



# Dynamic Stiffness Analysis of Graphene Sheets and Carbon Nanotubes

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## Abstract

Undamped natural frequencies and vibration modes are found for single layer graphene sheets and single wall carbon nanotubes, using a lattice model in which the dynamic stiffness matrix is obtained from an exact analytical solution of the governing differential member equations. The Wittrick-Williams algorithm enables any natural frequency to be found accurately and with certainty. Numerical results show reasonable agreement with finite element results, but some questions remain about which beam theory best approximates the atomic interactions. Solution times can be reduced considerably by using a repetitive analysis, but care must be taken to ensure satisfaction of the boundary conditions.

**Keywords:** graphene, carbon nanotubes, vibration, dynamic stiffness, periodic structures, Wittrick-Williams algorithm.

## 1 Introduction

It has recently been recognised that carbon based nanomaterials have great potential in advanced engineering applications on account of their exceptional mechanical, thermal and electrical properties [1, 2]. At the molecular level, these materials comprise two-dimensional hexagonal cells in which the carbon atoms are held together by massless covalent bonds. Arrays of cells can be formed into graphene sheets with a single layer (SLGS) or multiple layers (MLGS), or rolled into carbon nanotubes with a single wall (SWCNT) or multiple walls (MWCNT).

The method of molecular dynamics has been used to model the mechanical and vibrational behaviour of such structures [3]. This approach gives accurate predictions, but has high computational requirements due to its representation of inter-atomic potential functions. Continuum models based on plate and shell theories provide a faster alternative [4], and can be extended to include the effects of non-linear interactions such as van der Waals forces [5]. However continuum models

cannot fully represent the chiral structure of carbon nanotubes, and this is also a limitation of recent single beam models [6, 7].

Li and Chou [8] presented a lattice model based on the topology of the molecular structure which, while still having less computational rigour than molecular dynamics, includes the effects of chirality and can accurately model MLGS and MWCNT by including van der Waals forces [9]. In this model the carbon atoms are represented by point masses. They are connected by covalent bonds, represented by massless space frame elements having extensional, flexural and torsional stiffness properties. Geometric and elastic properties of such elements have been obtained experimentally [10, 11] and have been used by various authors. For example, Arghavan and Singh have presented natural frequencies, which are typically of the order 1THz, for SLGS [12] and SWCNT [13] with a range of dimensions and boundary conditions. These results were obtained by applying standard finite element analysis to lattice models, using Bernoulli-Euler beam theory and ignoring the van der Waals forces.

This paper also applies lattice models to SLGS and SWCNT, but uses exact dynamic stiffness theory derived from analytical solutions of the governing differential equations. Results obtained using Bernoulli-Euler and Timoshenko beam theories are compared with the results of Arghavan and Singh, and the use of an efficient model employing repetitive geometry is explored.

## 2 Lattice models of carbon nanostructures

Graphene sheets and carbon nanotubes are represented by the lattice model of Figure 1 [14]. A carbon atom lies at each node of the lattice, and the edges of the hexagons represent space frame elements with the properties listed in Table 1.

The two-dimensional geometry of a SLGS can be observed directly from Figure 1. The structure repeats in both the horizontal and vertical directions, and can therefore be modelled by multiple repetitions of the portion shown bold in the lower left-hand corner of the figure. This repeating portion has four nodes and six connections, three of which run from its own nodes to nodes in adjacent repeating portions.

A SWCNT can be modelled using the same repeating portion. Its three-dimensional geometry is obtained by rotating the lattice of Figure 1 into a circular tube so that the vector  $\mathbf{C}_\theta$ , known as the chiral vector, becomes the circumference. The structure is therefore rotationally periodic and also repeats in the translational direction  $\mathbf{T}_\theta$ .

The chiral vector can be expressed in terms of the vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  in Figure 1, by

$$\mathbf{C}_\theta = n\mathbf{a}_1 + m\mathbf{a}_2 \equiv (n, m) \quad (1)$$

where  $n$  and  $m$  are integers with  $0 \leq |m| \leq n$ . The angle  $\theta$  (here shown in degrees) between  $\mathbf{C}_\theta$  and  $\mathbf{a}_1$  is known as the chiral angle. Analysis of Figure 1 shows that the vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  each have magnitude  $a = L\sqrt{3}$ , and that

