Multiwalled carbon nanotubes: the thicker, the softer



IIJIMA ET AL. (1996)

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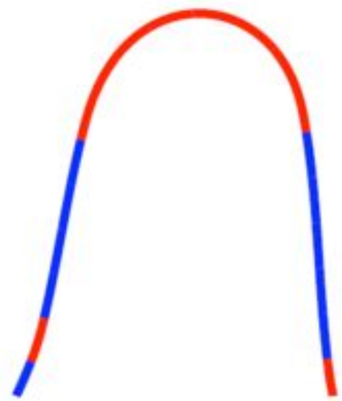
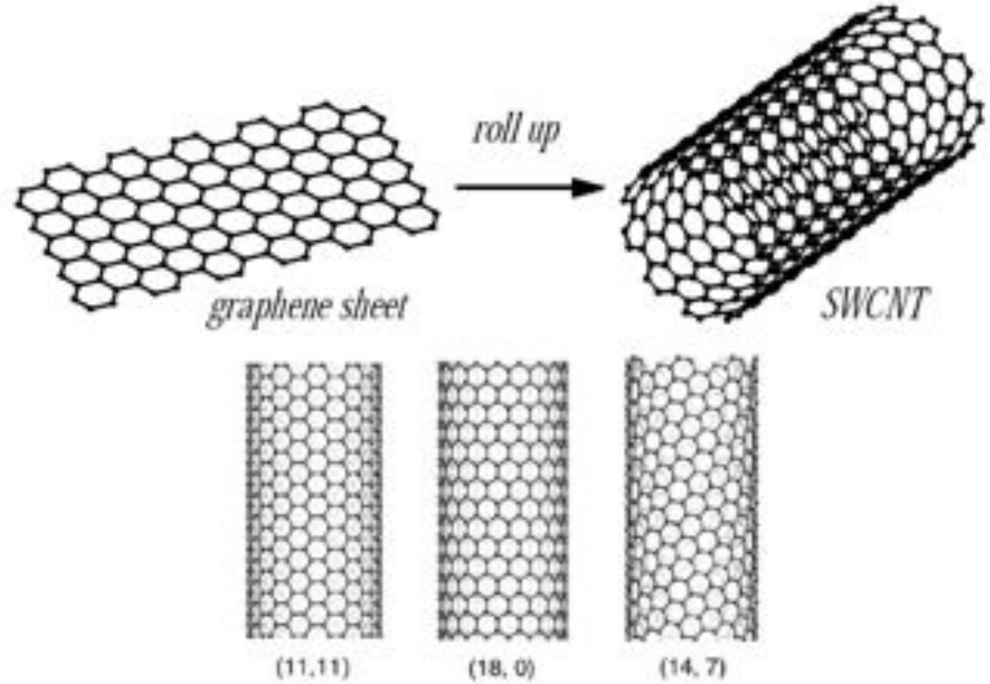
Universitat Politècnica de Catalunya (Spain)

