BENDING BEHAVIOUR OF SINGLE-LAYERED GRAPHENE NANOSHEETS WITH VACANCY DEFECTS

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Abstract:

The paper at hand deals with the single layered graphene sheets. In particular, the influence of the vacancy location and the density of vacancies on the bending behavior are investigated. The nanomechanical model is based on the structural mechanics approach with covalent bonds modeled as beam finite elements. The used graphene sheet model is described in detail and the obtained results are presented and thoroughly discussed.

1 Introduction

Discovered in 2004, graphene nanosheets quickly drew intensive research interests, with a total number of publications rapidly approaching that of nanotubes [1]. Although some extraordinary electronic mobility and thermal properties have been established, for this research superlative mechanical properties are of prime importance. In particular, graphene sheets are the thinnest material known to the current science. On the other side, its tensile strength surpasses steel by the factor of 100. Such high strength is not an obstacle for stretching properties since it is bent very easily – a property not typically exhibited by high strength materials. Therefore, precisely the last issue – bending behavior, is in the focus of the paper at hand.

To analyze mechanical behavior of graphene, two numerical tools are readily available. Molecular dynamics is a powerful tool for performing the most complex simulations. An alternative is, so called, structural mechanics approach, already successfully applied to the carbon nanotube models [2, 3, 4, 5, 6]. Although it may be argued that it lacks generality of the molecular dynamics, it has a significant advantage – analyses are done with standard beam finite elements, thus enabling analysis with usual finite element codes. Consequently, since the structural mechanics approach is an established technique in nanotube applications, it is the logical choice for the mechanical analysis of the graphene sheet as well.

Previous research of graphene dealing with mechanical properties is frequently concerned with the evaluation of material parameters like Young's modulus or Poission's ratio, see [7, 8]. Research with an extension to the influence of vacancies is given in [9]. The latter analysis was carried out for in-plane loading of graphene nanosheets with the emphasis on the influence of vacancies on Young's modulus. Applications to the buckling and vibration analyses followed [10, 11], also based on the structural mechanics approach. Fracture analysis was carried out in [12].

So, in contrast to [9], the goal of this paper is to evaluate bending properties of single-layered graphene nanosheets in the presence of vacancy defects. Of particular interest is the assessment of the influence of both number of vacancies and their corresponding positions. A numerical procedure is

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used in the structural mechanics approach, thus enabling us to easy experiment with different loading types and support conditions.
The outline of the paper is as follows. The second section presents basics of the structural mechanics approach. The third section gives some particulars of the used graphene sheet model, with the emphasis on the vacancies, loading and supports. The fourth section presents results in detail while the final section summarizes basic findings.

2 Finite element modeling of single-layered nanosheets

A graphene sheet consists of carbon atoms arranged in the hexagonal lattice ("chicken wire" pattern). Covalent sp^2 bonds act on carbon atoms. The vibrational potential energy due to these interactions is usually additively decomposed into stretching, bending, dihedral angle torsion, out of plane torsion and van der Waals parts. The stretching part U_r is mathematically described as:

$$U_r = \frac{1}{2}k_r\left(r - r_0\right)^2 = \frac{1}{2}k_r\left(\Delta r\right)^2, \qquad (1)$$

the bending potential energy U_θ:

$$U_\theta = \frac{1}{2}k_\theta\left(\theta - \theta_0\right)^2 = \frac{1}{2}k_\theta\left(\Delta\theta\right)^2, \qquad (2)$$

the torsion potential energy U_ϕ including both dihedral angle and out-of-plane torsion:

$$U_\phi = \frac{1}{2}k_\phi\left(\Delta\phi\right)^2. \qquad (3)$$

In the above equations, r and θ denote the distance between atoms and the bond angle after deformation, r_0 and θ_0 refer to the initial distance and the initial bond angle. The changes in the bond length, bond angle and angle change of bond twisting are described by Δr, $\Delta\theta$ and $\Delta\phi$. The material constants k_r, k_θ, k_ϕ represent the bond stretching force constant, the bond angle bending force constant and the torsional resistance of the chemical bond, respectively. Van der Waals energy is usually not considered in the analysis involving only one layer of graphene sheet.