Cross sectional area, $A$	$1.68794 \text{ \AA}^2$
Length of bond, $L$	$1.42 \text{ \AA}$
Polar moment of inertia, $J$	$0.45346 \text{ \AA}^4$
Moment of inertia, $I$	$0.22682 \text{ \AA}^4$
Young's modulus of elasticity, $E$	$5.488 \times 10^{-8} \text{ N\AA}^{-2}$
Shear modulus of rigidity, $G$	$8.711 \times 10^{-9} \text{ N\AA}^{-2}$
Mass of each carbon atom, $m_c$	$1.9943 \times 10^{-26} \text{ kg}$

Table 1. Properties of space frame elements

$$\mathbf{a}_1 \cdot \mathbf{a}_1 = a^2 \quad \mathbf{a}_2 \cdot \mathbf{a}_2 = a^2 \quad \mathbf{a}_1 \cdot \mathbf{a}_2 = a^2/2 \quad (2)$$

Hence the diameter of the nanotube is given by

$$D_\theta = |\mathbf{C}_\theta|/\pi = a\sqrt{n^2 + nm + m^2}/\pi \quad (3)$$

and

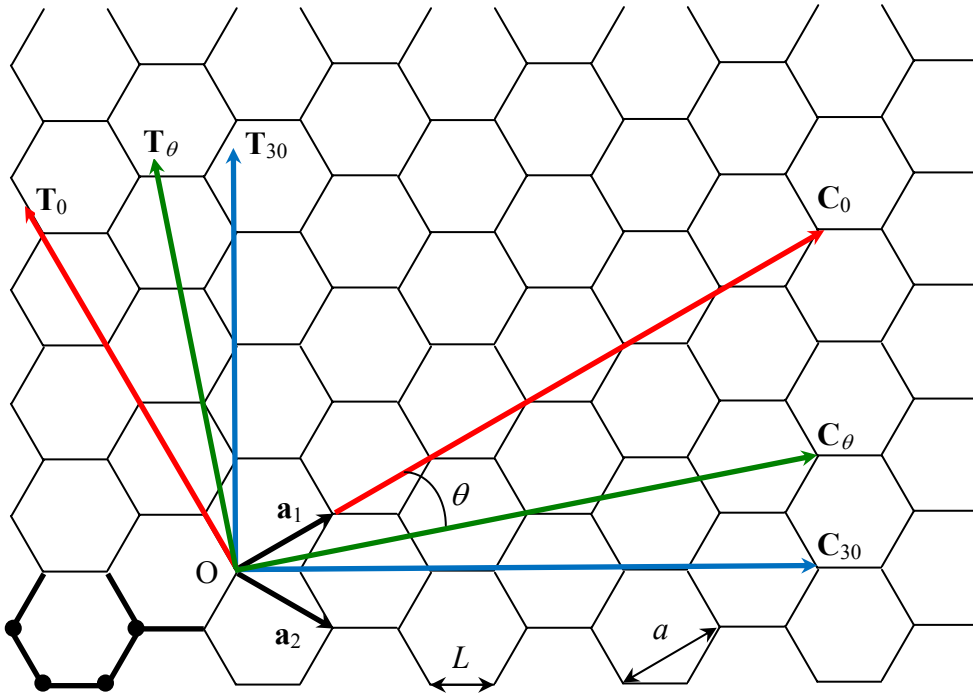


Figure 1: Geometry of lattice model, showing three examples of chiral vectors  $\mathbf{C}_\theta$  and the corresponding translational vectors  $\mathbf{T}_\theta$ .

$$\cos\theta = \frac{\mathbf{C}_\theta \cdot \mathbf{a}_1}{|\mathbf{C}_\theta||\mathbf{a}_1|} = \frac{2n + m}{2\sqrt{n^2 + nm + m^2}} \quad (4)$$

The chiral vectors shown in Figure 1 correspond to the cases

$$(n, m) = (6, 0) \quad (n, m) = (3, 3) \quad (n, m) = (4, 2) \quad (5)$$

and hence to the chiral angles

$$\theta = 0^\circ \quad \theta = 30^\circ \quad \theta = \cos^{-1}\left(\frac{5}{\sqrt{28}}\right) = 19.1^\circ \quad (6)$$

respectively. Based on the shape of the circumferential ring, a nanotube with chiral angle  $\theta = 0^\circ$ , for which  $m = 0$ , is said to have a zigzag configuration, while one with  $\theta = 30^\circ$ , for which  $m = n$ , has an armchair configuration. These two cases have additional symmetric characteristics which are lacking in other cases.

