Atomistic Mechanics of Nanoscale Structures: Static & Dynamic Analyses

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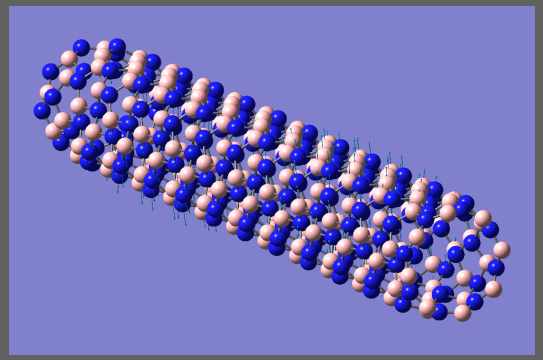
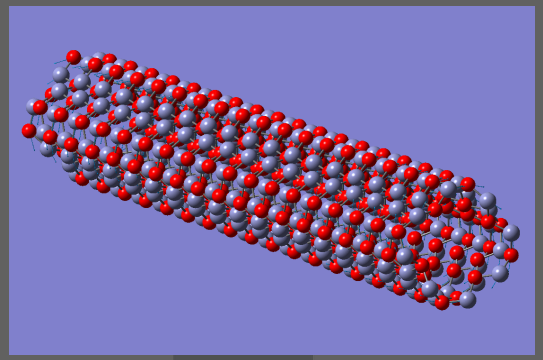
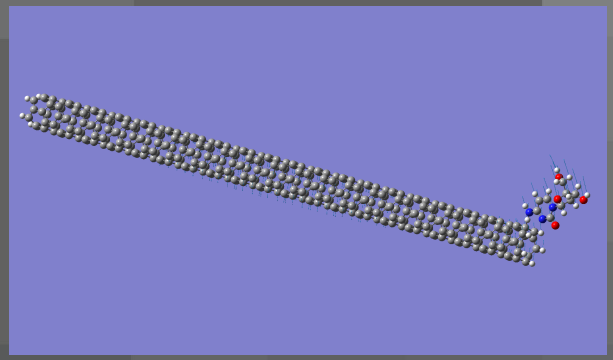
IISc Bangalore
13 January 2012







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College of Engineering

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Where is Swansea?

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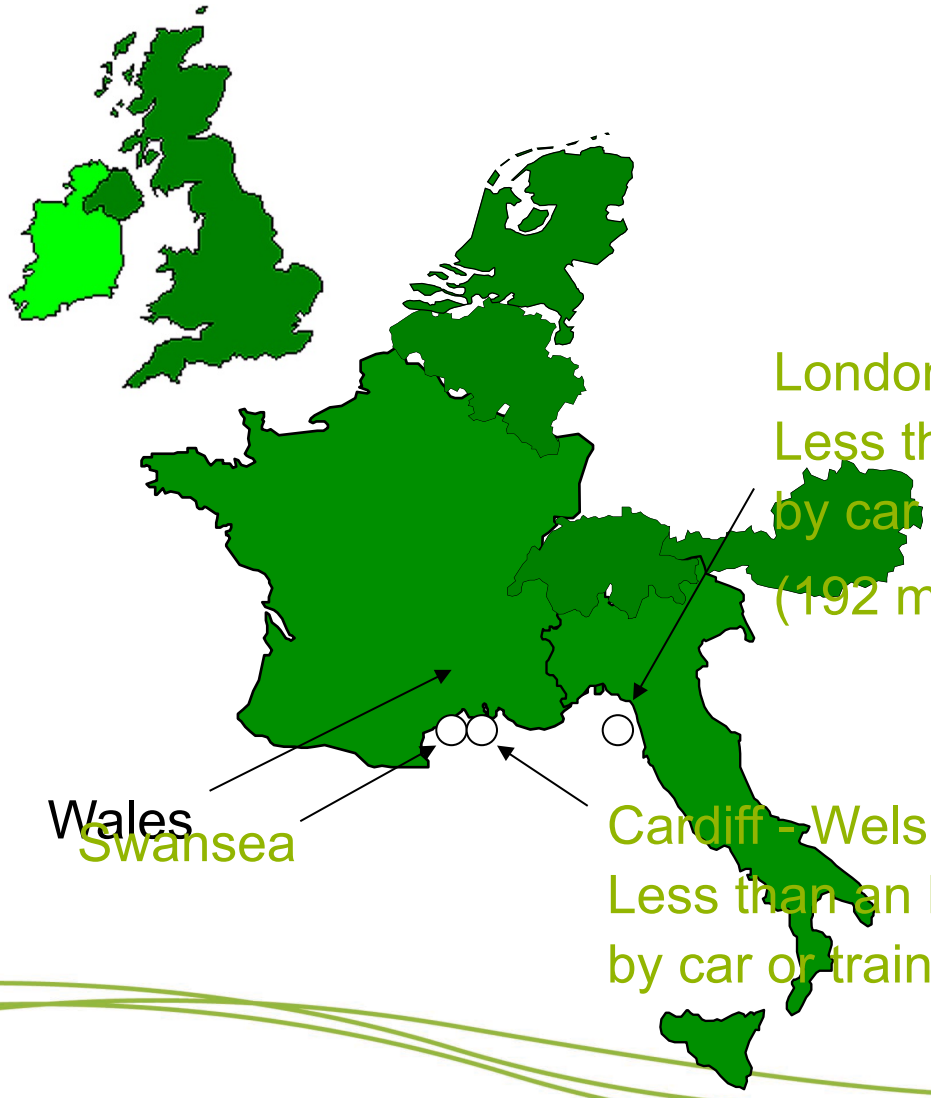

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- 29th UK university to be established
- King George V laid the foundation stone of the University in July 1920
- Now over 12,500 students - 1,800 international

Overview

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- Introduction
- Atomistic finite element method
- Carbon nanotubes: static and dynamic analysis, buckling
- Fullerenes: vibration spectra
- Graphene: static and dynamic analysis, composites
- Nanobio sensors: vibrating nanotube and graphene based mass sensor
- DNA mechanics
- Conclusions

Research Areas

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- Atomistic finite element method
- Nonlocal continuum mechanics for nanoscale objects
- Nanoscale bio sensors
- Uncertainty quantification in modelling and simulation
- Dynamic analysis of complex structures
- Vibration energy harvesting

Collaborators

- Prof F Scarpa (University of Bristol)
- Dr R Chowdhury, Dr C Wang, Dr A Gil, Prof P Rees (Swansea University).
- Dr T Murmu, Prof M McCarthy (University of Limerick)

Acknowledgements

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Carbon Nanotubes

Can we use continuum mechanics at the nanoslace?

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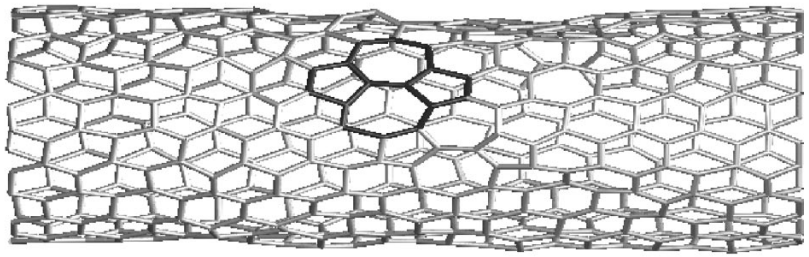
a)



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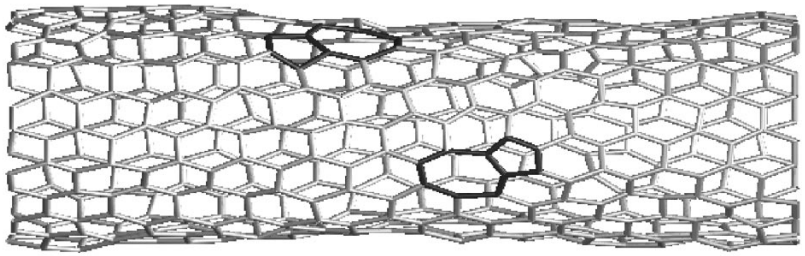

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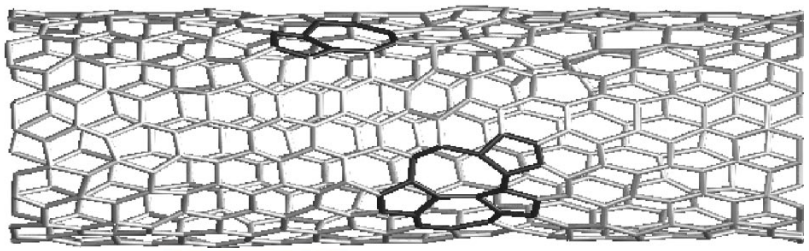

- What about the "holes"?
- Can we have an "equivalent" continuum model with "correct" properties?
- How defects can be taken into account ?

Which Young's modulus?

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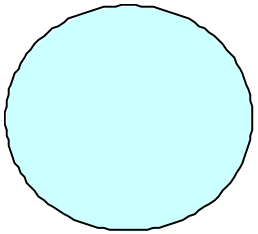
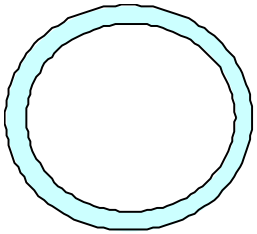
Effective



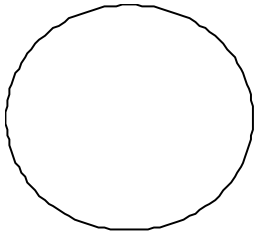
$$\bar{Y}_{11} = \frac{F}{\pi R^2 \varepsilon_{11}}$$

Longitudinal



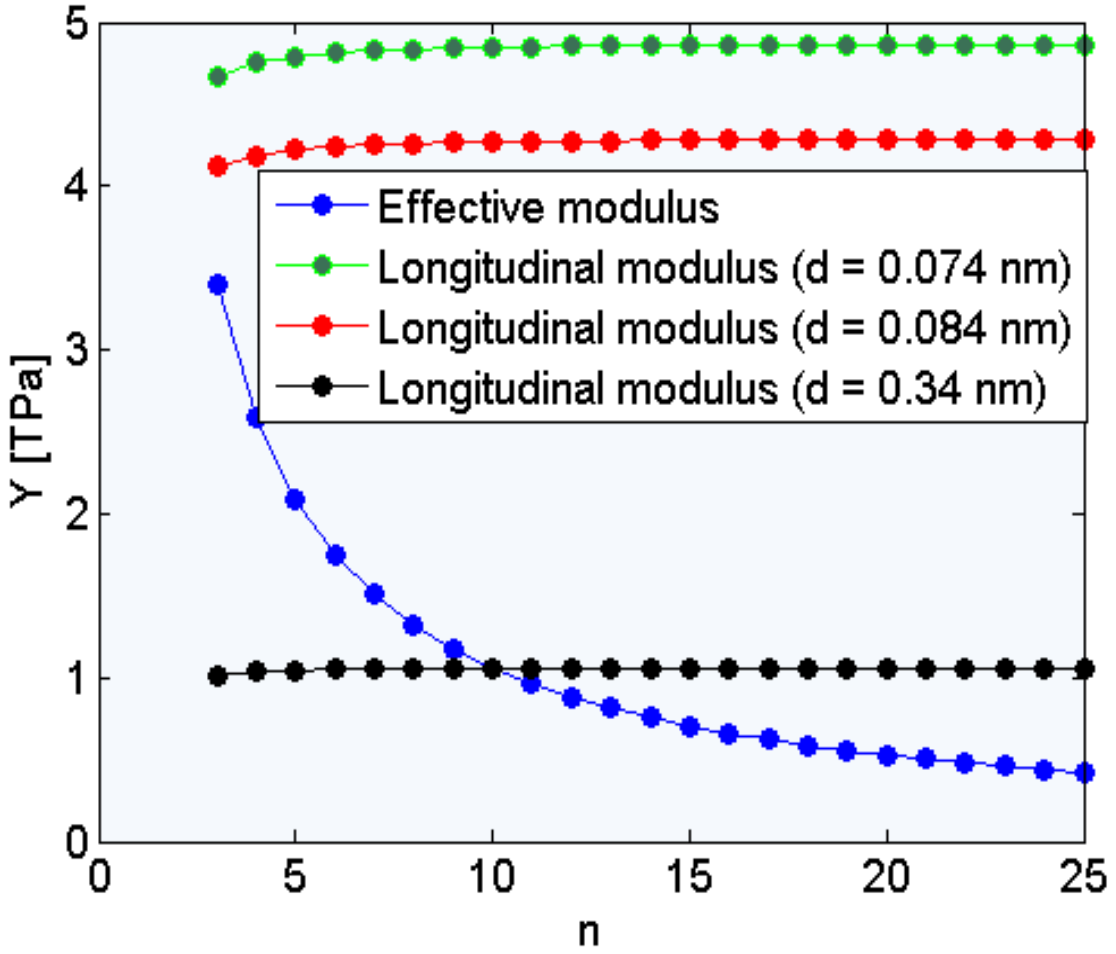
$$Y_{11} = \frac{F}{2\pi R d\, \varepsilon_{11}}$$

Surface



$$Y_{11}^{s} = \frac{F}{2\pi R\, \varepsilon_{11}}$$

Which Young's modulus?



Yakobson's paradox

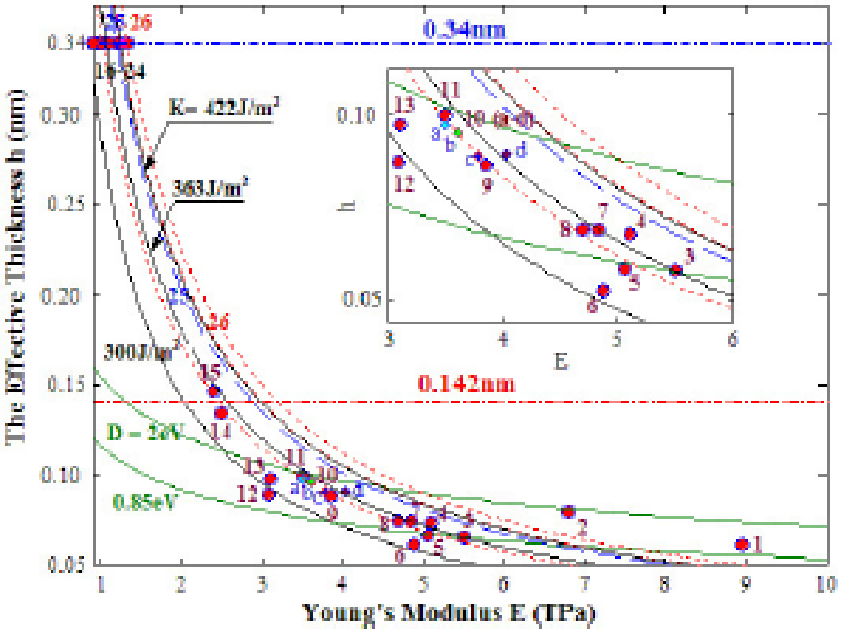


Figure 1. The effective thickness h, Young's modulus E, in-plane stiffness $K = \frac{Eh}{1-\nu^2} \approx Eh$ and the bending stiffness $D = \frac{Eh^3}{12(1-\nu^2)}$ obtained in the literature for SWCNTs, where ν is Poisson's ratio. Among the five solid lines two represent bending stiffness $D = \frac{Eh^3}{12(1-\nu^2)} \approx \frac{Eh^3}{12} = 0.85$ eV and 2 eV, respectively. The other three solid lines are associated with increasing in-plane stiffness $K = \frac{Eh}{1-\nu^2} \approx Eh = 300$, 360 and 422 J m^{-2}. Dots 10(a–d) are given by [9]. The models and sources of the dots in the figure are listed in table 1.

