and FEM, resulting in a better resemblance with MD, where ΔW are less than 5% for both cases of MD vs. FEM and MD vs. EL.

It is shown that discrepancies do exist, between elasticity (FEM, EL) and MD models. Assuming that MD calculation gives more reliable predictions on graphene deformation, the mismatches between the aforementioned method arise from the nature of the mechanics method employed where bending is dominant at small loads. For MD method, the predominant deformation mode for the single graphene layer is bond stretching, regardless of the extent of deformation. It is therefore anticipated that with multi-layered structures exhibiting resistance to bending, the mismatch could be diminished at small deformations. However, more calculation is needed to verify this point.

In conclusion, MD, EL, and FEM give consistent predictions for the elastic deformation of a graphene sheet, at large deformations of 10*h* when the mode of deformation is similar, i.e., stretching dominant. It is worthwhile to remark that the computational time involved in each model varies drastically. The analytical solution is by far the most efficient, followed by FEM which can usually be accomplish within roughly an hour, MD method is most time consuming, which may take hours or even days on a desktop PC with 400 MHz CPU before a optimized energy state is found.

Table 1. Mismatch (ΔW) between MD/MM+, EL, and FEM.

W_0	*MD/MM+ vs FEM*	*MD/MM+ vs EL*	*EL vs FEM*
1	8.55%	9.90%	1.51%
3	6.16%	6.37%	2.04%
5	4.04%	3.33%	3.19%
10	1.72%	3.47%	5.01%

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