### 3 Exact dynamic stiffness analysis of lattice structures

Exact expressions for the dynamic stiffness of vibrating uniform members were derived nearly 40 years ago [15] from analytical solutions of the governing differential equations. In contrast to common finite element formulations, separate stiffness and mass matrices are not used, and the dynamic effects are accounted for exactly in a single matrix whose elements are transcendental functions of the frequency. No assumptions are made about shape functions and hence any undamped natural frequency can be found exactly without the need to discretise members into finite elements. By making use of the Wittrick-Williams algorithm [16, 17] to locate eigenvalues with certainty, exact stiffness analysis was implemented in software for two-dimensional frame structures which also accounted for the effects of axial load [18], rotatory inertia and shear deflection [19].

In extending the analysis to three-dimensional frames [20], a very efficient computational procedure was developed for periodic structures in which analysis is performed for a single (base) repeating portion. The mode of vibration or buckling is assumed to repeat in the pattern

$$\mathbf{D}(j_1, j_2, j_3) = \mathbf{D}(0, 0, 0) \exp \left[ 2i\pi \left( \frac{n_1 j_1}{N_1} + \frac{n_2 j_2}{N_2} + \frac{n_3 j_3}{N_3} \right) \right] \quad (7)$$

where:  $i = \sqrt{-1}$ ;  $\mathbf{D}(j_1, j_2, j_3)$  is the displacement vector in the repeating portion located  $(j_1, j_2, j_3)$  bays in the three coordinate directions from the base repeating portion; the mode repeats over  $(N_1, N_2, N_3)$  bays in the three coordinate directions; and separate analysis is performed for each combination of harmonics

$$-\text{int}\left(\frac{N_k}{2}\right) \leq n_k \leq \text{int}\left(\frac{N_k}{2}\right) \quad (k = 1, 2, 3) \quad (8)$$

Complex arithmetic is required to assemble the stiffness matrix of any member which connects nodes in different repeating portions. The same form of repetitive analysis is applicable to rotationally periodic structures [21], which may also repeat in the translational direction.

It should be noted that Equation (7) assumes infinite repetition of the structure in linear directions, and so may only approximate the boundary conditions at the physical ends of the structure. Analysis for rotationally periodicity is exact.

## 4 Numerical examples

The computer program BUNVIS-RG [20] was used to find natural frequencies and vibration modes for a number of SLGS and SWCNT examples which had previously been analysed [12, 13] using a lattice model with Bernoulli-Euler finite element analysis. The space frame elements for all the examples had the properties listed in Table 1. For each example, analysis was performed using both Bernoulli-Euler (BE) and Timoshenko (Timo) beam theory.

### 4.1 Vibration of a single layer graphene sheet

The first example is a SLGS of width  $49.7\text{\AA}$  and height  $49.2\text{\AA}$ , i.e. such that the hexagonal cells of Figure 1 repeat 12 times in the horizontal direction and 20 times in the vertical direction. The sheet was assumed to be clamped on all four sides. Table 2 lists the first ten flexural and extensional natural frequencies, comparing the present analysis with the published results of Singh and Arghavan [22]. It is seen that, when Bernoulli-Euler beam theory is used, the natural frequencies found by the

Frequency number	Flexural			Extensional		
	BE	Timo	BE [22]	BE	Timo	BE [22]
1	0.1708	0.1700	0.1633	2.6563	2.0485	2.6114
2	0.3431	0.3402	0.3287	2.6721	2.0756	2.6184
3	0.3532	0.3501	0.3368	3.4933	2.2796	3.4158
4	0.5129	0.5068	0.4903	3.9739	2.9534	3.8986
5	0.6127	0.6046	0.5877	4.3824	3.1836	4.3117
6	0.6371	0.6284	0.6069	4.7950	3.2003	4.6838
7	0.7741	0.7614	0.7407	4.8315	3.3053	4.7411
8	0.7882	0.7750	0.7528	4.8492	3.9861	4.7503
9	0.9746	0.9560	0.9356	5.4147	3.9924	5.2961
10	1.0173	0.9969	0.9685	5.4247	4.0038	5.3504