Starting from potentials (1-3), Li and Chou [2] noticed similarities between these energies and energies used in structural mechanics of beams. For example, axial deformation of a homogenous beam with a constant cross section, loaded with constant axial force is governed by the potential:

$$U_A = \frac{1}{2}\frac{EA}{L}\left(\Delta L\right)^2, \qquad (4)$$

the bending energy where α denotes the rotational angle:

$$U_M = \frac{1}{2}\frac{EI}{L}\left(2\alpha\right)^2. \qquad (5)$$

and the torsional energy with $\Delta\beta$ is the relative rotation between the ends of the beam:

$$U_T = \frac{1}{2}\frac{GJ}{L}\left(\Delta\beta\right)^2. \qquad (6)$$

Similarity of eqs. (4-6) to the eqs. (1-3) is obvious. Identifying the material constants k_r, k_θ, k_ϕ as:

$$\frac{EA}{l} = k_r, \quad \frac{EI}{l} = k_\theta, \quad \frac{GJ}{l} = k_\phi, \qquad (7)$$

the covalent bond can be substituted by the simple beam finite element typically used in structural mechanics applications. This approach has been initially used in the analysis of carbon nanotubes, see [2-6] for several typical applications. Nowadays, it is also successfully applied to the problems involving graphene sheets, see [7-12].

3 Graphene sheet with vacancy defects

With a described model of covalent bonds at hand, graphene sheets with vacancy defects should be defined. We start from the zig-zag sheet models used in previous research [9], Fig. 1. As visible in Fig. 1, locations and density of vacancies are selected to provide adequate information about the behavior under various densities of vacancies as well as influences on their respective position on the graphene nanosheet. Analyzed sheets were made up of 29 x 17 hexagonal rings. A vacancy was simply modeled by the elimination of a

corresponding finite element node and three beam elements used for bonds simulation.
To provide a broader insight, the nanosheet is assumed to be supported in two different ways – simply supported on all sides and clamped on all sides, Fig. 2. Regarding loading, in all cases the graphene sheet is loaded with the uniform load acting on the direction parallel to the sheet normal and equally distributed among each finite element nodes, Fig. 2.

4 Results and discussion

Linear finite element simulations of graphene nanosheets bending under uniform normal load were performed and also maximal sheet