Authors	Method	Wall thickness (nm)	Young's modulus (TPa)
Lu[a]	Molecular dynamics	0.34	0.974
Hernández *et al.*[b]	Tight binding molecular dynamics	0.34	1.24
Odegard *et al.*[c]	Equivalent-continuum modeling	0.69	
Li and Chou[d]	Structural mechanics: stiffness matrix method	0.34	1.01
Jin and Yuan[e]	Molecular dynamics	0.34	1.238
Tserpes and Papanikos[f]	Structural mechanics: FE method	0.147	
Yakobson *et al.*[g]	Molecular dynamics	0.066	5.5
Zhou *et al.*[h]	Tight-binding model	0.074	5.1
Kudin *et al.*[i]	*Ab inito* computations	0.089	3.859
Tu and Ou-yang[j]	Local density approximation model	0.075	4.7
Vodenitcharova and Zhang[k]	Ring theory continuum mechanics	0.0617	4.88
Panatano *et al.*[l]	Continuum shell modeling	0.075	4.84
Goupalov[m]	Continuum model for long-wavelength phonons	0.087	
Wang *et al.*[n]	Ab *initio* calculation	0.0665	5.07

(Wang CY, Zhang LC, 2008. *Nanotechnology* **19**, 075705)
(Huang Y, Wu J, Hwang K C, 2006. *Phys. Rev. B* **74**, 245413)

Atomistic finite element method

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- Atomic bonds are represented by beam elements
- Beam properties are obtained by energy balance

$$U_{total} = U_r + U_\theta + U_\tau$$

$$U_r = \frac{1}{2} k_r (\Delta r)^2 \quad U_\theta = \frac{1}{2} k_\theta (\Delta\theta)^2 \quad U_\tau = \frac{1}{2} k_\tau (\Delta\phi)^2$$

$$U_{axial} = \frac{1}{2} K_{axial} (\Delta L)^2 = \frac{EA}{2L} (\Delta L)^2$$

$$U_{torsion} = \frac{1}{2} K_{torsion} (\Delta\beta)^2 = \frac{GJ}{2L} (\Delta\beta)$$

$$U_{bending} = \frac{1}{2} K_{bending} (2\alpha)^2 = \frac{EI}{2L} \frac{4+\Phi}{1+\Phi} (2\alpha)^2$$

Scarpa, F. and Adhikari, S., "A mechanical equivalence for the Poisson's ratio and thickness of C-C bonds in single wall carbon nanotubes", Journal of Physics D: Applied Physics, 41 (2008) 085306

Atomistic finite element method

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- All parameters of the beam can be obtained in closed-form:

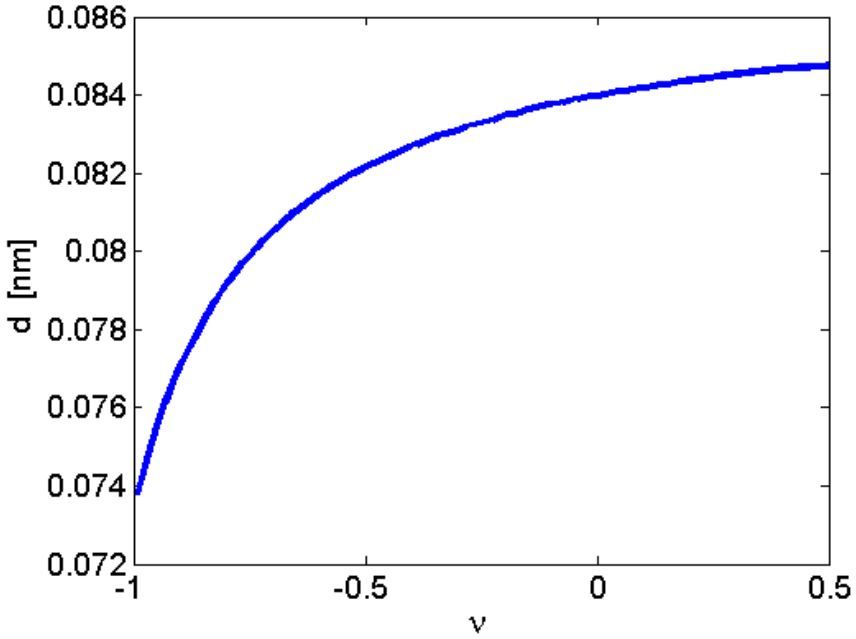
$$E = \frac{4k_r L}{\pi d^2}, \quad G = \frac{32k_\tau L}{\pi d^4}$$

$$\Phi = \frac{3k_r d^4\left(6+12\nu+6\nu^2\right)}{32k_\tau L^2\left(7+12\nu+4\nu^2\right)}$$

$$k_\theta = \frac{k_r d^2}{16}\frac{4\mathrm{A}+\mathrm{B}}{\mathrm{A}+\mathrm{B}} \qquad d < 2\sqrt{6}\sqrt{\frac{k_\tau}{k_r}}$$

$$\mathrm{A} = 112L^2k_\tau + 192L^2k_\tau\nu + 64L^2k_\tau\nu^2$$

$$\mathrm{B} = 9k_r d^4 + 18k_r d^4\nu + 9k_r d^4\nu^2$$



Scarpa, F. and Adhikari, S., "A mechanical equivalence for the Poisson's ratio and thickness of C-C bonds in single wall carbon nanotubes", Journal of Physics D: Applied Physics, 41 (2008) 085306

Atomistic Structural Mechanics

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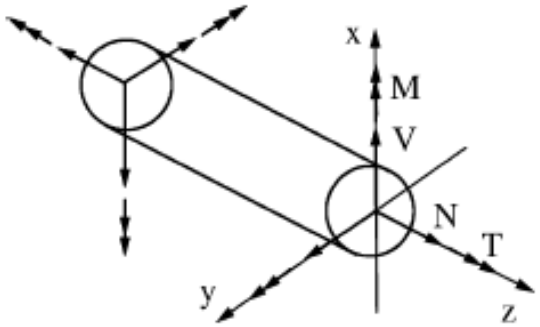
For space frames:



$$[\mathbf{K}]\{\mathbf{u}\} = \{\mathbf{f}\}$$

[K] → stiffness matrix
{u} → nodal displacement vector
{f} → nodal force vector

$$\mathbf{u} = [u_{xi}, u_{yi}, u_{zi}, \theta_{xi}, \theta_{yi}, \theta_{zi}, u_{xj}, u_{yj}, u_{zj}, \theta_{xj}, \theta_{yj}, \theta_{zj}]^{\mathrm{T}}$$

$$\mathbf{f} = [f_{xi}, f_{yi}, f_{zi}, m_{xi}, m_{yi}, m_{zi}, f_{xj}, f_{yj}, f_{zj}, m_{xj}, m_{yj}, m_{zj}]^{\mathrm{T}}$$

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{ii} & \mathbf{K}_{ij} \\ \mathbf{K}_{ij}^{\mathrm{T}} & \mathbf{K}_{jj} \end{bmatrix};$$

$$\mathbf{K}_{ii} = \begin{bmatrix} EA/L & 0 & 0 & 0 & 0 & 0 \\ 0 & 12EI_x/L^3 & 0 & 0 & 0 & 6EI_x/L^2 \\ 0 & 0 & 12EI_y/L^3 & 0 & -6EI_y/L^2 & 0 \\ 0 & 0 & 0 & GJ/L & 0 & 0 \\ 0 & 0 & -6EI_y/L^2 & 0 & 4EI_y/L & 0 \\ 0 & 6EI_x/L^2 & 0 & 0 & 0 & 4EI_x/L \end{bmatrix}$$

$$\mathbf{K}_{ij} = \begin{bmatrix} -EA/L & 0 & 0 & 0 & 0 & 0 \\ 0 & -12EI_x/L^3 & 0 & 0 & 0 & 6EI_x/L^2 \\ 0 & 0 & -12EI_y/L^3 & 0 & -6EI_y/L^2 & 0 \\ 0 & 0 & 0 & -GJ/L & 0 & 0 \\ 0 & 0 & 6EI_y/L^2 & 0 & 2EI_y/L & 0 \\ 0 & -6EI_x/L^2 & 0 & 0 & 0 & 2EI_x/L \end{bmatrix}$$

(Weaver Jr., W. and Gere, J.M., 1990. Matrix Analysis of Framed Structures. (third ed.),, Van Nostrand Reinhold, New York)

$$\mathbf{K}_{jj} = \begin{bmatrix} EA/L & 0 & 0 & 0 & 0 & 0 \\ 0 & 12EI_x/L^3 & 0 & 0 & 0 & -6EI_x/L^2 \\ 0 & 0 & 12EI_y/L^3 & 0 & 6EI_y/L^2 & 0 \\ 0 & 0 & 0 & GJ/L & 0 & 0 \\ 0 & 0 & 6EI_y/L^2 & 0 & 4EI_y/L & 0 \\ 0 & -6EI_x/L^2 & 0 & 0 & 0 & 4EI_x/L \end{bmatrix}.$$

Atomistic FE – bending deformation of SWCNTs

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Table 2. Bending modulus, thickness and Poisson's ratio for zigzag and armchair SWCNTs. Aspect ratio (tube length/tube diameter) is 20.

Radius (nm)	ν	d (nm)	E (TPa)	G (TPa)	Y_f (TPa)	ε_f
Zigzag						
0.378	0.0344	0.112	16.79	2.54	0.88	3.51×10^{-5}
0.777	0.0344	0.0853	16.77	7.61	1.078	1.84×10^{-5}
0.935	0.0344	0.0842	16.65	8.02	1.079	1.56×10^{-5}
1.1708	0.0344	0.0837	16.81	8.17	1.083	1.24×10^{-5}
Armchair						
0.246	0.0344	0.0773	19.7	11.25	2.7	2.51×10^{-5}
0.585	0.0344	0.0911	14.22	5.85	1.26	1.935×10^{-5}
0.883	0.0344	0.0841	16.65	8.02	1.15	1.54×10^{-5}
1.312	0.0344	0.0836	16.89	8.25	1.075	1.12×10^{-5}

(F Scarpa and S Adhikari, 2008. *J. Phys. D: App. Phys.*, 41, 085306)

Atomistic FE – bending deformation of SWCNTs bundles

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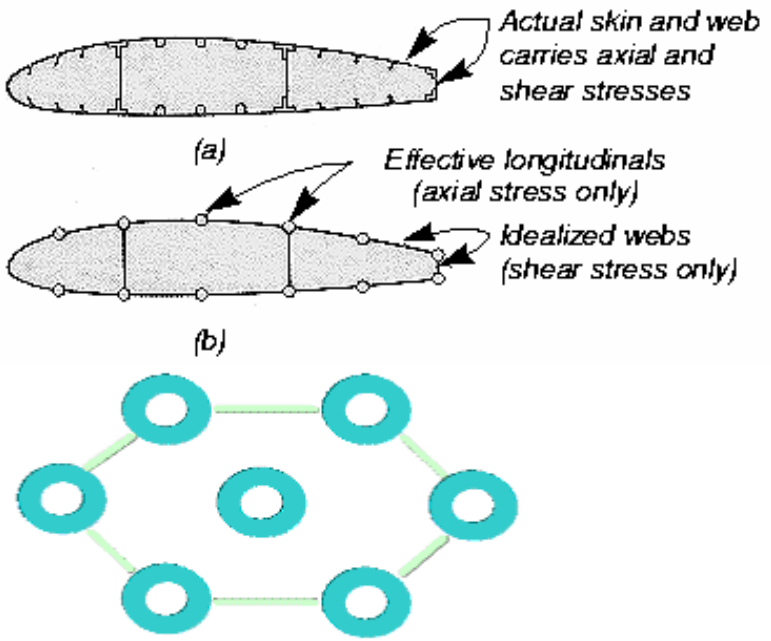
Similarity between hexagonal SWCNT packing bundle and structural idealization for wing boxes



Polar moment of inertia for each CNT:

$$I_c = \frac{\pi}{4}\left[\left(R+\frac{d}{2}\right)^4 - \left(R-\frac{d}{2}\right)^4\right] \qquad (1)$$

Polar moment of inertia for hexagonal packing:

$$I_{hex} = 4\left(I_c + \left(3\frac{l_0^2}{2}\right)^2 A_c\right) + 3I_c \qquad (2)$$

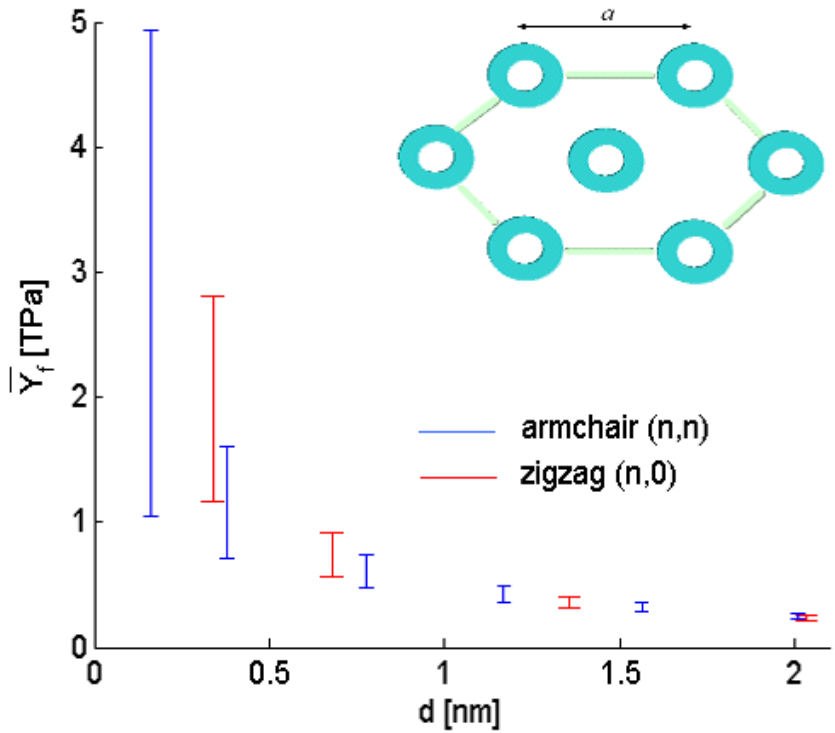
Flexural modulus of the nanbundle:

$$\bar{Y}_f = Y\frac{I_{hex}}{I_h} \qquad (3)$$

$$\bar{Y}_f = Y\left[\frac{20\sqrt{3}\pi R^3 d}{3(2R+t_{VdW})^4} + \frac{7\sqrt{3}\pi R d^3}{33(2R+t_{VdW})^4} + \frac{64\sqrt{3}\pi R^2 t_{VdW} d}{11(2R+t_{VdW})^4} + \frac{16\sqrt{3}\pi R t_{VdW}^2 d}{11(2R+t_{VdW})^4}\right]$$

(F Scarpa and S Adhikari, 2008. *J. Phys. D: App. Phys.*, 41, 085306)

Atomistic FE – bending deformation of SWCNTs bundles



(F Scarpa and S Adhikari, 2008. *J. Phys. D: App. Phys.*, 41, 085306)