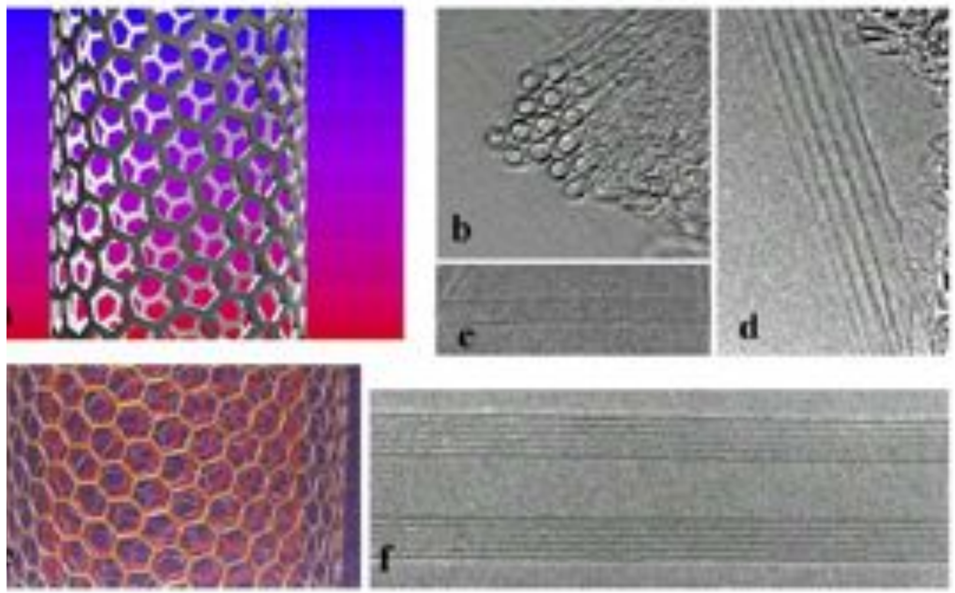
NanoSpain'09, Zaragoza, 2009



Introduction: CNTs Mechanics

CNTs come alone (SWCNTs), in bundles, or nested (MWCNTs).





..JAYAN& ZHOU, *Top. Appl. Phys.* (2001)

Unique structure and size, together with remarkable mechanical, electronic, thermal, chemical properties make them attractive in nanostructured materials and devices.

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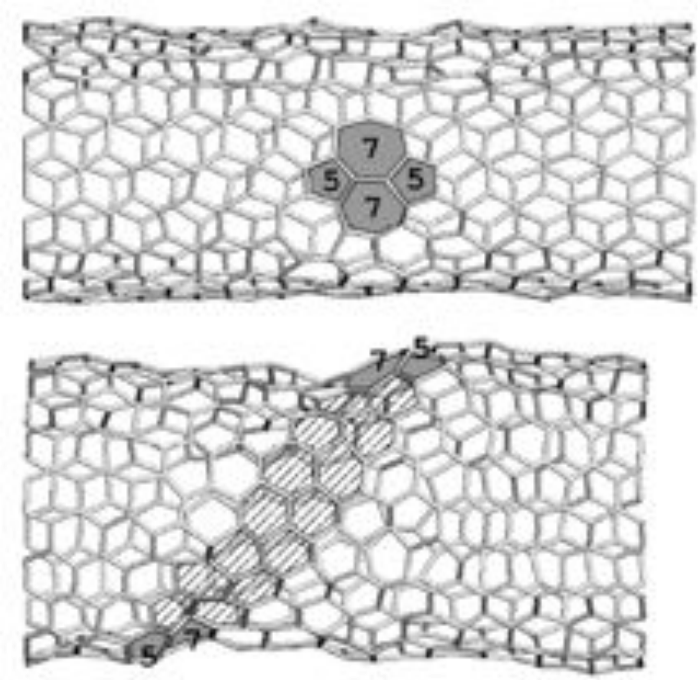
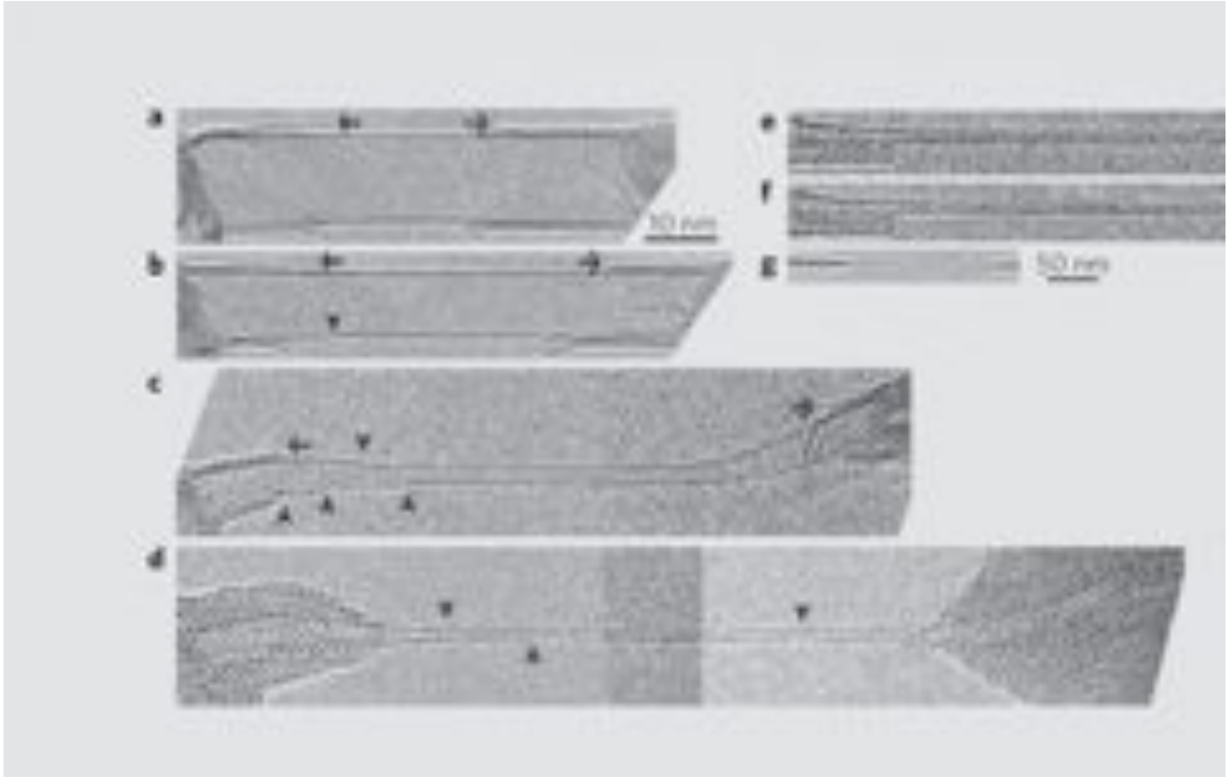
Introduction: CNTs Mechanics