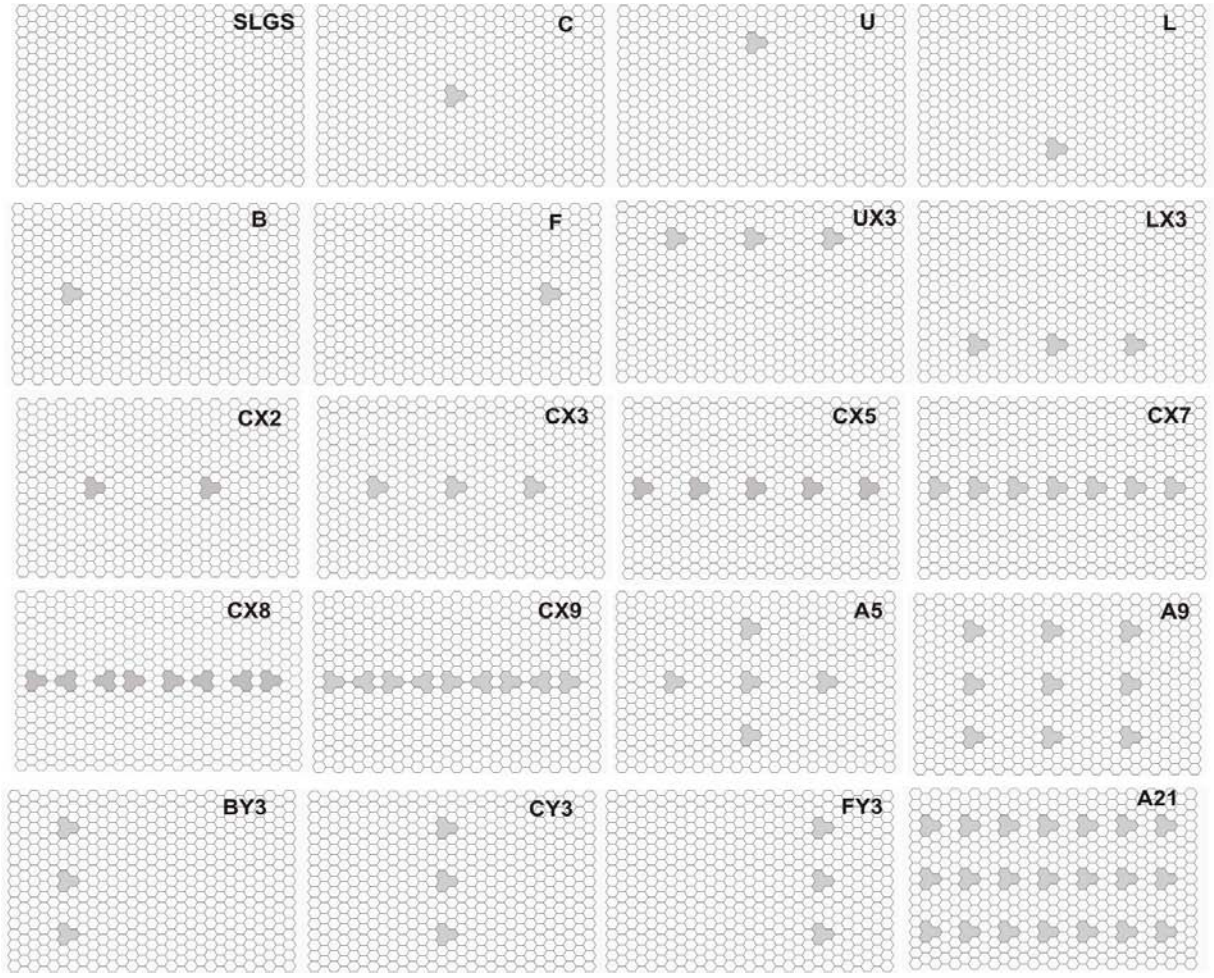

Figure 1. Graphene sheets – labels and vacancy positions, according to [9].

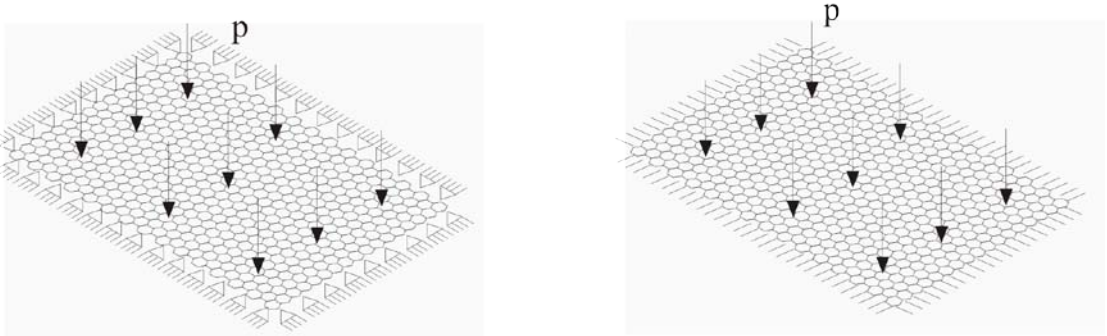

Figure 2. Graphene sheets – supports and loading.

displacements were monitored.
Sheet dimensions were 6,31597 nm x 4,182 nm. Applied loading was of pressure type with a value 0,1 nN/nm^2, equally distributed as equivalent nodal forces. The material constants k_r, k_θ and k_Φ in Eqs. (1-3) are taken from [4, 6]:

$$k_r = 938\ \text{kcal}/\text{mol}\,\text{Å}^2 = 651{,}72\ \text{nN}/\text{nm},$$

$$k_\theta = 126\ \text{kcal}/\text{mol}\,\text{rad}^2 = 0{,}875\ \text{nNnm}/\text{rad}^2,$$

$$k_\phi = 40\ \text{kcal}/\text{mol}\,\text{Å}^2 = 0{,}2779\ \text{nNnm}/\text{rad}^2.$$