Buckling of Carbon nanotubes

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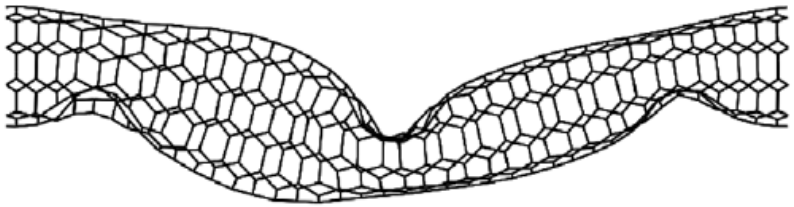
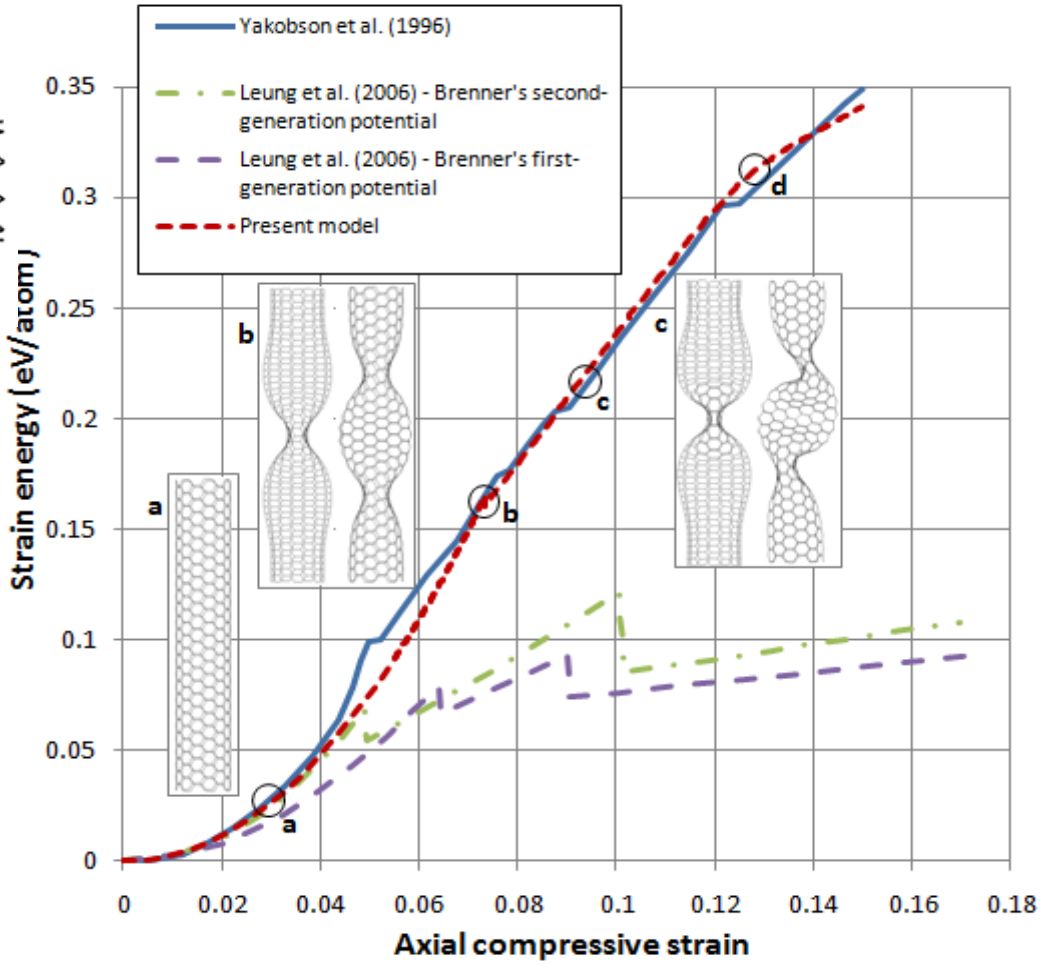


(a) Molecular dynamics

(b) Hyperplastic atomistic FE (Ogden strain energy density function)



Comparison of buckling mechanisms in a (5,5) SWCNT with 5.0 nm length.

Flores, E. I. S., Adhikari, S., Friswell, M. I. and Scarpa, F., "Hyperelastic axial buckling of single wall carbon nanotubes", Physica E: Low-dimensional Systems and Nanostructures, 44[2] (2011), pp. 525-529.

Carbon nanotubes with defects

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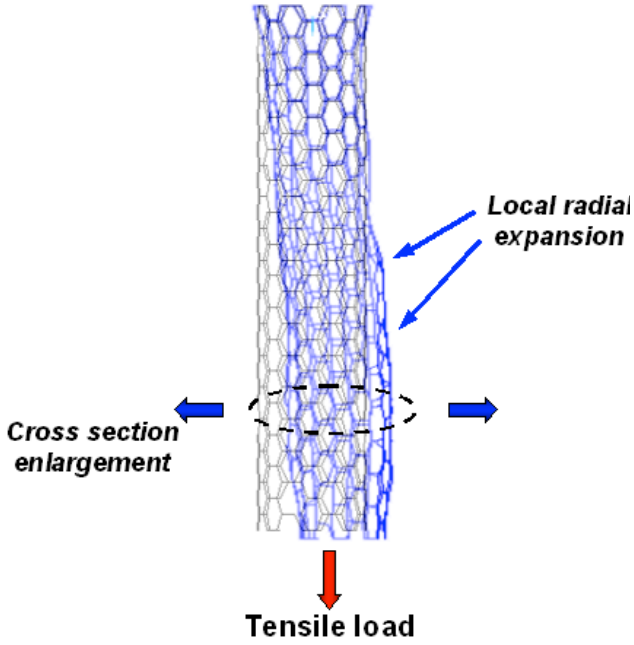
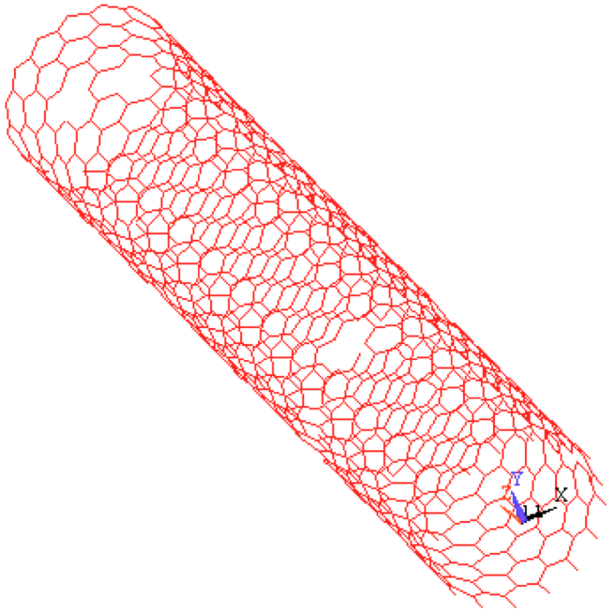
- We are interested in the changes in the mechanical properties





Scarpa, F., Adhikari, S. and Wang, C. Y., "Mechanical properties of non reconstructed defective single wall carbon nanotubes", *Journal of Physics D: Applied Physics*, 42 (2009) 142002

Carbon nanotubes with defects

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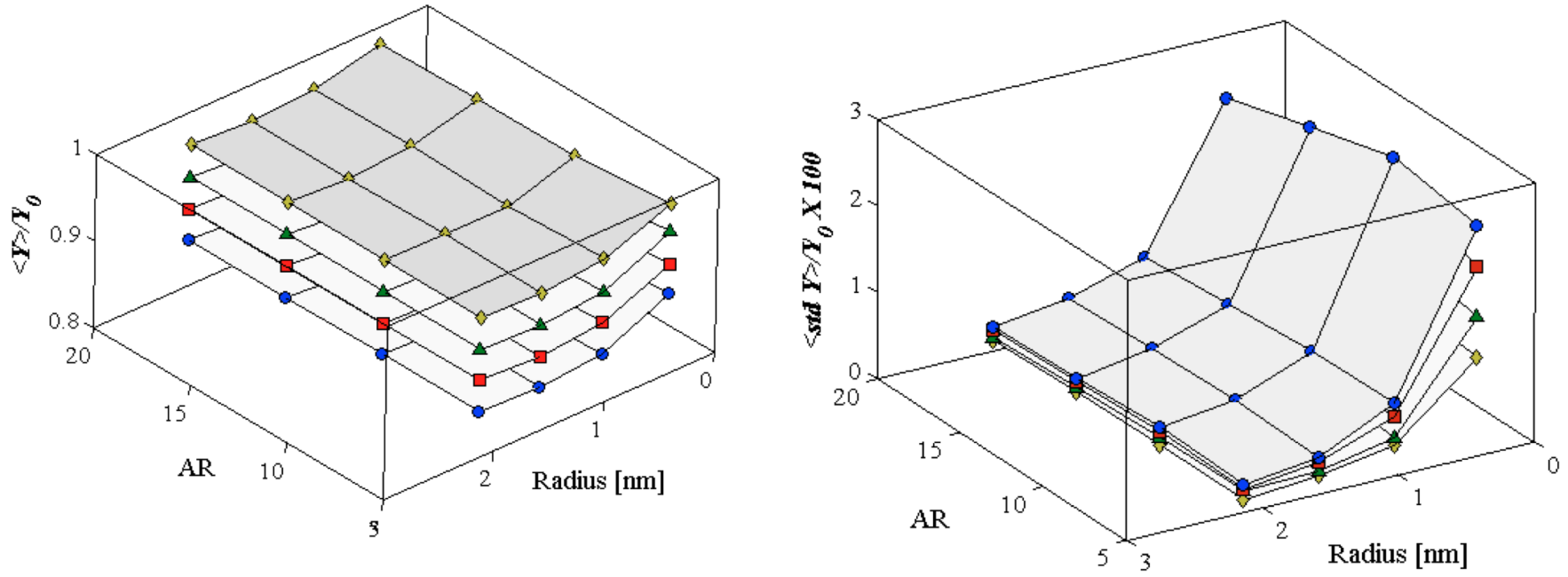

(a) Ratio between mean of axial Young's modulus and pristine stiffness and (b) between standard deviation of the Young's modulus against pristine Young's modulus for armchair (n,n). Pristine Young's modulus Y_0: 2.9, 1.36, 0.91, 0.67 TPa for a thickness d = 0.084 nm. ● = 2 % NRV; ■ = 1.5 % NRV; ▲= 1 % NRV; ♦= 0.5 % NRV

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Fullerene

Vibration spectra of fullerene family

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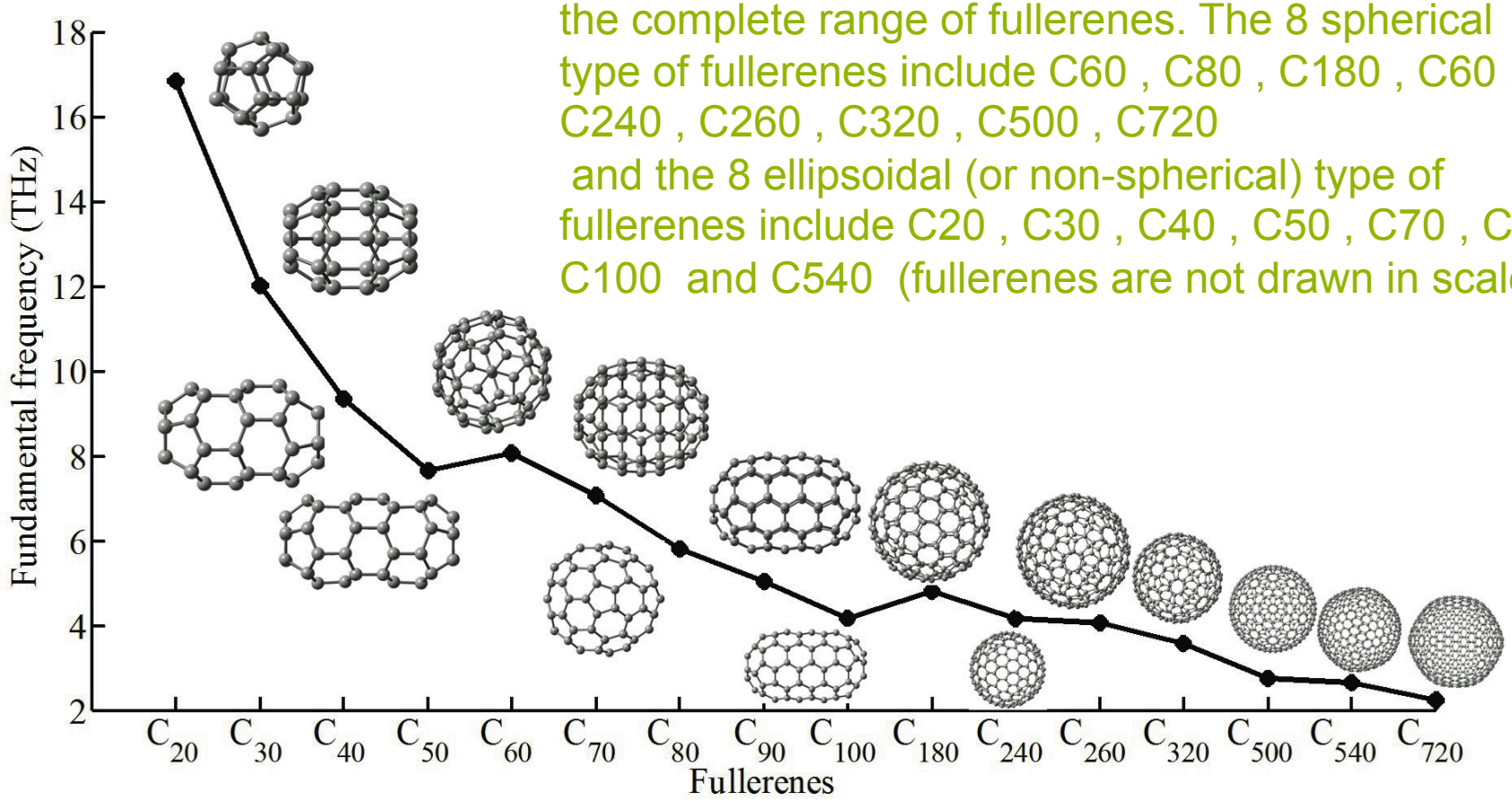
The variation of the first natural frequency across the the complete range of fullerenes. The 8 spherical type of fullerenes include C60 , C80 , C180 , C60 , C240 , C260 , C320 , C500 , C720
and the 8 ellipsoidal (or non-spherical) type of fullerenes include C20 , C30 , C40 , C50 , C70 , C90 , C100 and C540 (fullerenes are not drawn in scale).



Adhikari, S. and Chowdhury, R., "Vibration spectra of fullerene family", Physics Letters A, 375[22] (2011), pp. 1276-1280.

