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Mechanical Characteristics of Carbon Nanotubes: *Micropolar Elasticity Models and Molecular Dynamics Simulations under Torsion and Bending*

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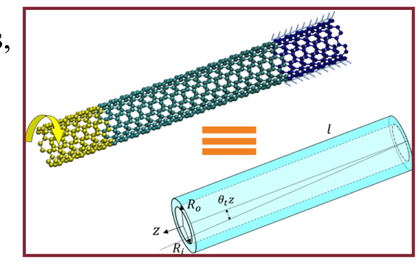
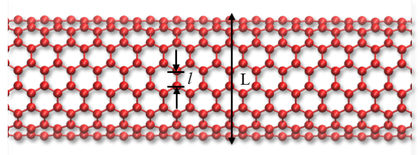
Introduction

- Carbon nanotubes (CNTs) have many actual and potential applications in different fields of engineering (e.g. sensors, actuators, springs, resonators, reinforcement elements, probes) thanks to their outstanding mechanical, optical, thermal and electrical properties.
- The efficient application of carbon nanotubes in nanodevices and nanomaterials requires a comprehensive understanding of their mechanical properties.
- Although atomistic simulations provides a deep insight into nanoscopic phenomena, the computational burden increases progressively as system scale enlarges. With the use of continuum models evaluated in accordance with atomistic simulations we can benefit from the efficiency of continuum modeling while preserving the accuracy of simulation.
- Observations reports size-dependent behaviour in CNTs which should be accounted for, where smart applications are desired.
- The size-dependency stems from CNTs internal structures which is comparable to the macroscopic length.





scale effects → Classical continuum theory (crossed out)

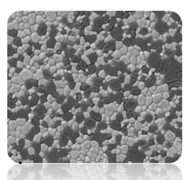
Non-local (non-classical) continuum → Preserve the memory of material's internal structure through internal scale parameter

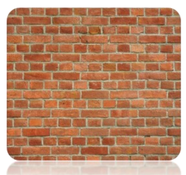
Molecular Dynamics Simulation (MD)

- Using MD both **bending** and **torsional** deformations are applied on two sets of eight armchair and zigzag single-walled CNTs with mean diameters ranging from d = 6.3 to 16.2 Å.
- The aspect ratio (length/mean diameter), is fixed at 5, however, the independency of bending and torsional rigidities to the aspect ratio is ensured.

Micropolar Theory

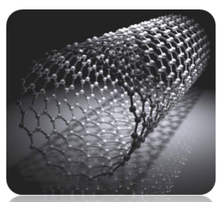
In micropolar theory, material particles are described in terms of both their positions and orientations. Micropolar theory has been successfully used to describe a wide range of materials with internal structures like brick masonry walls, particulate composites, polycrystals, porous materials. In this works the applicability of micropolar theory and couple stress theory to model size dependency in CNTs are evaluated.


polycrystals


Brick-masonry walls


Particulate composites

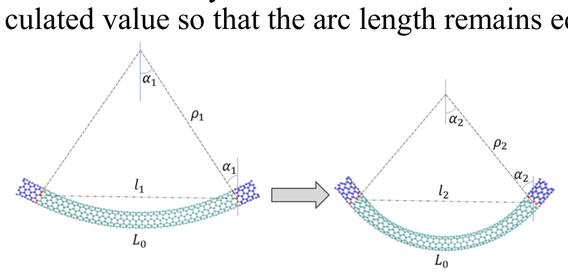

Porous materials


Carbon nanotubes

Degrees of Freedom:	u_i, ϕ_i
Kinematic relation:	$\varepsilon^{M}_{ij} = u_{i,j} + e_{ijk}\phi_k \qquad \chi_{kj} = \phi_{k,j}$
Equilibrium equation:	$\sigma^{M}_{ij,j} = 0, \qquad \mu_{kj,j} - e_{ijk}\sigma^{M}_{ij} = 0$
Constitutive equation: (Isotropic Elasticity)	$\sigma^{M}_{ij}(\mathbf{x}) = \lambda\varepsilon^{M}_{kk}(\mathbf{x})\delta_{ij} + (\mu+\chi)\varepsilon^{M}_{ij}(\mathbf{x}) + \mu\varepsilon^{M}_{ji}(\mathbf{x}),$ $\mu_{kj}(\mathbf{x}) = \alpha\chi_{ii}(\mathbf{x})\delta_{kj} + \beta\chi_{jk}(\mathbf{x}) + \gamma\chi_{kj}(\mathbf{x})$