To obtain beam element properties, eq. (7), Young's modulus E is taken to be 1 nN/nm^2, while the other structural mechanics parameters of the beam element, such as the cross sectional area A, moments of inertia I_1, I_2, the torsional constant J and the shear modulus G are calculated and given in a Table 1.
Obtained results are presented in Fig. 3-7 and Tab. 2. Fig. 3 and Tab. 2 summarize the most important results. Figs. 4 and 5 give deformed views of selected graphene sheets – a pristine sheet (SLGS) and the one with most vacancy defects – A21. Obviously, the larger number of vacancies in a sheet, the larger the maximal vertical displacement as well. As expected, the minimal displacement was obtained for the pristine graphene sheets (SLGS). The maximal increase in vertical displacement compared to the pristine sheet occurs for the A21 sheet type and is almost 10% in the case of clamped sheet, while the value of about 14% is obtained for a simply supported sheet. Also, single defects that are not located at the centre - sheets U, L, B, F, do not seem to significantly contribute to the increase in the vertical displacement, especially in the clamped case.
It is also found that the curve of the influence of vacancy defects on the centerline on the maximal vertical displacement, Fig. 6, has the steepest slope for the first defect. The increase in the number of vacancies at the centerline does naturally increase vertical displacement, although the trend seems to be slow in the beginning. However, Fig. 6 clearly points out that the defect on the center of the nanosheet has the most pronounced influence. The introduction of additional two defects on the centerline (CX3) has negligible influence since vertical displacement for C and CX3 type of defects

Table 1. Beam element properties.

Cross sectional area, A:	92,544 nm^2
Moments of inertia, I_1, I_2:	0,1243 nm^4
Torsional constant, J:	0,10277 nm^4
Shear modulus, G:	0,384 nN/nm^2

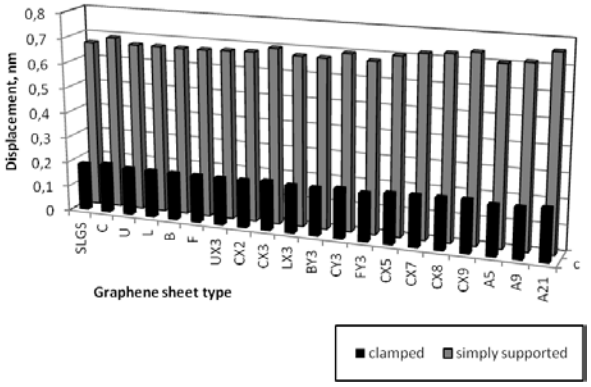

Figure 3. Maximal displacement for two types of support conditions listed for each vacancy defect type.

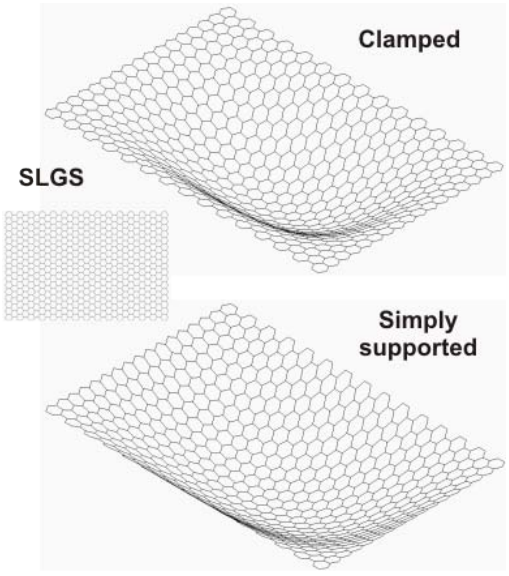

Figure 4. Deformed view of pristine sheet (SLGS) for a simply supported sheet and clamped sheet.

are almost equal. If the similar analysis is performed with respect to the density of vacancies, Fig. 7, the same trends can be noticed. As in the previous case, the most marked influence is observed for the first vacancy.