Table 2. Natural frequencies (THz) of a SLGS clamped on all four sides

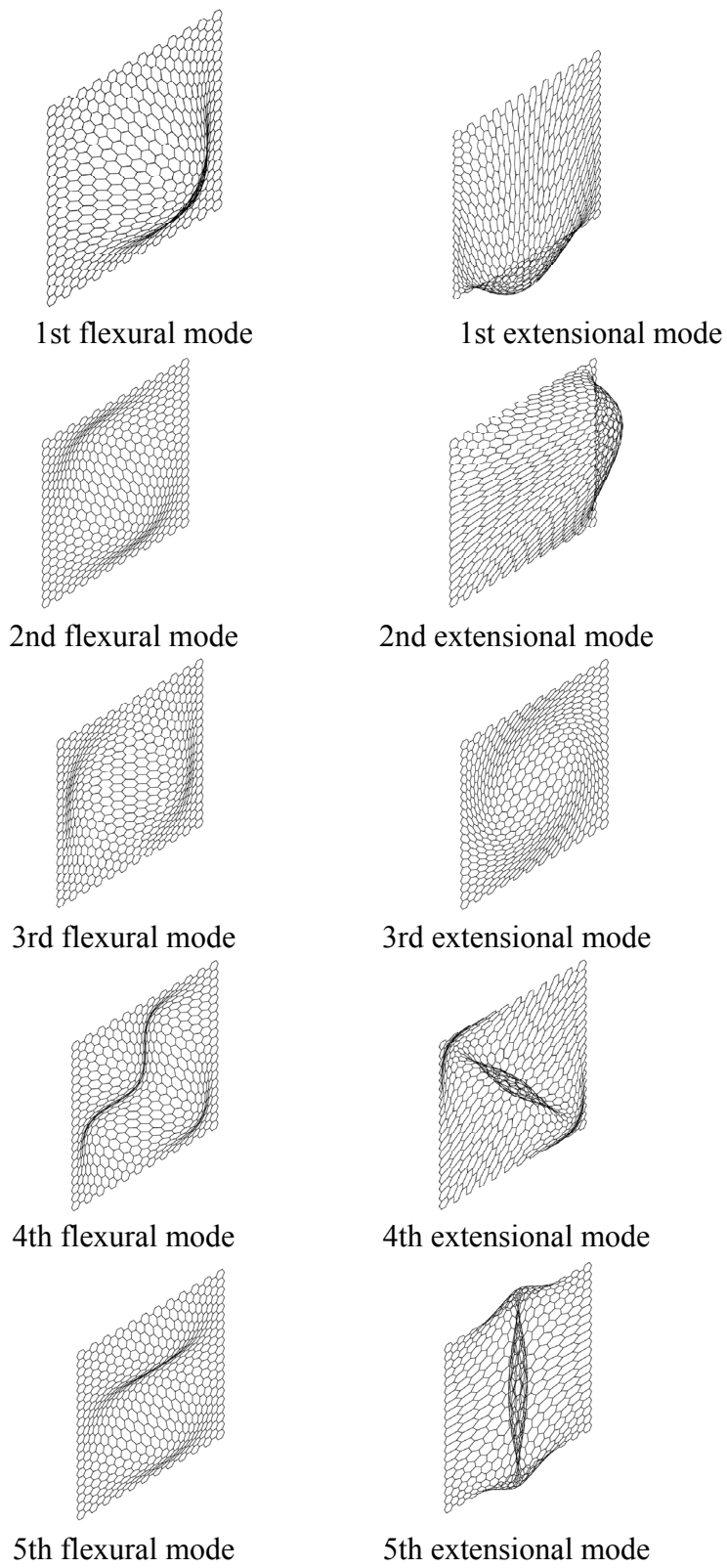


Figure 2: Vibration modes of a SLGS clamped on all four sides.

two methods agree well, the flexural natural frequencies to within about 5% and the extensional natural frequencies to about 2%, the results from the present method being consistently higher. Introduction of Timoshenko beam theory reduced the natural frequencies (as expected), by just 2% for the flexural natural frequencies but by up to 30% for the extensional natural frequencies. Figure 2 shows the first five flexural and extensional vibration modes, which show very good agreement with those of [22].

Solution times on a (slow) Sun workstation averaged 51 seconds per natural frequency found. Use of the repetitive analysis summarised in Equations (7) and (8) reduced the size of the structure analysed from 984 nodes to just the 4 nodes of a repeating portion. However, the repetitive analysis is better suited to modelling structures with simply supported edges, and could only provide approximate results for this example with clamped edges. Nevertheless, indications are that the solution time per natural frequency found would be reduced by about two orders of magnitude when using such analysis on examples for which it was appropriate.