Bending Deformation

- To apply pure bending and avoid spurious axial strain, a novel method is proposed, in which after every small incremental rotation of both ends, the two ends moves at a calculated value so that the arc length remains equal to the initial length of the tube

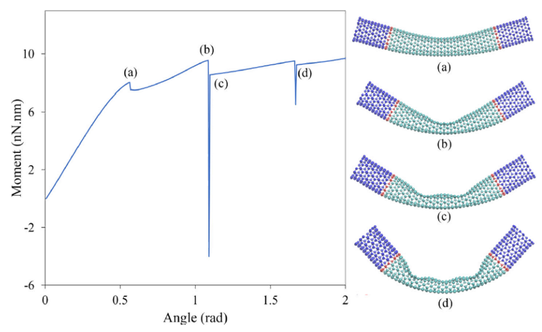


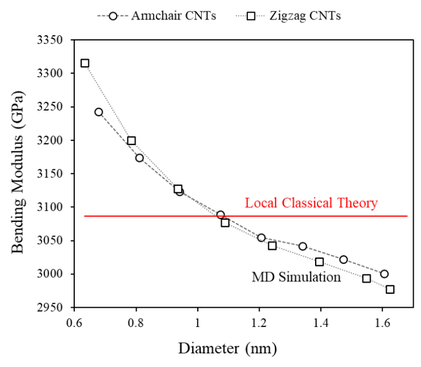
$$\rho_1(2\alpha_1) = \rho_2(2\alpha_2) = L_0 \qquad l_1 = 2\rho_1 \sin\alpha_1 \quad l_2 = 2\rho_2 \sin\alpha_2$$

$$\Delta l = \frac{1}{2}(l_1 - l_2) = \frac{1}{2}L_0\left(\frac{\sin\alpha_1}{\alpha_1} - \frac{\sin\alpha_2}{\alpha_2}\right)$$

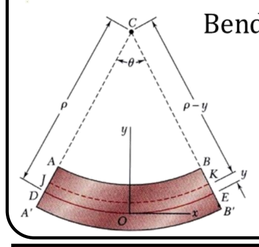
Size dependency in bending modulus of CNTs

- Using the linear part of the moment curve versus bending angle, the bending rigidities and the bending modulus for each CNT diameter is calculated.
- A size-dependency in the bending modulus is observed which can not be described with classical theory.





pure bending of a circular cylinder in non-classical theories



Bending Modulus = E Ω

where

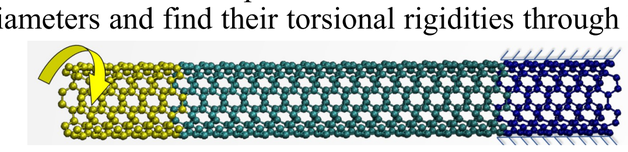
Micropolar : $\Omega_m = 1 + \frac{8N^2}{1+\nu}\left[\frac{1-(\beta/\gamma)^2}{(\delta R_i)^2 + (\delta R_o)^2} + \frac{(\nu+\beta/\gamma)^2}{8N^2(1-\nu) + \xi(\delta R_i, \delta R_o)}\right]$

Constrained micropolar theory: $\Omega_{cm} = 1 + 8(1-\nu)\frac{l_b^2}{R_o^2 + R_i^2}$

Modified couple stress theory: $\Omega_{cs} = \frac{M\rho}{EI} = 1 + \frac{2l^2}{R_o^2 + R_i^2}$

Torsional Deformation

- Torsional deformation are also performed on a set of armchair and zigzag nanotubes with different diameters and find their torsional rigidities through molecular dynamics simulations.