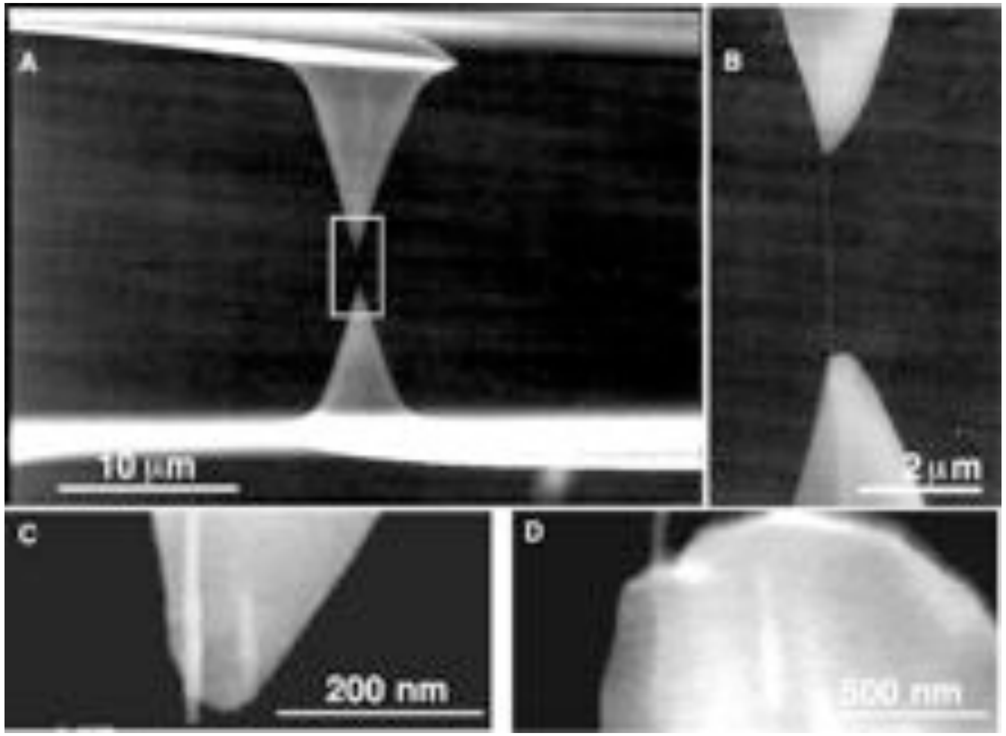
Nardelli et al, *PRL* (1996)