Frequency number	Clamped-free			Clamped-clamped		
	BE	Timo	BE [13]	BE	Timo	BE [13]
1	0.0709	0.0558	0.0694	0.4467	0.3479	0.4175
2	0.0709	0.0558	0.0694	0.4467	0.3479	0.4175
3	0.4216	0.3276	0.4124	1.1278	0.8607	1.0570
4	0.4216	0.3276	0.4124	1.1278	0.8607	1.0570
5	0.7153	0.4747	0.7039	1.4814	0.9803	1.4166
6	1.0169	0.7887	1.0028	2.0121	1.5127	1.8896
7	1.0985	0.8424	1.0744	2.0121	1.5127	1.8896
8	1.0985	0.8424	1.0744	2.0952	1.6368	2.0179

Table 3. Natural frequencies (THz) of a (6,0) zigzag SWCNT

Frequency number	Clamped-free			Clamped-clamped		
	BE	Timo	BE [13]	BE	Timo	BE [13]
1	0.0768	0.0593	0.0733	0.4471	0.3409	0.4135
2	0.0768	0.0593	0.0733	0.4471	0.3409	0.4141
3	0.4432	0.3383	0.4232	1.0911	0.8211	1.0163
4	0.4432	0.3383	0.4238	1.0911	0.8211	1.0230
5	0.6356	0.4287	0.6058	1.2949	0.8752	1.2126
6	0.9863	0.7531	0.9451	1.8975	1.4180	1.7779
7	1.1180	0.8453	1.0700	1.8975	1.4180	1.8062
8	1.1180	0.8453	1.0744	1.9943	1.5283	1.8756

Table 4. Natural frequencies (THz) of a (4,4) armchair SWCNT

## 4.2 Vibration of single walled carbon nanotubes

Natural frequencies and vibration modes were next found for two SWCNT examples which were previously analysed by Arghavan and Singh [13]. The structures had a zigzag configuration with  $\theta = 0^\circ$  and  $\mathbf{C}_\theta = \mathbf{C}_0 = (6,0)$ , and an armchair configuration with  $\theta = 30^\circ$  and  $\mathbf{C}_\theta = \mathbf{C}_{30} = (4,4)$ , respectively. The zigzag SWCNT had six repeating portions around the circumference, giving a diameter  $D_\theta = 4.70\text{\AA}$ , and length  $51.83\text{\AA}$  (i.e. 12 repeating portions). The armchair SWCNT had four repeating portions around the circumference, giving a diameter  $D_\theta = 5.42\text{\AA}$ , and length  $54.11\text{\AA}$  (i.e. 22 repeating portions). Each example was solved for both clamped-free (C-F) and clamped-clamped (C-C) boundary conditions. Results for the two examples are given in Tables 3 and 4, respectively, where it is noted that (due to symmetry) flexural natural frequencies occur in pairs while extensional natural frequencies are single-fold. Bernoulli-Euler results from the present method are consistently higher than those of [13], by between 2% and 8%. The use of Timoshenko beam theory reduces all of these natural frequencies substantially, by up to 35%. Selected vibration modes are shown in Figures 3 and 4, and show very good agreement with those of [13].

## 5 Concluding remarks

Undamped natural frequencies and vibration modes have been found for single layer graphene sheets and single wall carbon nanotubes, using a lattice model in which the dynamic stiffness matrix is obtained from an exact analytical solution of the governing differential member equations. The analysis therefore avoids the use of arbitrary shape functions and discretisation into finite elements. The Wittrick-Williams algorithm ensures that any natural frequency can be found accurately and with certainty.

Numerical results for the flexural natural frequencies of a graphene sheet, clamped on all four sides, and of two carbon nanotubes show good agreement with finite element results from the literature, when Bernoulli-Euler beam theory is used. But when Timoshenko theory is applied, the extensional natural frequencies for the graphene sheet, and all the natural frequencies for the nanotubes, are considerably lower. The vibration modes show good agreement with finite element results.

Solution times are acceptable, and can be reduced substantially by taking advantage of the repetitive nature of such structures. However, care must be taken to ensure that the assumptions made in the repetitive analysis are compatible with the boundary conditions at the edges of the structure.