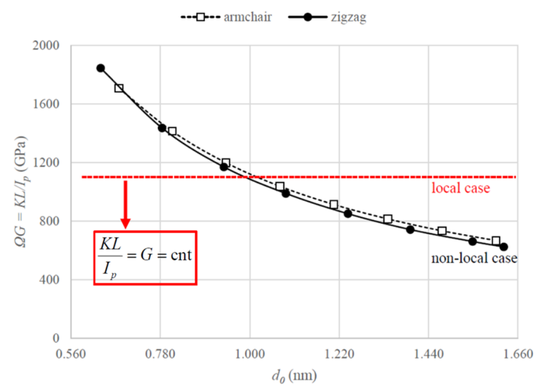


Size dependency in shear modulus of CNTs

- Torsional rigidity and subsequently the shear modulus are calculated and again a dependency of shear modulus to the diameter is recognized.

$$K_t = \partial^2 U/\partial\theta^2$$

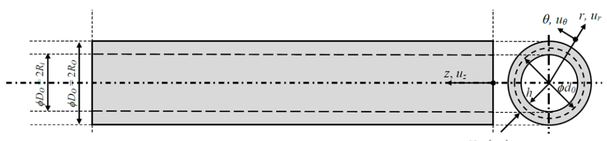
$$\text{Shear Modulus} = K_t L_0 / I_p$$



pure torsion of a circular cylinder in non-classical theories

Displacement and microrotation fields

$$u_r = 0, \quad u_\theta = \theta_t r z, \quad u_z = 0, \quad \phi_r = \theta_t \Phi(r), \quad \phi_\theta = 0, \quad \phi_z = \theta_t z$$



Strain and Curvatures $\varepsilon_{\theta z} = -\theta_t\Phi(r), \ \varepsilon_{z\theta} = \theta_t(r + \Phi(r)), \ \chi_{rr} = \theta_t\Phi'(r), \ \chi_{\theta\theta} = \theta_t\frac{\Phi(r)}{r}, \ \chi_{zz} = \theta_t$

Constitutive Eq. + Equilibrium Eq. → $r^2\Phi''(r) + r\Phi'(r) - (1 + p^2r^2)\Phi(r) - \frac{p^2}{2}r^3 = 0 \quad \Phi(r) = AI_1(pr) + BK_1(pr) - r/2$

Shear Modulus = G Ω

Micropolar : $\Omega_h G = G\left(1 + \frac{(4l_t)^2}{(d_0+h)^2 - (d_0-h)^2}\right) + \frac{64A(p\alpha\eta_1^I + \kappa\eta_2^I) + 64B(p\alpha\eta_1^{II} - \kappa\eta_2^{II})}{p((d_0+h)^4 - (d_0-h)^4)}$

Modified couple stress theory: $\Omega_s G = G\left(1 + 6\left(\frac{2l_t}{d_0}\right)^2\frac{1 - \frac{4}{3}\psi X}{1 - \psi X}\right)$

Optimization problem

- Non-linear optimization approach is performed aiming to minimize the difference between bending/torsional rigidities obtained from MD simulations and continuum models

$$F_{obj} = \left|\frac{(\text{Bending or Torsional Rigidity})_{MD} - (\text{Bending or Torsional Rigidity})_{continuum}}{(\text{Bending or Torsional Rigidity})_{MD}}\right|$$

principle of non-negative energy → $0 \le E, -1 < \nu \le 0.5, \quad 0 \le l_b, 0 \le N \le 1, \ -1 \le \frac{\beta}{\gamma} \le 1$ (bending) $\quad 0 \le G\ (\text{GPa}), \ 0 \le N \le 1, \quad 0 \le \psi \le 1.5, \ 0 \le l_t\ (\text{nm}),$ (torsion)

Vodenitcharova and Zhang criterion: → $0 \le h \le 1.42$

Results and Conclusion

- The size dependency in bending/shear modulus is best captured by micropolar theory, which can preserving the memory of internal structure via additional material parameters.
- Although the prediction by modified couple stress theory are not as successful as micropolar theory, a sufficient accuracy is still provided despite its simplified formulations.
- Since micropolar theory inherently accounts for the relative rotations related to the skew-symmetric part of the stress/strain tensor, The superiority of micropolar theory to couple stress theory suggests the presence of asymmetric stress/strains in the problem.
- An evident deficiency of classical Cauchy theory is observed.
- The value of the bending characteristic length, l_b, is directly correlated to the carbon-carbon bond length (≈ 1.4 Å) while the value of the torsional characteristic length, l_t, is related to the hexagonal lattice structure
- The obtained parameters from torsion is consistent to those from bending proving the competency of our method which is independent of the loading protocol.

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