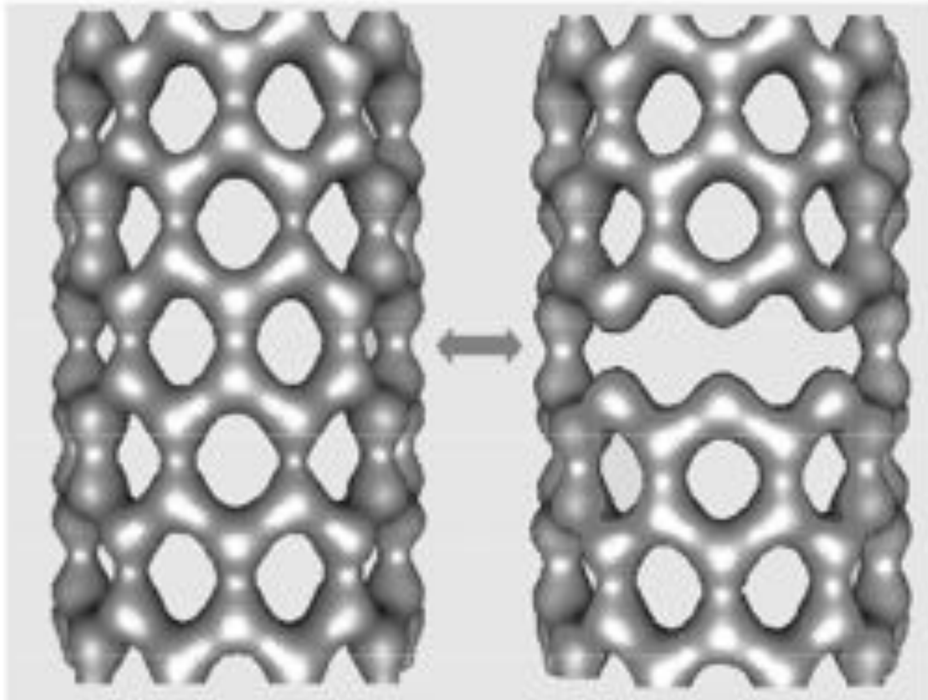
Huang et al, *Nature* (2006)

CNTs can experience plasticity at high temperatures...

Introduction: CNTs Mechanics



Yu et al, *Science* (2000)