Thin shell theory

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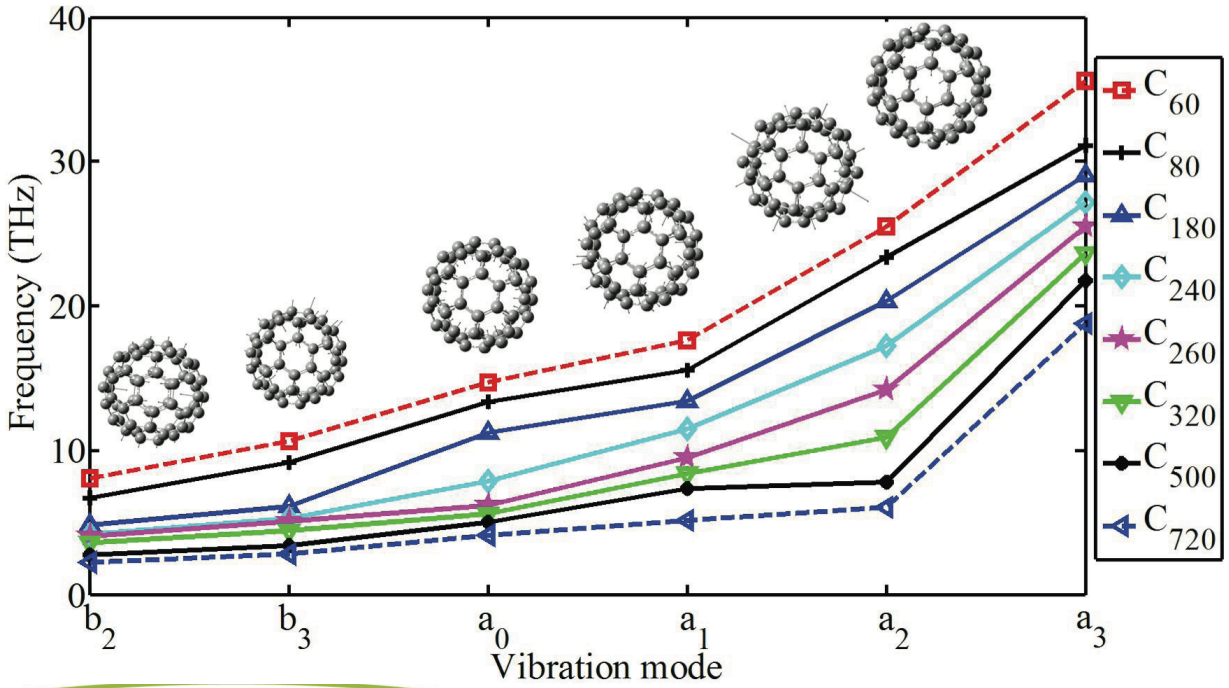
The natural frequencies of spherical fullerenes can be given by

$$\omega_{n1,2}^2 = \frac{E}{R^2\rho}\Omega_{n1,2}^2 \qquad \Omega_{n1,2}^2 = \frac{1}{2(1-\mu^2)}\{n(n+1)+1+3\mu \pm \sqrt{[n(n+1)+1+3\mu]^2 - 4(1-\mu^2)[n(n+1)-2]}\}$$



Atomistic Simulation vs Shell theory

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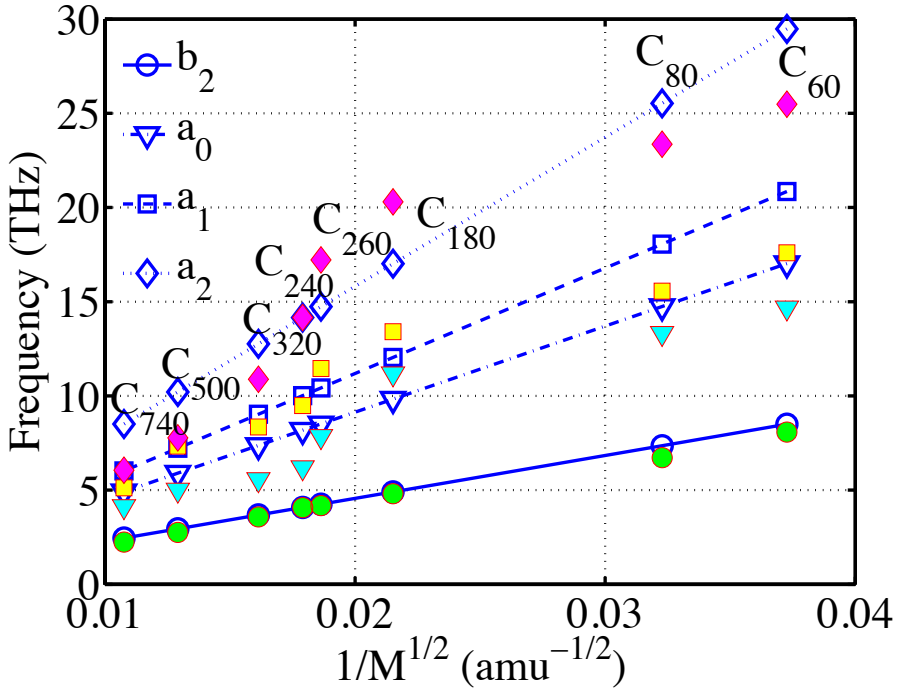
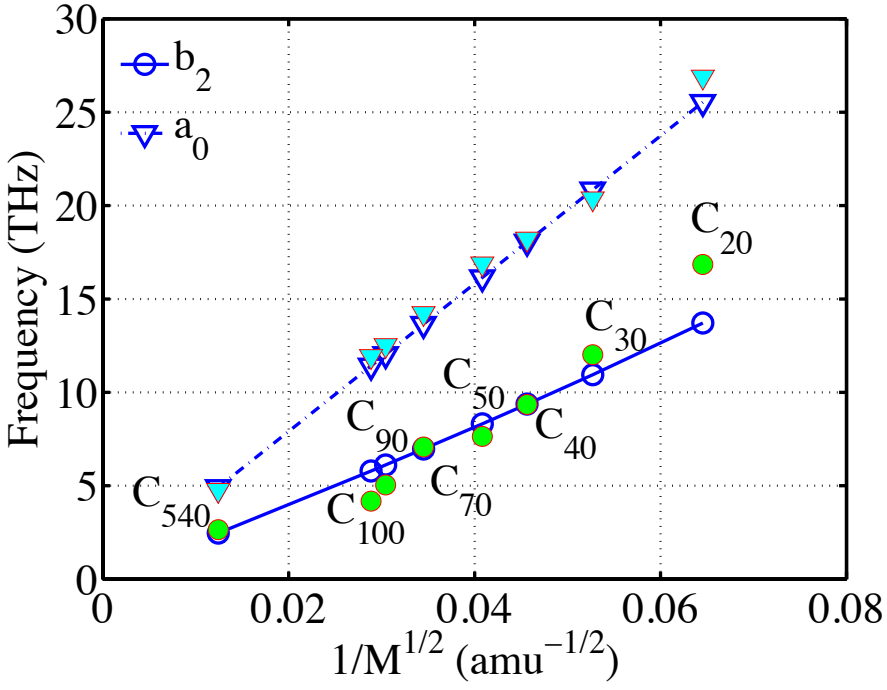


Spherical type fullerenes



Ellipsoidal type fullerenes

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Graphene

College of Engineering

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Atomistic FE – in-plane SLGS

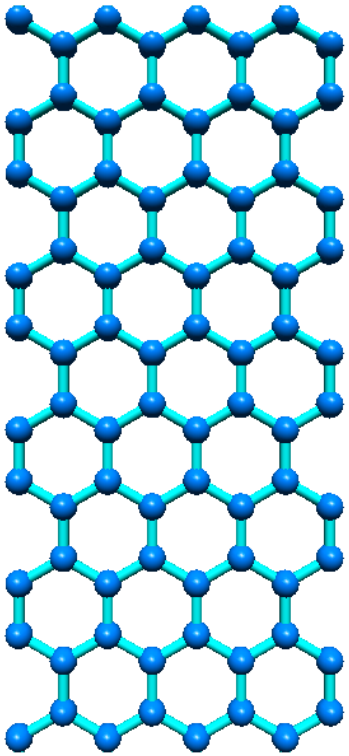

Table 5. Graphene data from literature and present work.

Author	Y_1 (TPa nm)	Y_2 (TPa nm)	ν_{12}	ν_{21}	d (Å)
Tu and Ou-Yang [45]		0.348		0.34	0.74
Zhou *et al* [46]		0.377		0.24	0.74
Yakobson *et al* [47]		0.363		0.19	0.66
Caillerie *et al* [25]		0.277		0.26	N/A
Brenner *et al* [15]		0.235		0.41	0.62
Huang *et al* [17]		0.243		0.397	0.57
Kudin *et al* [13]		0.345		0.149	0.84
Chang and Gao [50]		0.360		0.16	3.4
Cho *et al* [48]		0.386		0.195	3.35
Sakhaee-Pour [34]		0.337–0.354		1.129–1.441	3.4
Hemmasizadeh *et al* [24]		0.124		0.19	1.317
Blakslee *et al* [58]		0.342		0.16	3.35
Lee *et al* [60]		0.335		N/A	3.35
Reddy *et al* [23]	0.228	0.277	0.43	0.52	3.4
Present FE honeycomb (AMBER)	0.517	0.342	0.523	0.509	0.82–0.99
Present FE honeycomb (Morse)	0.546	0.408	0.551	0.577	0.86–0.87
Present EHM stretching–hinging (AMBER)		0.297		0.211	0.84
Present EHM stretching–hinging (Morse)		0.384		0.213	0.74
Present EHM stretching–hinging-shear (AMBER)		0.144		0.617	0.84
Present EHM stretching–hinging-shear (Morse)		0.169		0.653	0.74
Present EHM-all deformation mechanisms (AMBER)		0.064		0.830	0.84
Present EHM-all deformation mechanisms (Morse)		0.074		0.848	0.74

(F Scarpa, S Adhikari, A S Phani, 2009. *Nanotechnology* 20, 065709)

Atomistic FE vs Continuum – SLGS

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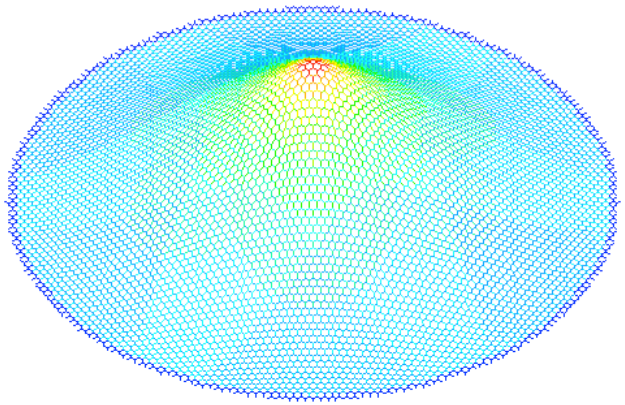
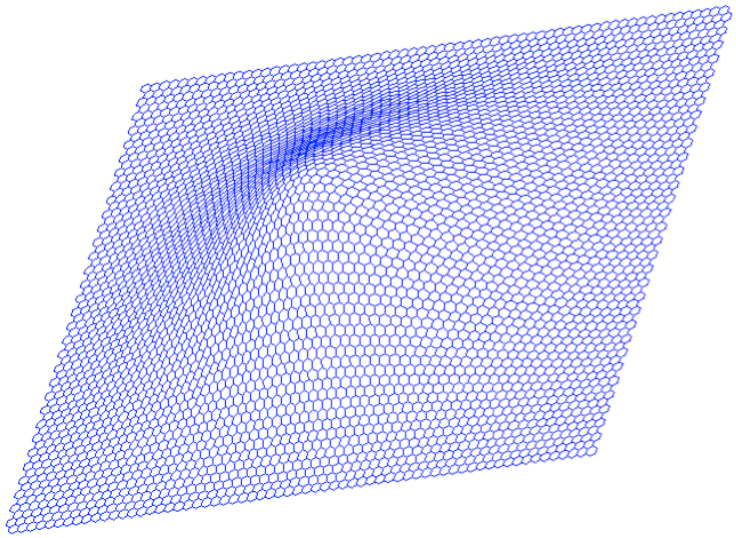


Circular SLGS (R = 9: 5 nm) under central loading. Distribution of equivalent membrane stresses.



Deformation of rectangular SLGS (15.1 x 13.03 nm^2) under central loading.

Scarpa, F., Adhikari, S., Gil, A. J. and Remillat, C., "The bending of single layer graphene sheets: Lattice versus continuum approach", Nanotechnology, 21[12] (2010), pp. 125702:1-9.

Axtomistic FE vs Continuum – SLGS

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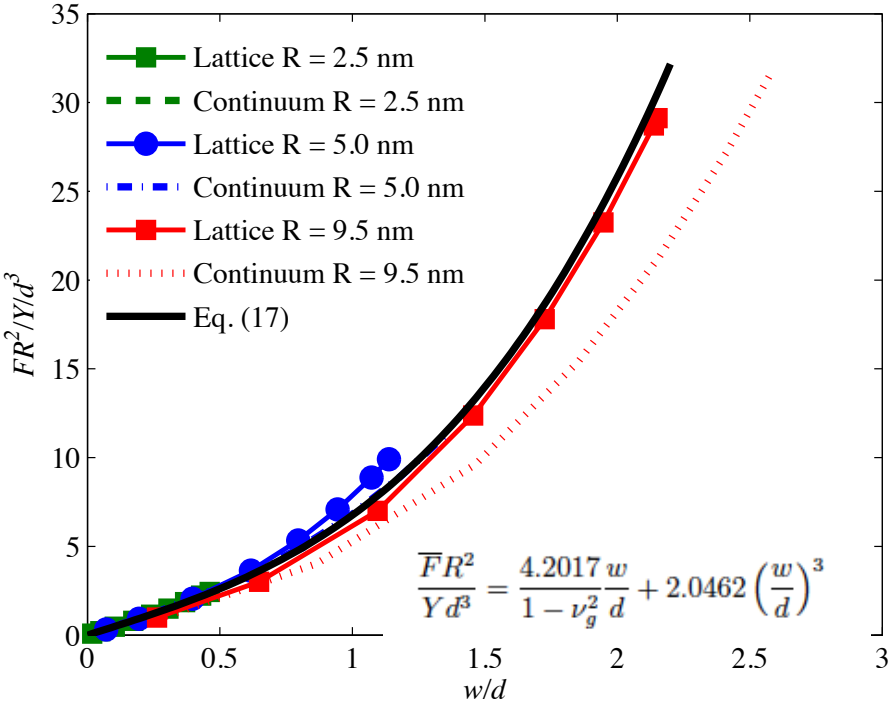
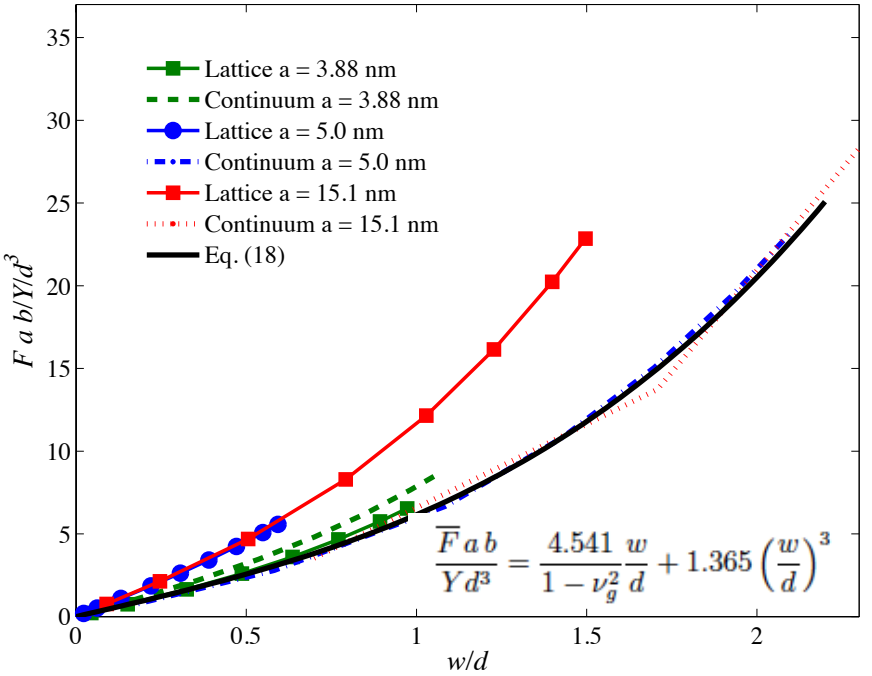
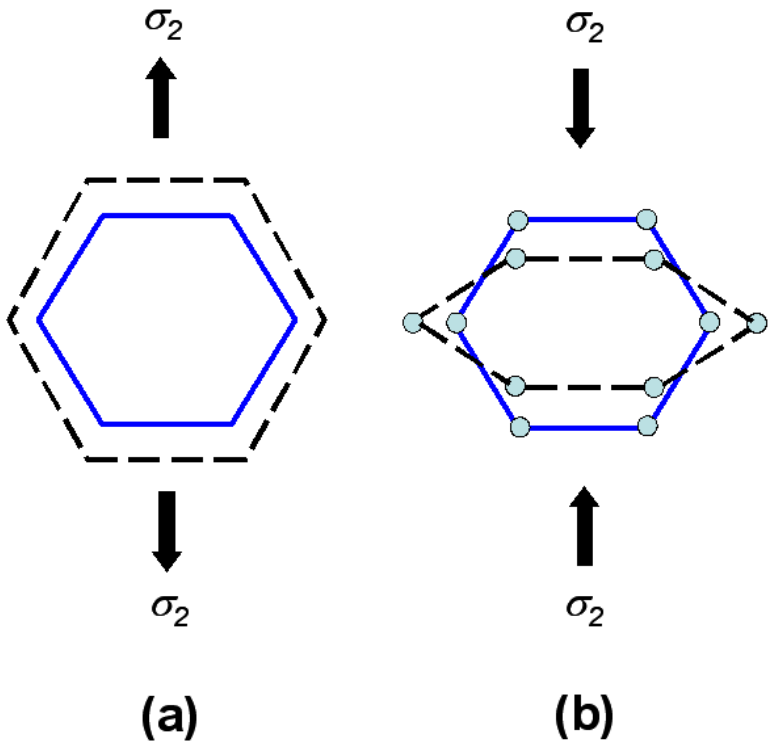




Comparison of the nondimensional force vs. nondimensional out-of-plane displacement for circular and rectangular lattice and continuum SLGS.