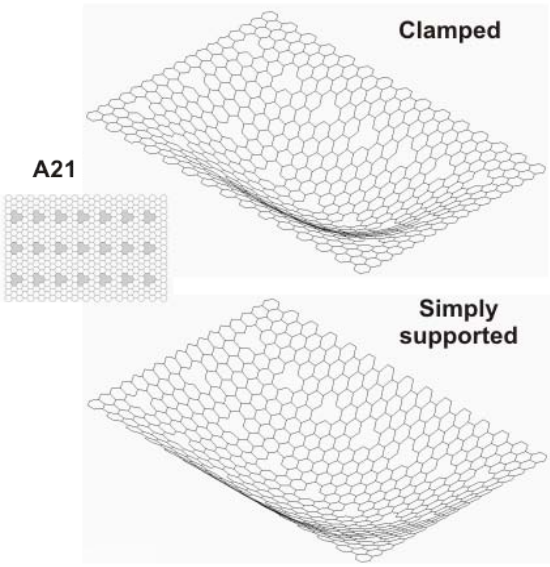

Figure 5. Deformed view of defected sheets (A21) for a simply supported sheet and clamped sheet.

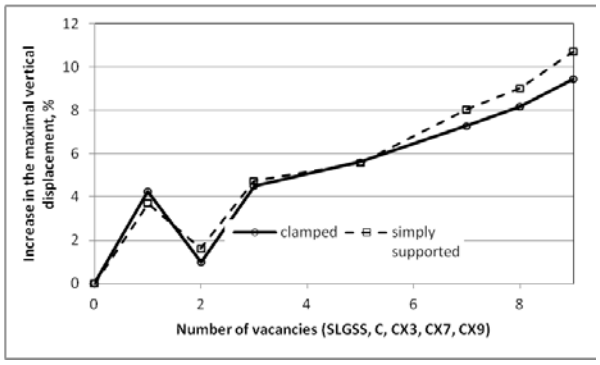

Figure 6. Influence of vacancy defects at the centerline on the maximal displacement.

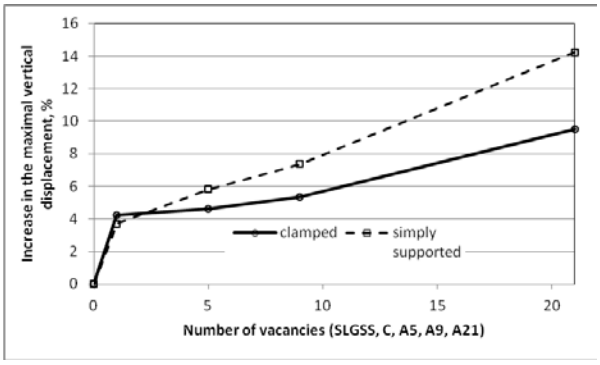

Figure 7. Influence of density of vacancies on the maximal displacement.

Table 2. Vertical displacement and increase in the vertical displacement with respect to the SLGS for graphene sheets.

	Vert. displacement, nm		increase, %	
Sheet type	clamped	simply supported	clamped	simply supported
SLGS	0,1905	0,6643	0,0	0,0
C	0,1986	0,6889	4,3	3,7
U	0,1906	0,6681	0,1	0,6
L	0,1906	0,6681	0,1	0,6
B	0,1908	0,6678	0,2	0,5
F	0,1909	0,6686	0,2	0,6
UX3	0,1912	0,6728	0,4	1,3
CX2	0,1924	0,6751	1,0	1,6
CX3	0,1991	0,6957	4,5	4,7
LX3	0,1912	0,6728	0,4	1,3
BY3	0,1912	0,6723	0,4	1,2
CY3	0,1987	0,6959	4,3	4,8
FY3	0,1917	0,6741	0,6	1,5
CX5	0,2012	0,7014	5,6	5,6
CX7	0,2044	0,7177	7,3	8,0
CX8	0,2061	0,7242	8,2	9,0
CX9	0,2085	0,7357	9,4	10,7
A5	0,1993	0,7029	4,6	5,8
A9	0,2007	0,7133	5,4	7,4
A21	0,2086	0,7588	9,5	14,2

5 Conclusion

The paper presented an efficient structural mechanics model for the nano-scale analysis of single-layered graphene sheets. The crucial idea in the paper was to investigate the influence of numbers of vacancies and their positions on the graphene sheets on the bending deformation. The defect in the center of the nanosheet proved to exert the most pronounced influence on the bending behavior. Since the real graphene sheets always include some kind of vacancy defects, these results should provide useful safety guidelines in the numerical analysis of such nanostructures.

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