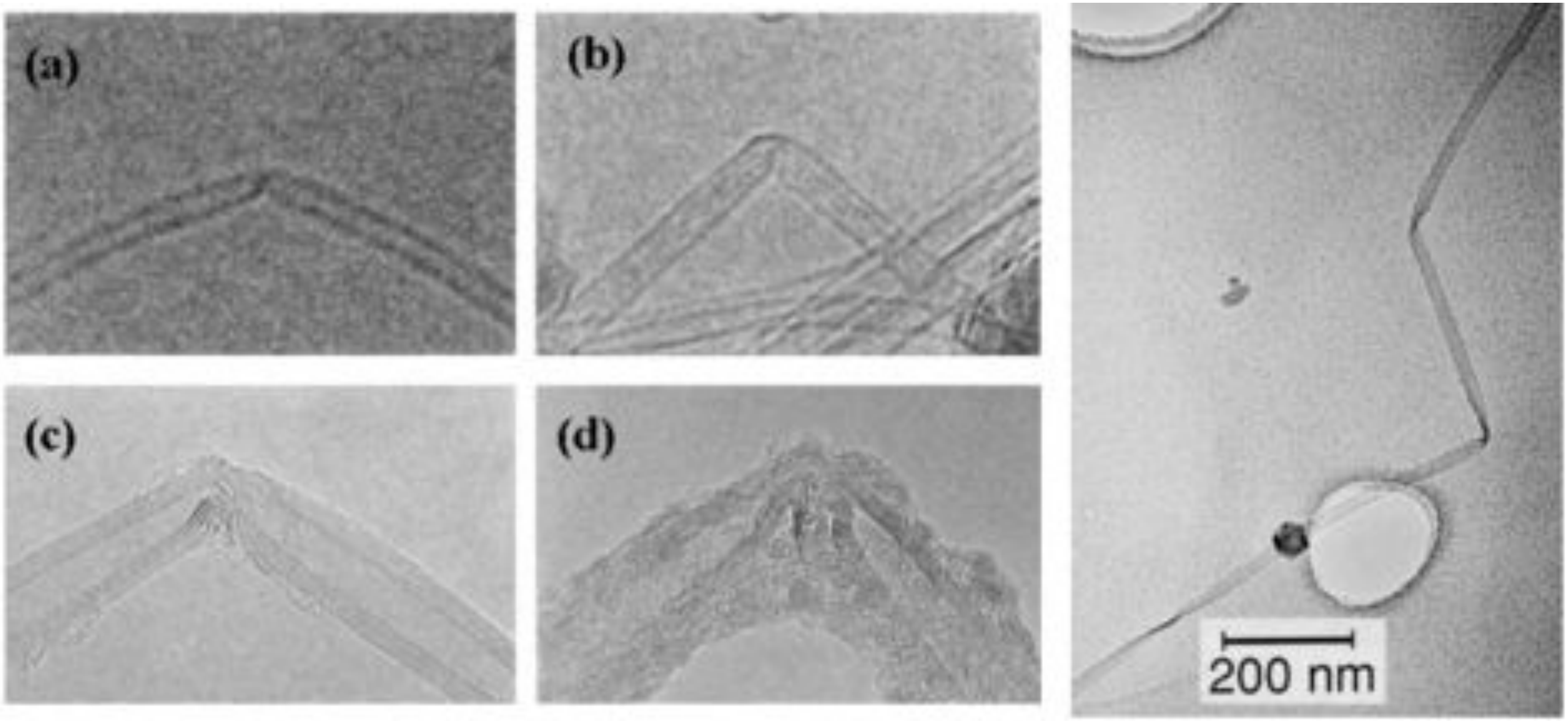
Dumitrica et al, *J. Chem. Phys* (2003)

or fracture at room temperature...

Introduction: CNTs Mechanics

Because of the hollow geometry and crystalline perfection and stability, they are extremely resilient and undergo reversibly very large deformations with buckling.

Very rich nonlinear elasticity



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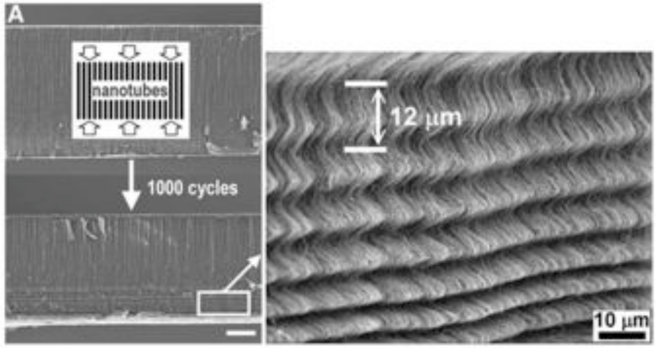
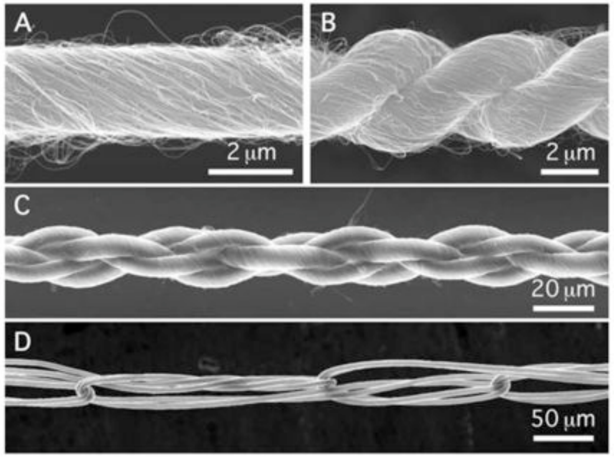
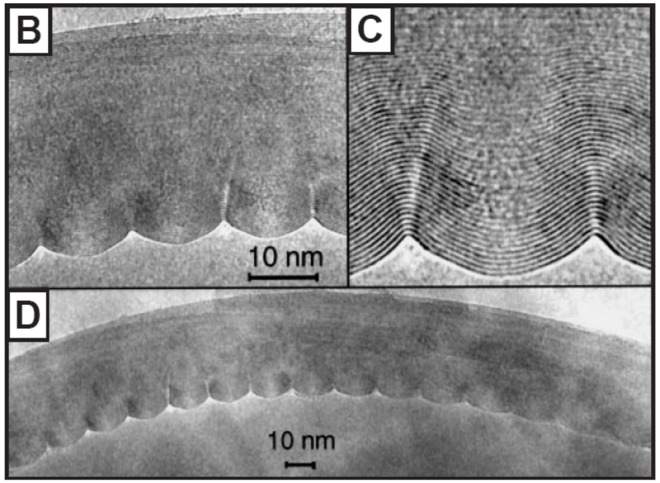
Multiscale mechanics