The literature reports that lattice models give a reasonably accurate representation of carbon nanostructures, and the analysis is considerably faster than that required by a more robust approach such as molecular dynamics modelling. Previous authors have assumed Bernoulli-Euler beam theory for the lattice members. The present work has shown that allowing for rotatory inertia and shear deflection produces significantly lower results for carbon nanotubes. In the context of conventional structures this observation would provide a strong argument for the use of



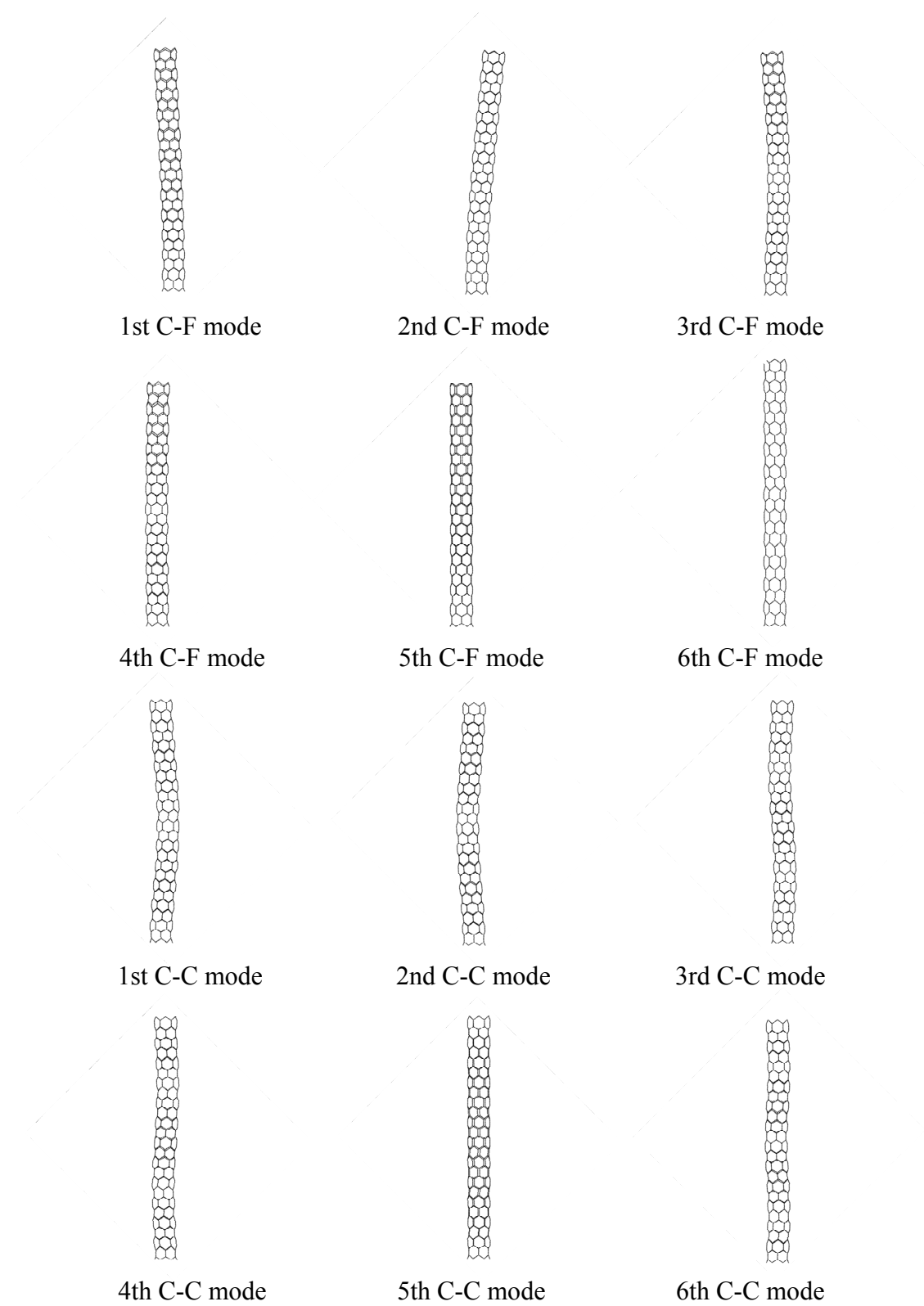


Figure 3: Vibration modes of a (6,0) zigzag SWCNT.