Analytical approach for SLGS – honeycomb structure



C-C bonds deform under stretching and hinging

$$K_h = \frac{8k_\tau}{d^2}$$ Hinging constant related to thickness d

Applying averaging of stretching and hinging deformation over unit cell:

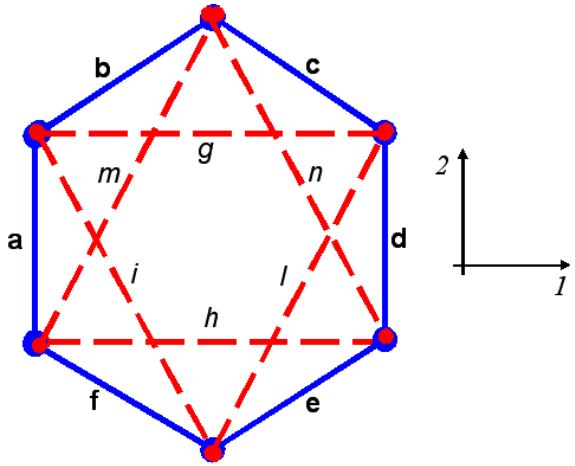
$$E_1 = \frac{4\sqrt{3}k_r K_h}{3d\left(k_r + 3K_h\right)} \qquad E_2 = \frac{4\sqrt{3}k_r K_h}{3d\left(k_r + 3K_h\right)}$$

$$\nu_{21} = \nu_{12} = \frac{1 - K_h/k_r}{1 + 3K_h/k_r} \qquad G_{12} = \frac{\sqrt{3}K_h k_r}{3d\left(k_r + K_h\right)}$$

- Isotropic for "infinite" graphene sheet
- Orthotropic for finite size graphene and considering edge effects

F Scarpa, S Adhikari, A S Phani, 2009. *Nanotechnology* **20,** 065709

Analytical approach for SLGS – honeycomb structure



Unit cell made by rods withstanding axial and bending deformation

$$Y_{\mathbf{a-f}} = \frac{4Lk_r}{\pi d_s^2}$$ Equivalent Young's modulus for axial members

$$Y_{g-n} = \frac{16k_\theta}{\pi L d_b^2}$$ Equivalent Young's modulus for axial members

A **Rigidity** matrix is obtained using a lattice continuum modelling of space frames → equivalence with plane stress formulation for a plane sheet:

$$E = \frac{1}{d_{\max}} \frac{4\sqrt{3}}{9L^2}\left(k_r L^2 + 12k_\theta\right) \quad \nu = \frac{1}{3}$$

F Scarpa, S Adhikari, A S Phani, 2009. *Nanotechnology* **20,** 065709
(L Kollár and I Hegedús. Analysis and design of space frames by the Continuum Method. Developments in Civil Engineering, 10. Elsevier, Amsterdam, 1985)

Atomistic FE – Bilayer Graphene

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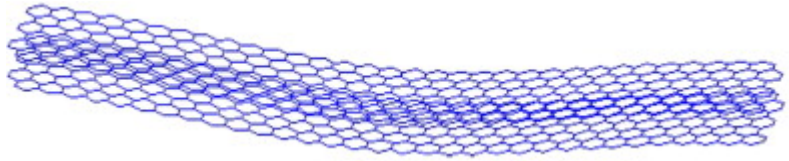

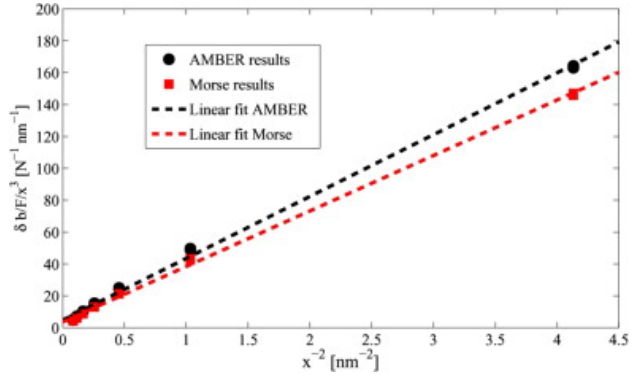

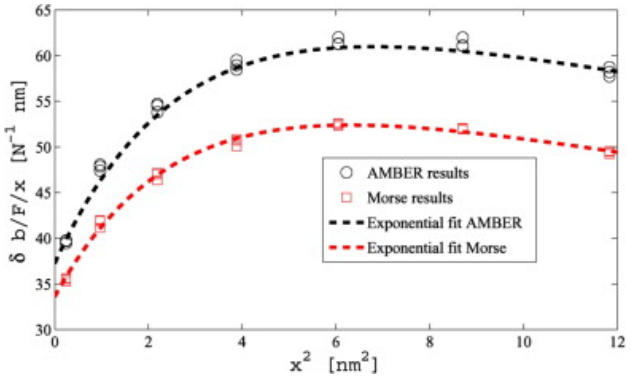

- Equivalent to structural "sandwich" beams
- C-C bonds in graphene layers represented with classical equivalent beam models
- "Core" represented by Lennard-Jones potential interactions:

$$F_{ij} = -12\epsilon\left[\left(\frac{r_{min}}{y}\right)^{13} - \left(\frac{r_{min}}{y}\right)^{7}\right]$$

r_{min} = 0.383 nm
ε = 2.39 meV

Dimensions [nm × nm]	E_f [TPa]	G_{LJ} [TPa]	Force model
7.99 × 0.92	0.371	0.0142	AMBER
7.99 × 1.35	0.379	0.0143	AMBER
7.99 × 2.63	0.371	0.0143	AMBER
7.99 × 0.92	0.531	0.0161	Morse
7.99 × 1.35	0.535	0.0161	Morse
7.99 × 2.63	0.520	0.0160	Morse

E_f =0.5 TPa (I.W. Frank, D.M. Tanenbaum, A.M. van der Zande, P.L. McEuen, J. Vac. Sci. Technol. B 25 (2007) 2558)

Scarpa, F., Adhikari, S. and Chowdhury, R., "The transverse elasticity of bilayer graphene", Physics Letters A, 374[19-20] (2010), pp. 2053-2057.

Mechanical vibration of SLGS

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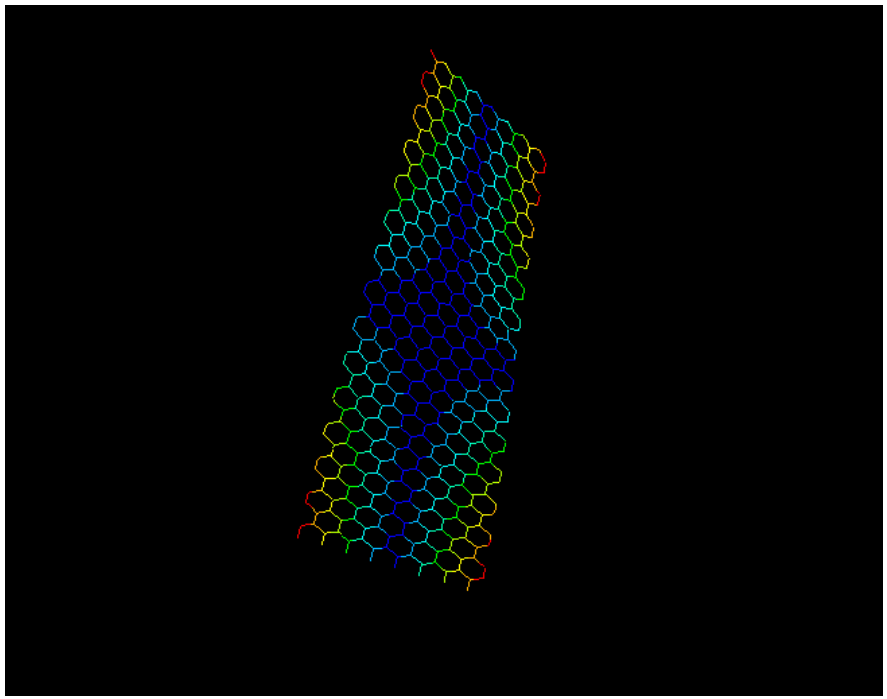
Lumped mass matrix:

$$[\mathbf{M}]_{\mathbf{e}} = diag\left[\ \frac{m_e}{3} \quad \frac{m_e}{3} \quad \frac{m_e}{3} \quad 0 \quad 0 \quad 0\ \right]$$

Minimisation of the Hamiltonian for the ith mode:

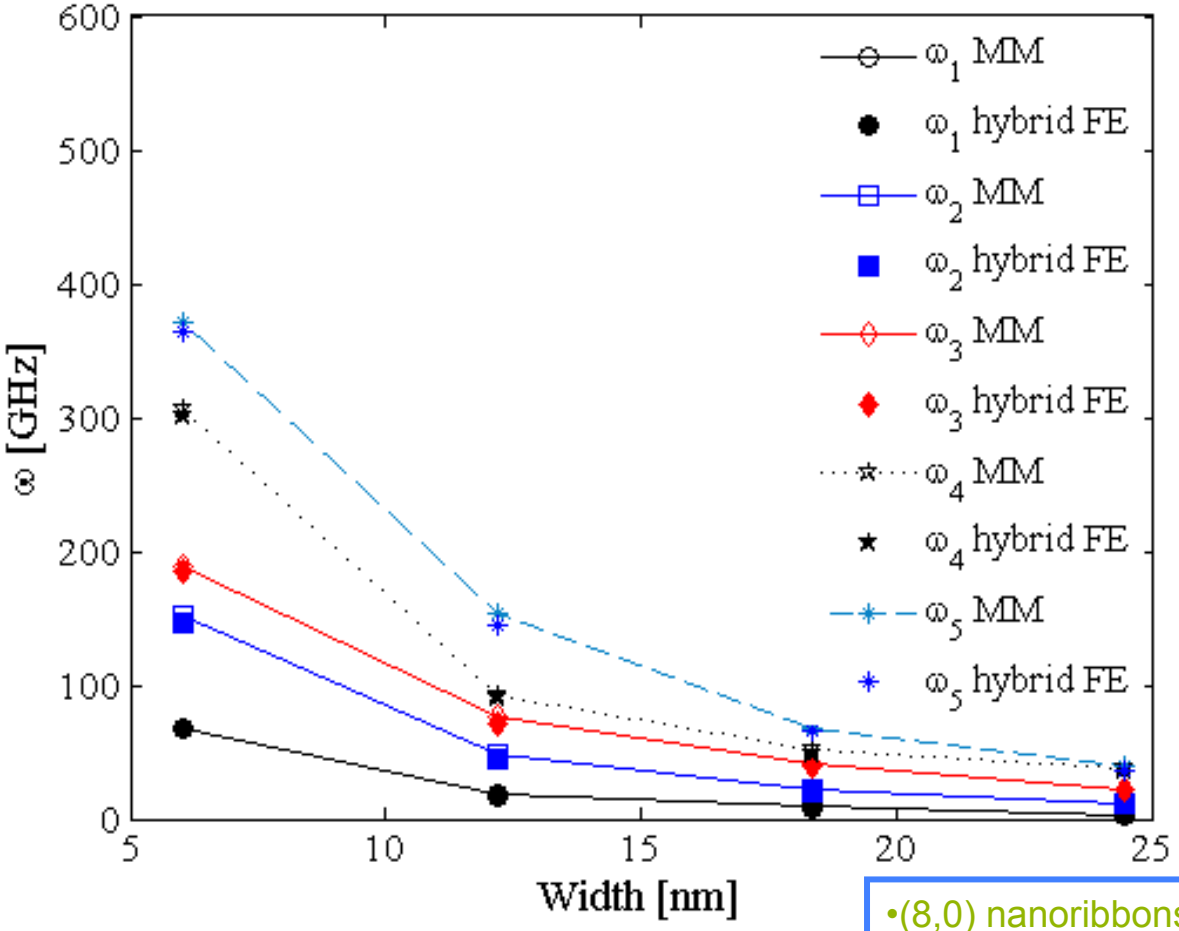
$$H_i = \frac{1}{2}\{\mathbf{\Phi}\}_i^T [\mathbf{M}] \{\mathbf{\Phi}\}_i \times \omega_i^2 + \frac{1}{2}\{\Phi\}_i^T [\mathbf{K}] \{\Phi\}_i = \omega_i^2$$

Comparison against Molecular Mechanics model based on the eigenvalue analysis of the system Hessian matrix



Scarpa, F., Chowdhury, R., Kam, K., Adhikari, S. and Ruzzene, M., "Wave propagation in graphene nanoribbons", Nanoscale Research Letters, 6 (2011), pp. 430:1-10.
Chowdhury, R., Adhikari, S., Scarpa, F. and Friswell, M. I., "Transverse vibration of single layer graphene sheets", Journal of Physics D: Applied Physics, 44[20] (2011), pp. 205401:1-11.

Mechanical vibration of SLGS



- (8,0) nanoribbons with different lengths
- Errors between 2 and 3 %
- Average thickness d = 0.077 nm

Graphene composites

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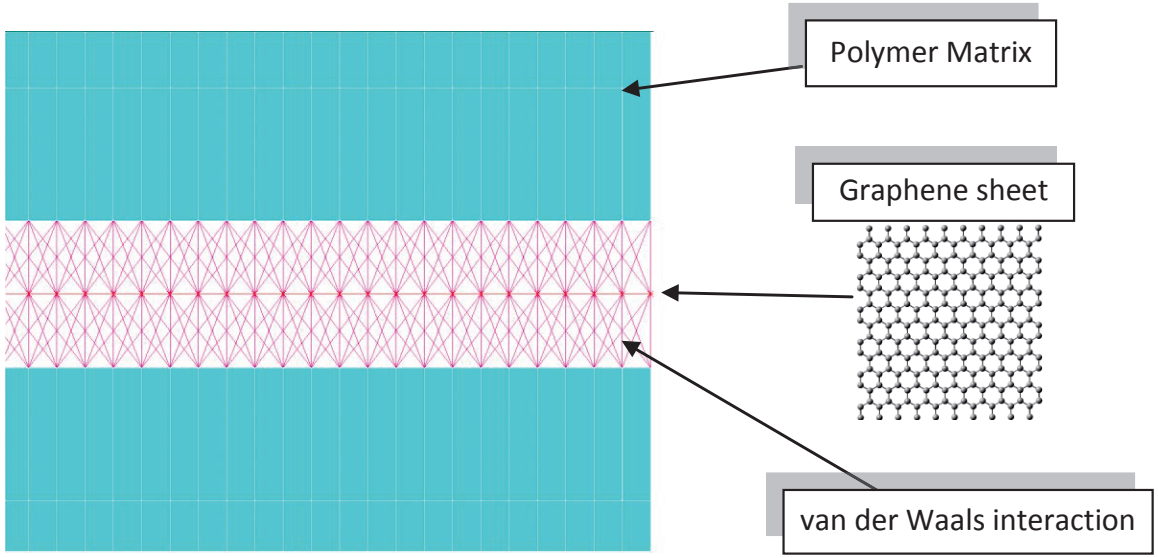

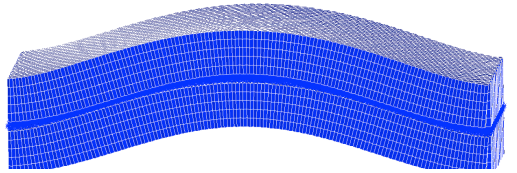

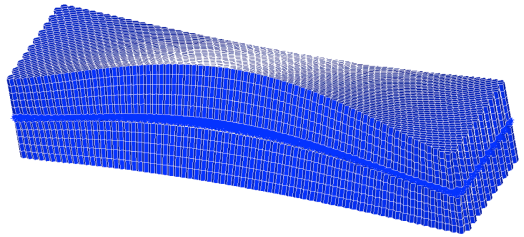

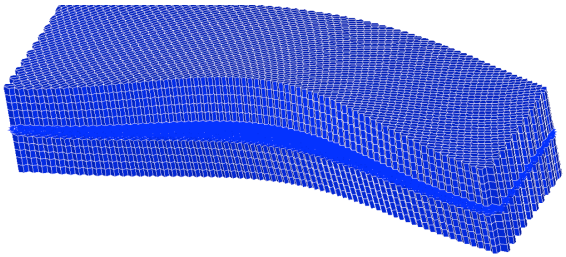

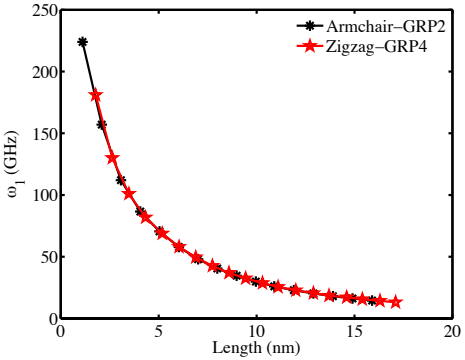

Chandra, Y., Chowdhury, R., Scarpa, F., Adhikari, S. and Seinz, J., "Multiscale modeling on dynamic behaviour of graphene based composites", Materials Science and Engineering B, in press.

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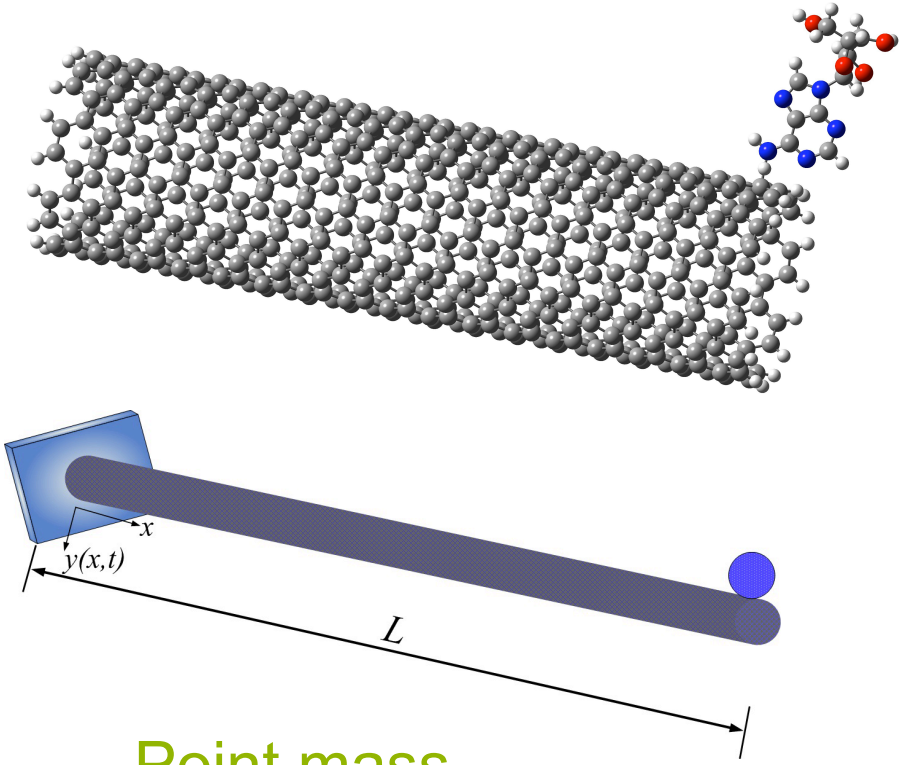
Nanobio Sensors

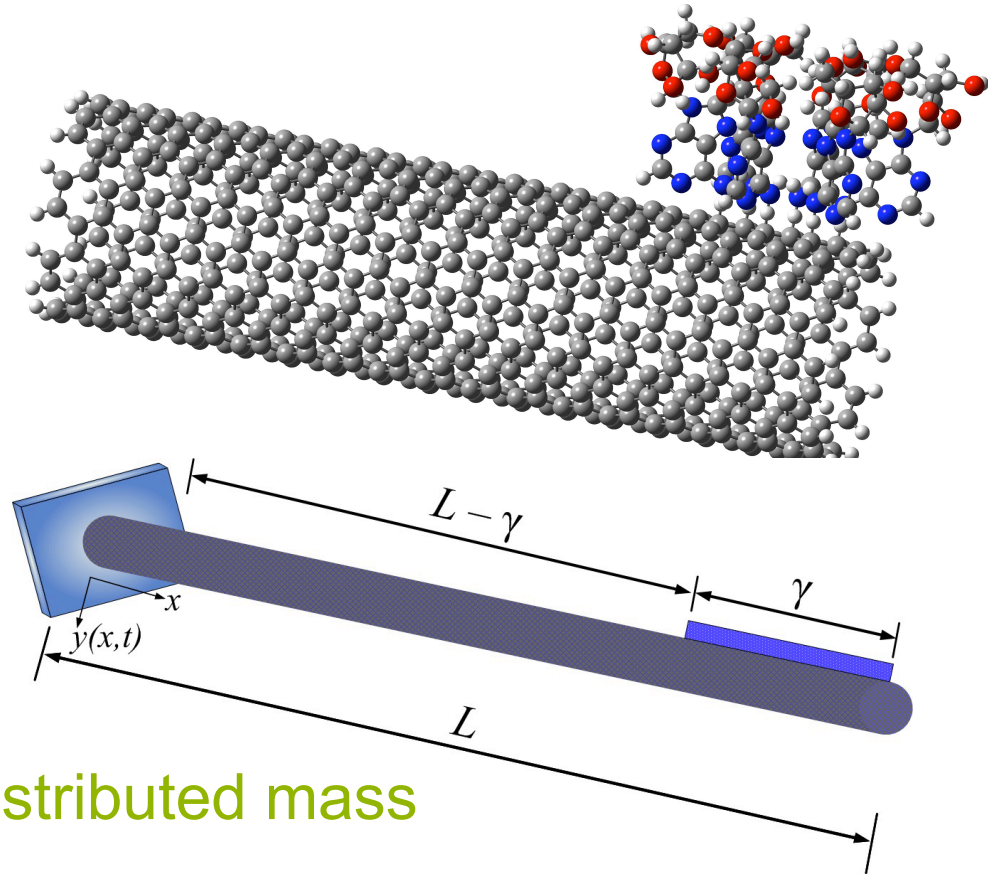
Vibration based mass sensor: CNT

Swansea University
Prifysgol Abertawe



Point mass

Chowdhury, R., Adhikari, S. and Mitchell, J., "Vibrating carbon nanotube based bio-sensors", Physica E: Low-dimensional Systems and Nanostructures, 42[2] (2009), pp. 104-109.



Distributed mass

Adhikari, S. and Chowdhury, R., "The calibration of carbon nanotube based bio-nano sensors", *Journal of Applied Physics*, 107[12] (2010), pp. 124322:1-8

Vibration based mass sensor: CNT

Swansea University
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The equation of motion of free-vibration: $$EI\frac{\partial^4 y(x,t)}{\partial x^4} + \rho A\frac{\partial^2 y(x,t)}{\partial t^2} = 0$$

The resonance frequencies: $$f_j = \frac{\lambda_j^2}{2\pi}\sqrt{\frac{EI}{\rho A L^4}} \qquad \cos\lambda\cosh\lambda + 1 = 0$$

The Mode shapes: $$Y_j(\xi) = (\cosh\lambda_j\xi - \cos\lambda_j\xi) - \left(\frac{\sinh\lambda_j - \sin\lambda_j}{\cosh\lambda_j + \cos\lambda_j}\right)(\sinh\lambda_j\xi - \sin\lambda_j\xi)$$

where

$$\xi = \frac{x}{L}$$

We use energy principles to obtain the frequency shift due to the added mass.

Vibration based mass sensor: CNT

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Natural frequency with the added mass:

$$f_n = \frac{1}{2\pi}\sqrt{\frac{k_{eq}}{m_{eq}}} = \frac{\beta}{2\pi}\frac{c_k}{\sqrt{1+c_m\Delta M}}$$

where

$$\beta = \sqrt{\frac{EI}{\rho A L^4}}$$

the stiffness calibration constant

$$c_k = \sqrt{\frac{I_3}{I_1}}$$

and the mass calibration constant

$$c_m = \frac{I_2}{I_1}$$

Identification of the added mass

$$f_n = \frac{f_{0_n}}{\sqrt{1+c_m\Delta M}} \tag{22}$$

The frequency-shift can be expressed using Eq. (22) as

$$\Delta f = f_{0_n} - f_n = f_{0_n} - \frac{f_{0_n}}{\sqrt{1+c_m\Delta M}} \tag{23}$$

From this we obtain

$$\frac{\Delta f}{f_{0_n}} = 1 - \frac{1}{\sqrt{1+c_m\Delta M}} \tag{24}$$

Rearranging gives the expression

$$\Delta M = \frac{1}{c_m\left(1-\frac{\Delta f}{f_{0_n}}\right)^2} - \frac{1}{c_m} \tag{25}$$

Vibration based mass sensor: CNT

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Mass of a nano object can be detected from the frequency shift Δf

$$M = \frac{\rho AL}{c_m}\frac{(c_k^2\beta^2)}{(c_k\beta - 2\pi\Delta f)^2} - \frac{\rho AL}{c_m}$$

$$I_1 = \int_0^1 Y_j^2(\xi)\mathrm{d}\xi = 1.0$$

$$I_2 = \frac{1}{\gamma}\int_{\xi=1-\gamma}^1 Y_j^2(\xi)\mathrm{d}\xi; \quad 0 \le \gamma \le 1$$

$$I_3 = \int_0^1 Y_j''^2(\xi)\mathrm{d}\xi = 12.3624$$

$$c_k = \sqrt{\frac{I_3}{I_1}} = 3.5160 \quad \text{and} \quad c_m = \frac{I_2}{I_1}$$

TABLE I. The stiffness (c_k) and mass (c_m) calibration constants for CNT based bio-nano sensor. The value of γ indicates the length of the mass as a fraction of the length of the CNT.

Mass size	Cantilevered CNT		Bridged CNT	
	c_k	c_m	c_k	c_m
Point mass ($\gamma \to 0$)	3.5160152	4.0	22.373285	2.522208547
$\gamma = 0.1$		3.474732666		2.486573805
$\gamma = 0.2$		3.000820053		2.383894805
$\gamma = 0.3$		2.579653837		2.226110255
$\gamma = 0.4$		2.212267400		2.030797235
$\gamma = 0.5$		1.898480438		1.818142650
$\gamma = 0.6$		1.636330135		1.607531183
$\gamma = 0.7$		1.421839146		1.414412512
$\gamma = 0.8$		1.249156270		1.248100151

Adhikari, S. and Chowdhury, R., "The calibration of carbon nanotube ba bio-nano sensors", *Journal of Applied Physics*, **107**[12] (2010), pp. 124322:1-8

Vibration based mass sensor: CNT

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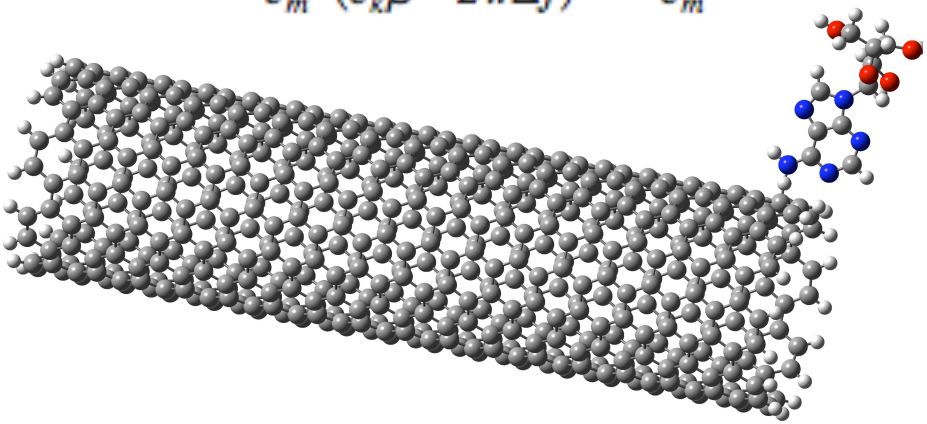
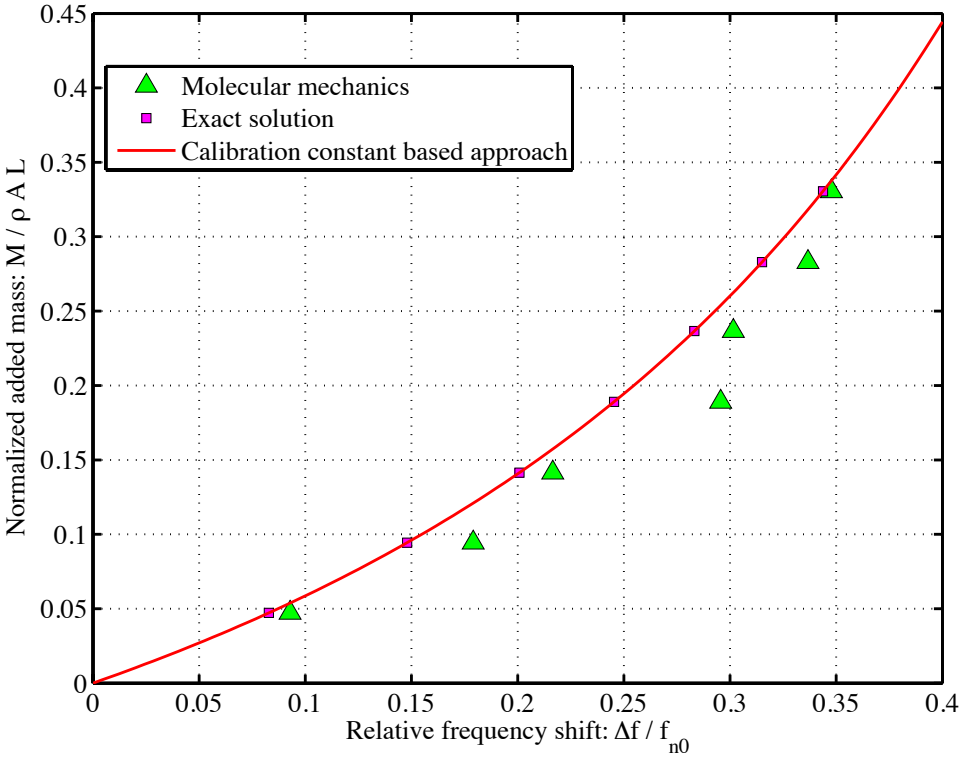
Mass of a nano object can be detected from the frequency shift Δf

$$M = \frac{\rho A L}{c_m} \frac{(c_k^2 \beta^2)}{(c_k \beta - 2\pi \Delta f)^2} - \frac{\rho A L}{c_m}$$