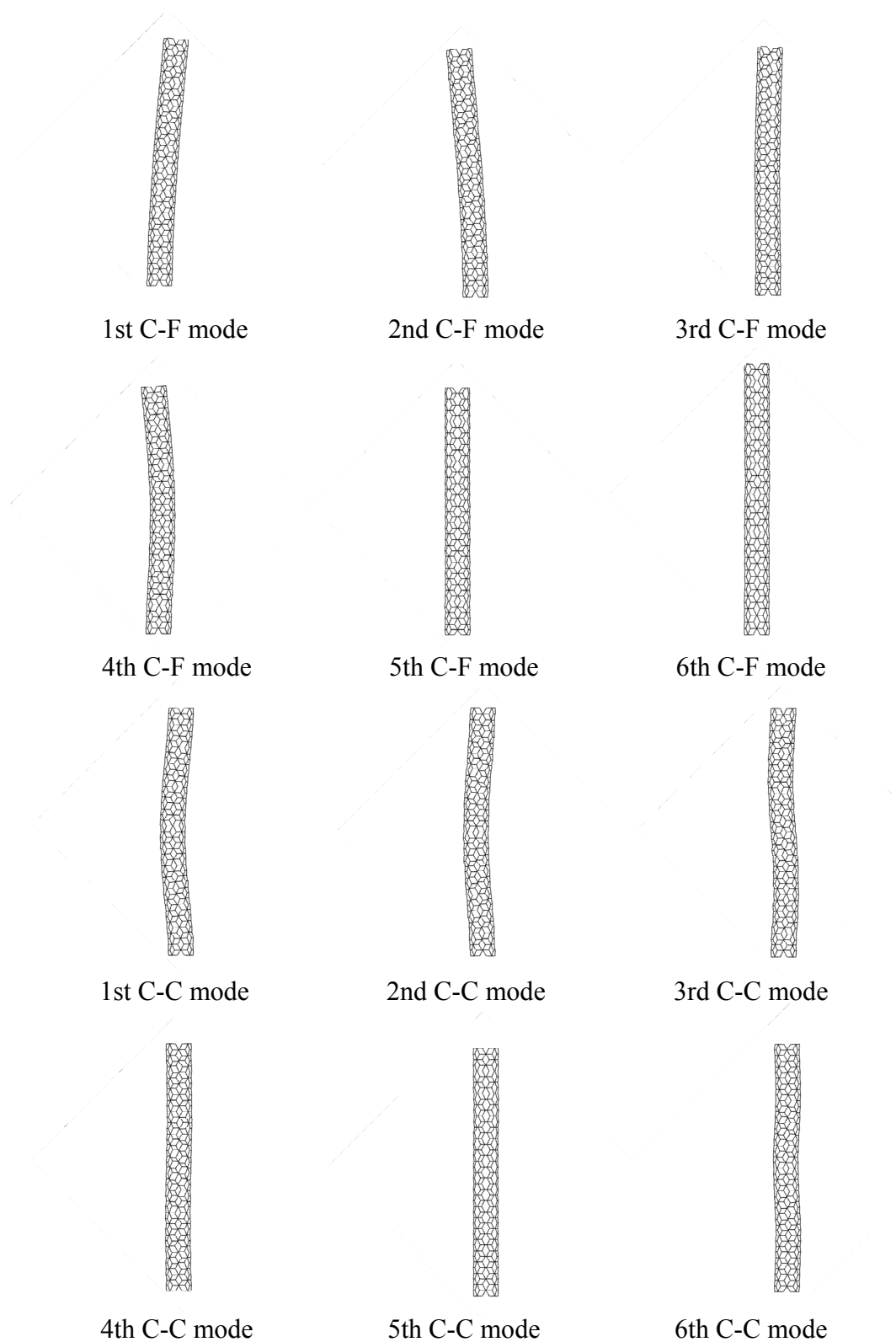


Figure 4: Vibration modes of a (4,4) armchair SWCNT.

Timoshenko beam theory. However, because the lattice model is used here as an approximation to the true atomic interactions, the nature of this approximation needs to be addressed in order to determine whether effects corresponding to rotatory inertia and shear deflection can occur. The choice of an appropriate beam theory for the lattice model therefore remains an open question.

The examples studied have been confined to single layer graphene sheets and single wall carbon nanotubes. It is expected that accuracy would be lost in applying the present analysis to multiple layer sheets and multiple wall nanotubes, because the lattice model does not take account of interaction effects such as van der Waal's forces. It is proposed to consider how such effects might be included in the governing differential equations which are solved to construct the dynamic stiffness matrix.