CNT with deoxythymidine



Adhikari, S. and Chowdhury, R., "The calibration of carbon nanotube based bio-nano sensors", *Journal of Applied Physics*, **107**[12] (2010), pp. 124322:1-8

Vibration based mass sensor: Graphene

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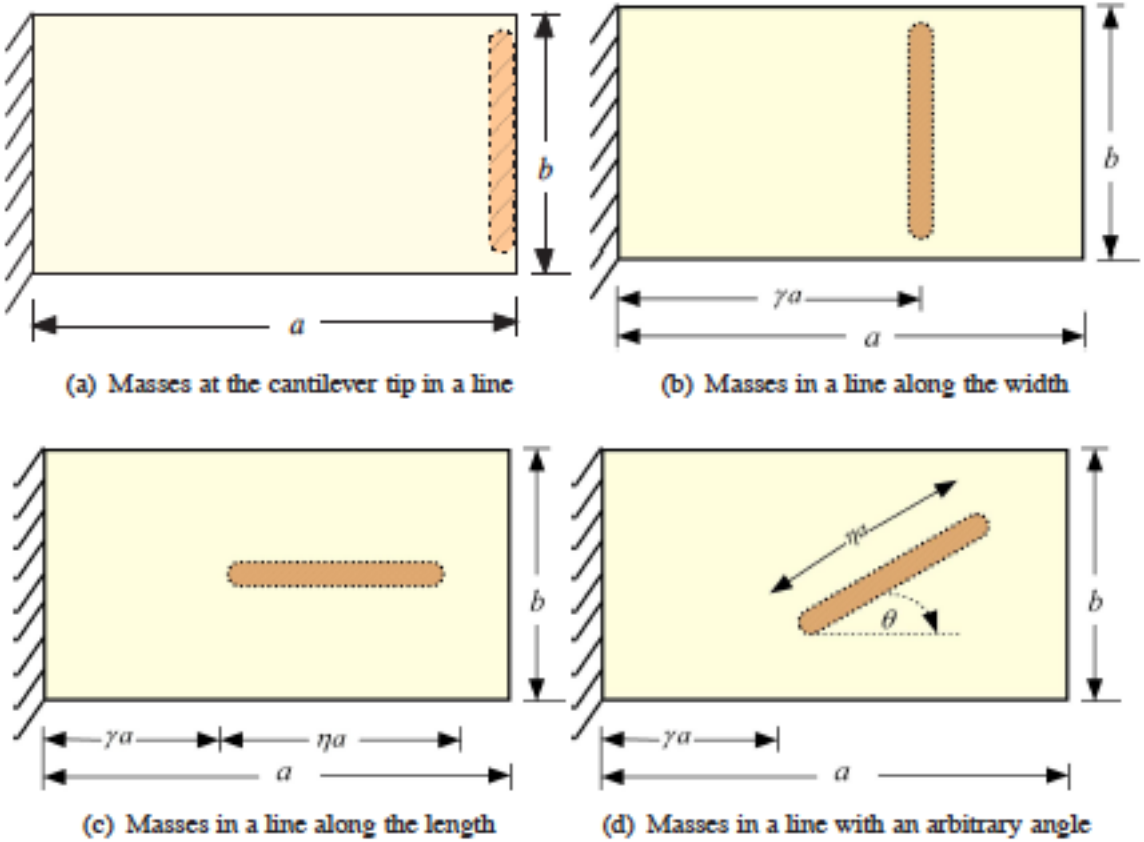
Vibrating graphene sheets can be used as sensors with different mass arrangements



Vibration based mass sensor: Graphene

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Relative added mass:

$$\mu = \frac{1}{c_n\left(1-\frac{\Delta f}{f_0}\right)^2} - \frac{1}{c_n}$$

Table 1: The calibration constants for SLGS based bio-nano sensor due to four possible configurations of attached mass.

Mass arrangement	Calibration constant c_n
Case (a): Masses are at the cantilever tip in a line	$2\pi/(3\pi-8)$
Case (b): Masses are in a line along the width	$2\pi(1-\cos(\pi\gamma/2))^2/(3\pi-8)$
Case (c): Masses are in a line along the length	$(3\pi\eta+[\sin((\gamma+\eta)\pi)-\sin(\gamma\pi)]-8[\sin((\gamma+\eta)\pi/2)-\sin(\gamma\pi/2)])/\eta(3\pi-8)$
Case (d): Masses are in a line with an arbitrary angle θ	$(3\pi\eta\cos(\theta)+[\sin((\gamma+\eta\cos(\theta))\pi)-\sin(\gamma\pi)]-8[\sin((\gamma+\eta\cos(\theta))\pi/2)-\sin(\gamma\pi/2)])/\eta\cos(\theta)(3\pi-8)$

Vibration based mass sensor: Graphene

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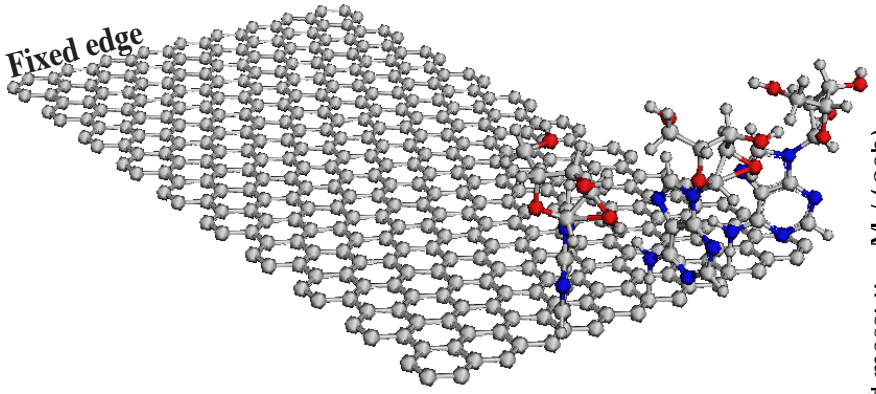
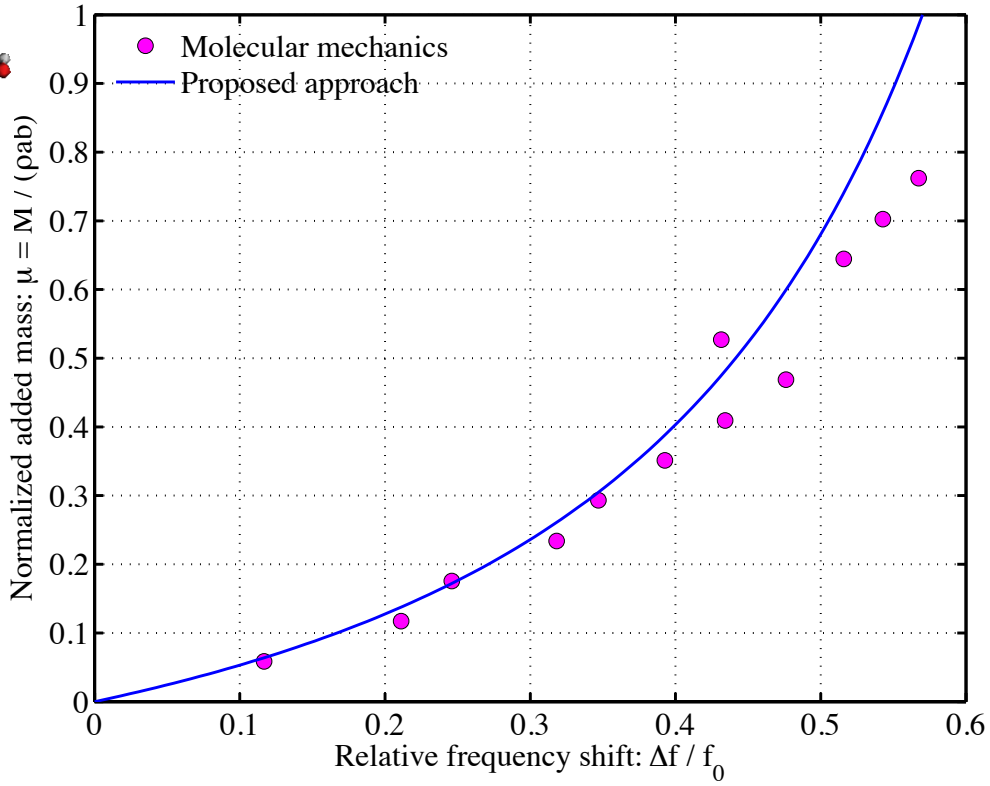
Vibrating graphene sheets can be used as sensors with different mass arrangements



SLGS with adenosine



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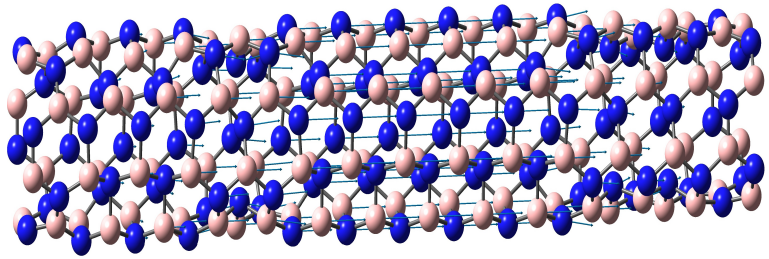
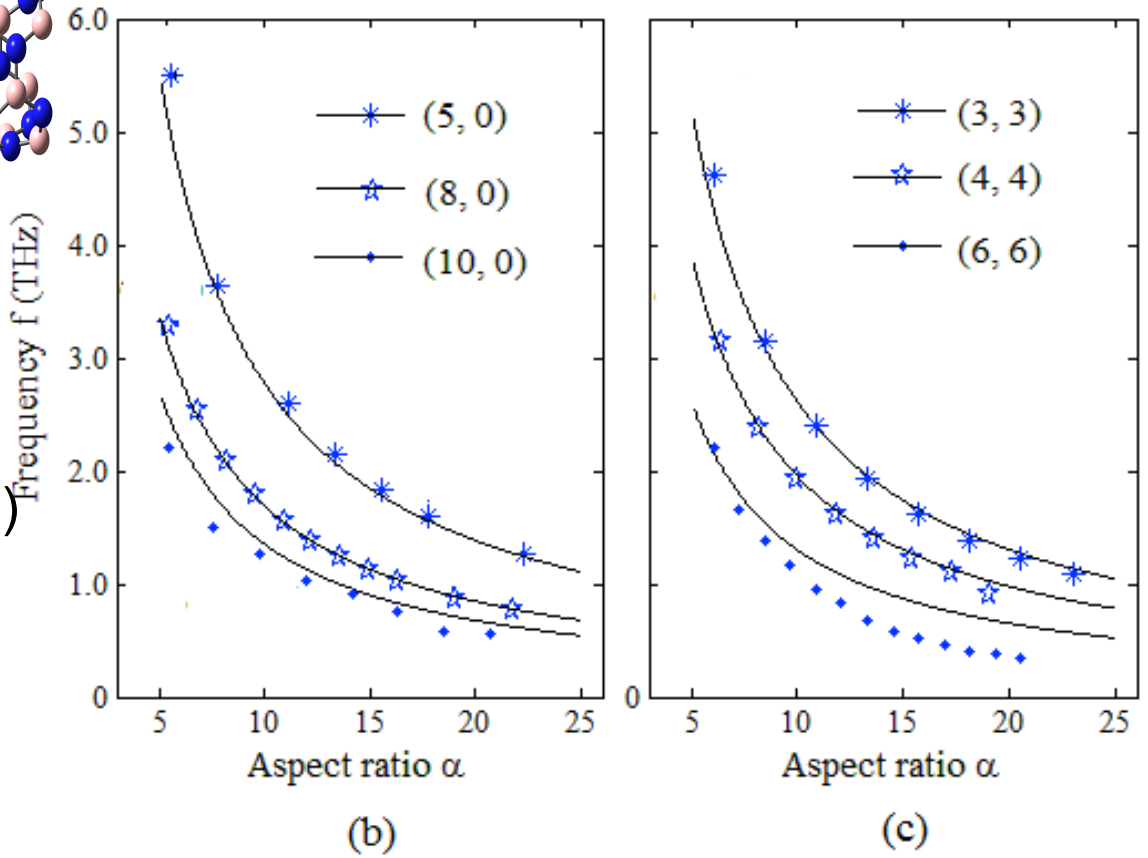
Boron Nitride Nanotube and Nanosheets

Axial vibration of BNNT



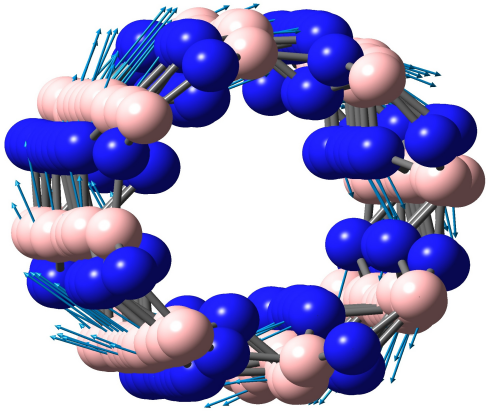
(a)

(a) Axial vibration and its associated frequency of (b) zigzag and (c) armchair BNNTs given by the MM simulations (discrete dots) and a column model with Young's modulus 1*TPa* (solid lines).



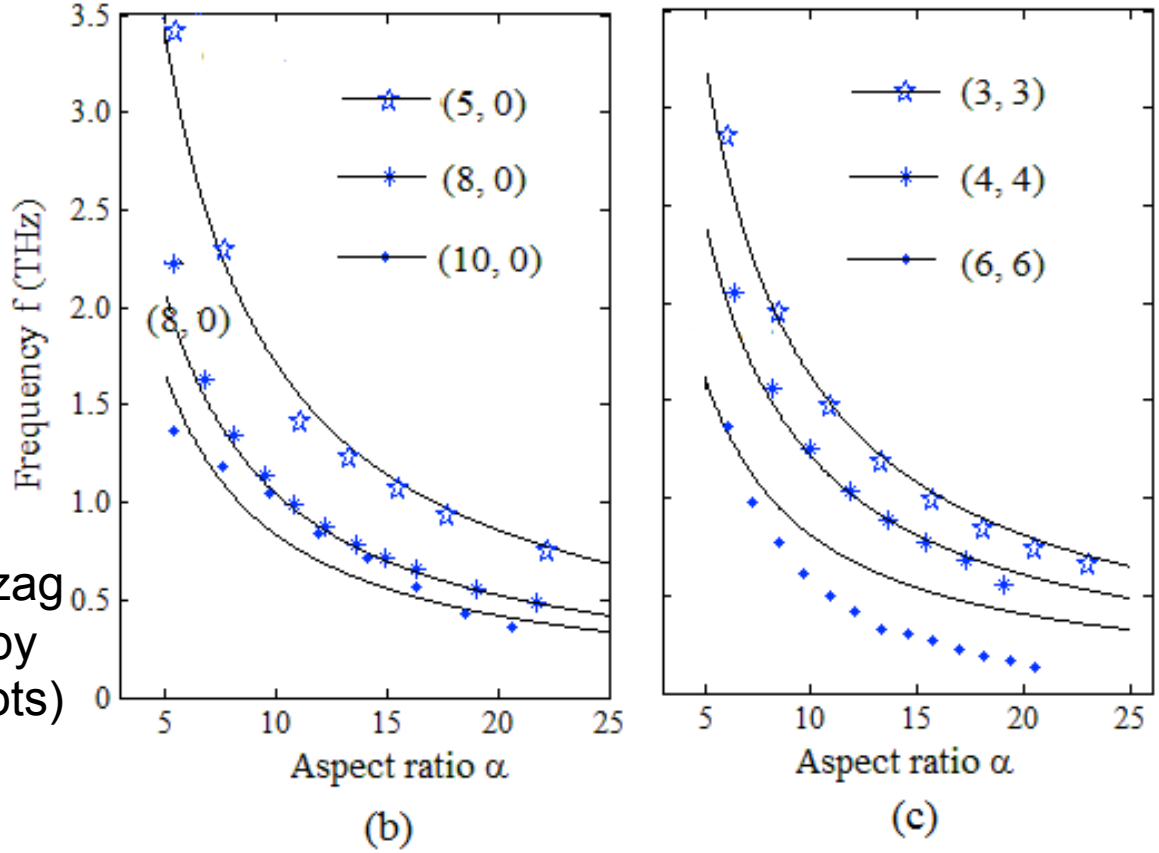
Chowdhury, R., Wang, C. W., Adhikari, S. and Scarpa, F., "Vibration and symmetry-breaking of boron nitride nanotubes", Nanotechnology, 21[36] (2010), pp. 365702:1-9.

Torsional vibration of BNNT



(a)

(a) Torsional vibration and its associated frequency of (b) zigzag and (c) armchair BNNTs given by the MM simulations (discrete dots) and a column model with shear modulus 0.41TPa (solid lines).



Chowdhury, R., Wang, C. W., Adhikari, S. and Scarpa, F., "Vibration and symmetry-breaking of boron nitride nanotubes", Nanotechnology, 21[36] (2010), pp. 365702:1-9.

Optimised shape of BNNT

Swansea University
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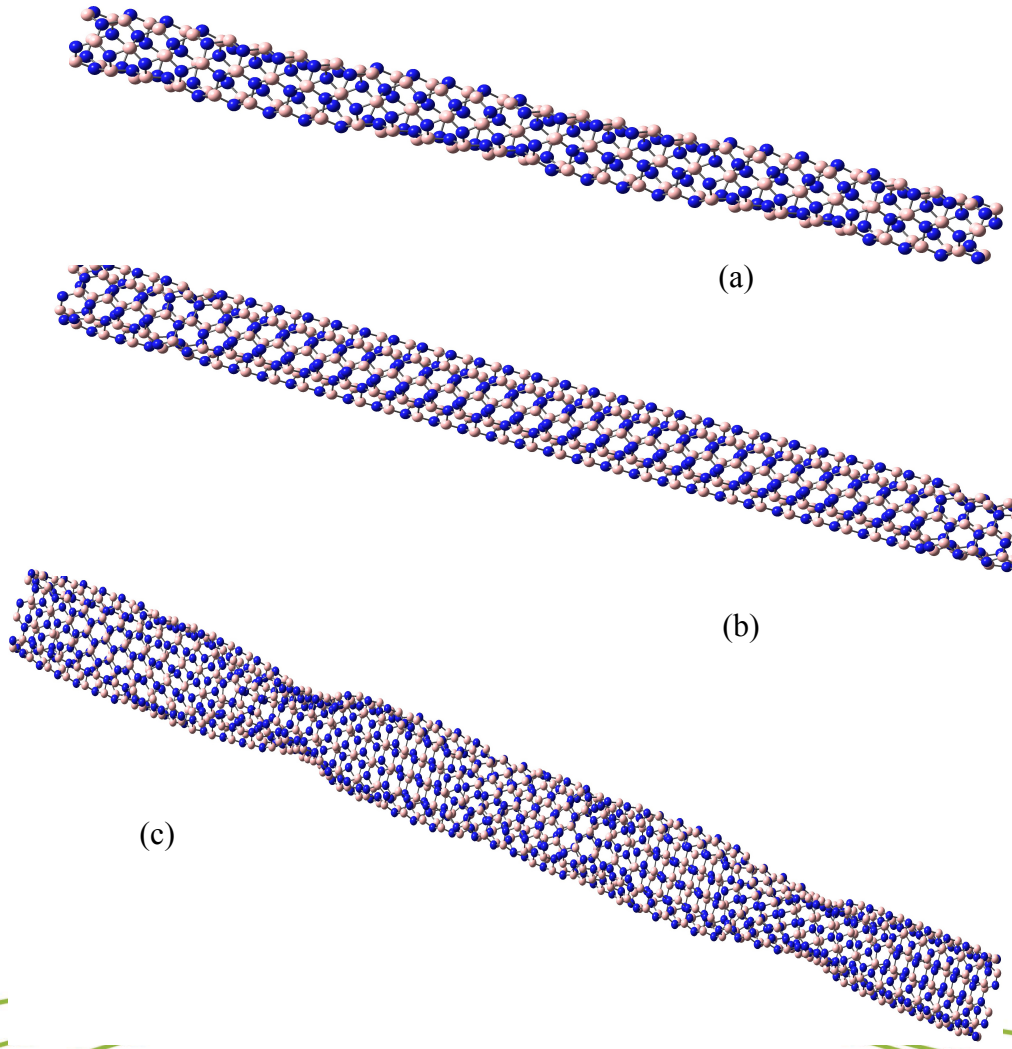

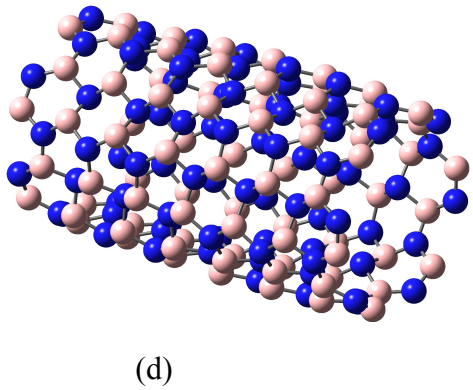

Optimized configuration of armchair BNNTs: (a) (3, 3), (b) (4,4) and (c) (6,6) with the aspect ratio 15, and (d) short (6, 6) with the aspect ratio 2.

Mechanical property of BN Sheets

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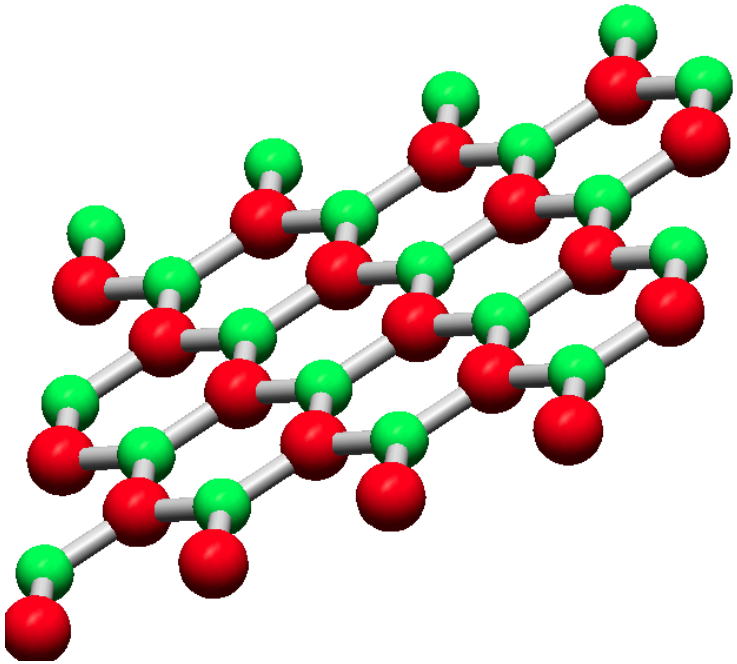

$$\bar{Y} = \frac{8\sqrt{3}\,C_\rho}{18 + \tau_{BN}^2 \left(\frac{C_\rho}{C_\theta}\right)}$$

$$\bar{\nu} = \frac{\tau_{BN}^2 \left(\frac{C_\rho}{C_\theta}\right) - 6}{18 + \tau_{BN}^2 \left(\frac{C_\rho}{C_\theta}\right)}$$

$$\bar{G} = \frac{2\sqrt{3}\,C_\rho}{3 + 18\,\tau_{BN}^2 \left(\frac{C_\rho}{C_\theta}\right)}$$

Example of armchair (4, 0) BN sheet. Boron atoms are in red, nitrogen atoms are in green.

Boldrin, L., Scarpa, F., Chowdhury, R., Adhikari, S. and Ruzzene, M., "Effective mechanical properties of hexagonal boron nitride nanosheets", Nanotechnology, 22[50] (2011), pp. 505702:1-7.

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DNA Mechanics

Atomistic FE of DNA

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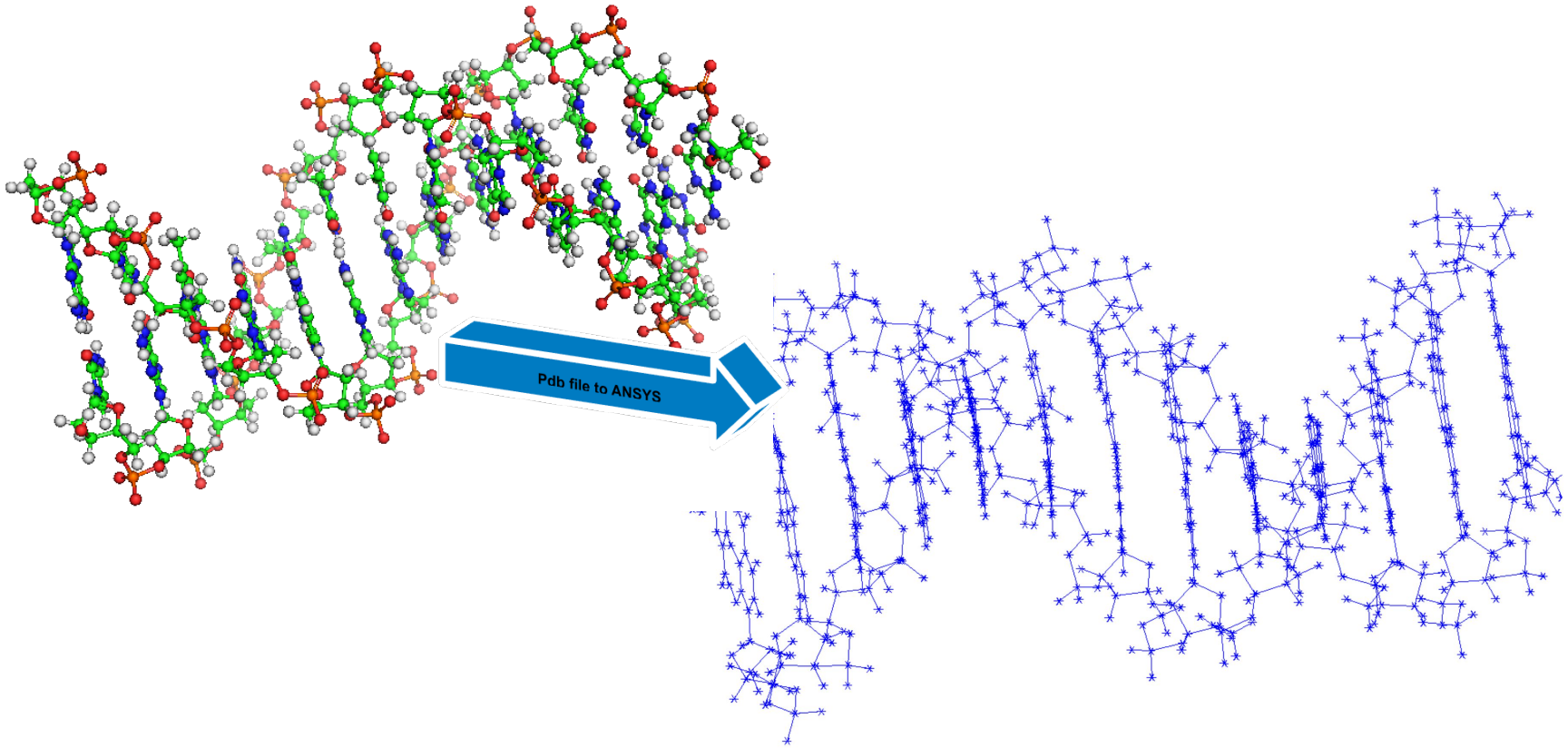
From protein data bank file to ANSYS input file – **a new code for automatic translation**



Atomistic FE of DNA

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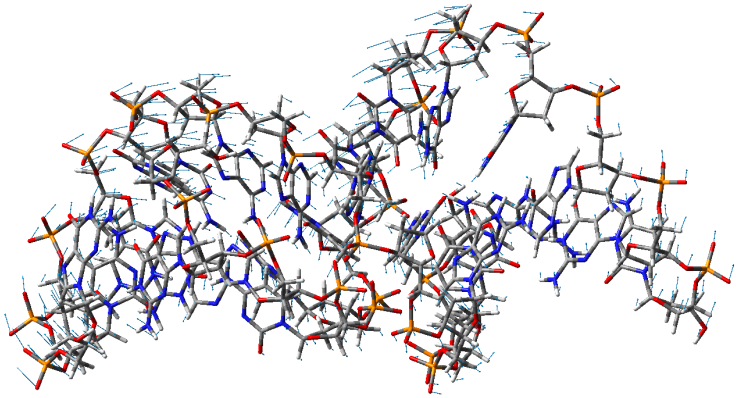
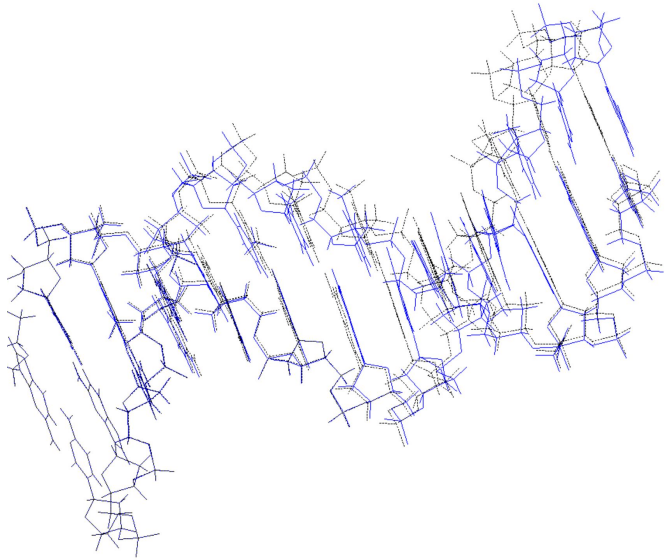
Material properties of the beams are obtained depending on the nature of the bonds



Mode 3 (MM:33.679; FE 38.768 GHz)



Mode 6 (MM:111.696; FE 112.71 GHz)

Conclusions

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- Atomistic finite element method is developed for general nanosalce structures:
  - Carbon nanotube
  - Fullerenes
  - Graphene
  - Nanoscale bio sensors
- Programs have been written to convert pdb files to Finite Element geometry file and material properties
- Encouraging results compared to MM simulation were obtained
- Future: nonlinearity, large-scale problems such as proteins & nanocomposites, molecular dynamic simulations, experimental validation

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