## References

- [1] K.S. Novoselov, D. Jiang, F. Schedin, T.J. Booth, V.V. Khotkevich, S.V. Morozov, A.K. Geim, "Two-dimensional atomic crystals", *Proceedings of the National Academy of Sciences of the United States of America*, 102(30), 10451-10453, 2005.
- [2] S. Iijima, "Helical microtubules of graphite carbon", *Nature*, 354(6348), 56-58, 1991.
- [3] S. Iijima, C. Brabec, A. Maiti, J. Bernholc, "Structural flexibility of carbon nanotubes", *Journal of Chemical Physics*, 104(5), 2089-2092, 1996.
- [4] X.Q. He, S. Kitipornchai, K.M. Liew, "Resonance analysis of multi-layered graphene sheets used as nanoscale resonators", *Nanotechnology*, 16(10), 2086-2091, 2005.
- [5] X.Q. He, M. Eisenberger, K.M. Liew, "The effect of van der Waals interaction modeling on the vibration characteristics of multiwalled carbon nanotubes", *Journal of Applied Physics*, 100(12), 124317, 2006.
- [6] I. Elishakoff, D. Pentaras, "Fundamental natural frequencies of double-walled carbon nanotubes", *Journal of Sound and Vibration*, 322(4-5), 652-664, 2009.
- [7] Y.G. Hu, K.M. Liew, Q. Wang, "Nonlocal elastic beam models for flexural wave propagation in double-walled carbon nanotubes", *Journal of Applied Physics*, 106(4), 044301, 2009.
- [8] C. Li, T.W. Chou, "A structural mechanics approach for the analysis of carbon nanotubes", *International Journal of Solids and Structures*, 40(10), 2487-2499, 2003.
- [9] C. Li, T.W. Chou, "Elastic moduli of multi-walled carbon nanotubes and the effect of van der Waals forces", *Composites Science and Technology*, 63(11), 1517-1524, 2003.
- [10] W.D. Cornell, P. Cieplak, C.I. Bayly, I.R. Gould, K.M. Merz, D.M. Ferguson, D.C. Spellmeyer, T. Fox, J.W. Caldwell, P.A. Kollman, "A second generation force field for the simulation of proteins, nucleic acids, and organic molecules", *Journal of the American Chemical Society*, 117(19), 5179-5197, 1995.

- [11] W.L. Jorgensen, D.L. Severance, "Aromatic-aromatic interactions: free energy profiles for the benzene dimer in water, chloroform, and liquid benzene", *Journal of the American Chemical Society*, 112(12), 4768-4774, 1990.
- [12] S. Arghavan, A.V. Singh, "Atomic lattice structure and continuum plate theories for the vibrational characteristics of graphene", *Journal of Applied Physics*, 110(8), 084308, 2011.
- [13] S. Arghavan, A.V. Singh, "On the vibrations of single-walled carbon nanotubes", *Journal of Sound and Vibration*, 330(13), 3102-3122, 2011.
- [14] R. Saito, G. Dresselhaus, M.S. Dresselhaus, "Physical Properties of Carbon Nanotubes", Imperial College Press, London, 2003.
- [15] V. Kolousek, "Dynamics in Engineering Structures", Butterworths, London, 1973.
- [16] W.H. Wittrick, F.W. Williams, "A general algorithm for computing natural frequencies of elastic structures", *Quarterly Journal of Mechanics and Applied Mathematics*, 24(3), 263-284, 1971.
- [17] W.H. Wittrick, F.W. Williams, "An algorithm for computing critical buckling loads of elastic structures", *Journal of Structural Mechanics*, 1(4), 497-518, 1973.
- [18] F.W. Williams, W.P. Howson, "Compact computation of natural frequencies and buckling loads for plane frames", *International Journal for Numerical Methods in Engineering*. 11(7), 1067-1081, 1977.
- [19] W.P. Howson, J.R. Banerjee, F.W. Williams, "Concise equations and program for exact eigensolutions of plane frames including member shear", *Advances in Engineering Software*, 5(3), 137-141, 1983.
- [20] M.S. Anderson, F.W. Williams, "Natural vibration and buckling of general periodic lattice structures", *AIAA Journal*, 24(1), 163-169, 1986.
- [21] F.W. Williams, "An algorithm for exact eigenvalue calculations for rotationally periodic structures", *International Journal for Numerical Methods in Engineering*, 23(4), 609-622, 1986.
- [22] A.V. Singh and S. Arghavan, "Extensional and flexural modes of vibration of single layer graphene sheets by lattice structure and continuum plate theories", *Proceedings of the 8th International Symposium on Vibrations of Continuous Systems*, Whistler, Canada, 48-50, 2011.