Cao et al, *Science* (2005)



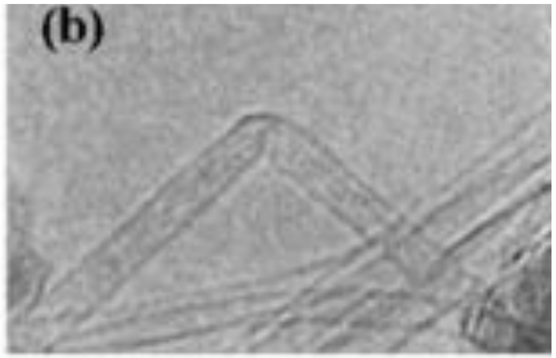


Baughman et al, *Science* (2004)
10's of microns



Poncharal et al, *Science* (1999)
100's of nanometers

Build large scale models from microscopic models to reduce empiricism and uncertainty



Iijima et al (1996)
nanometers

Baughman et al, *Science* (2002)
Amstrongs

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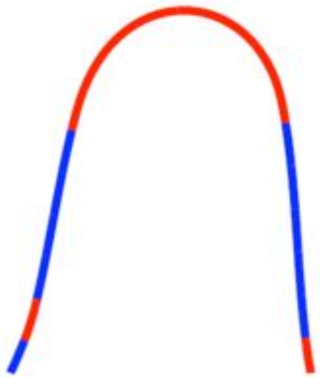
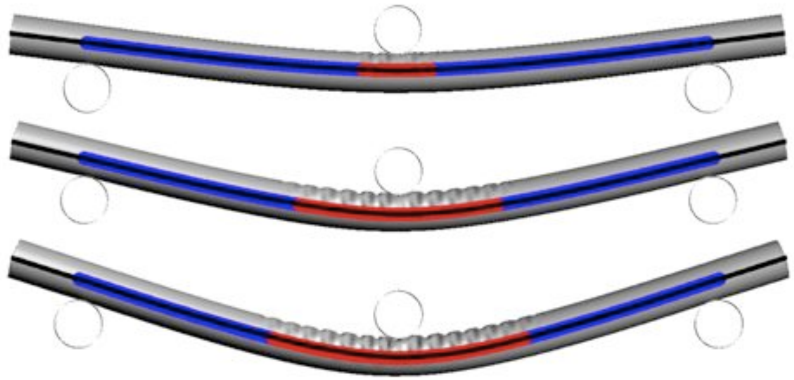
Multiple-scale analysis

Continuum surface models from atomistic models Arroyo & Belytschko, JMPS (2002)

Mechanics of thick multiwalled CNTs through scaling laws

Mesoscopic models, phase-transforming elastica





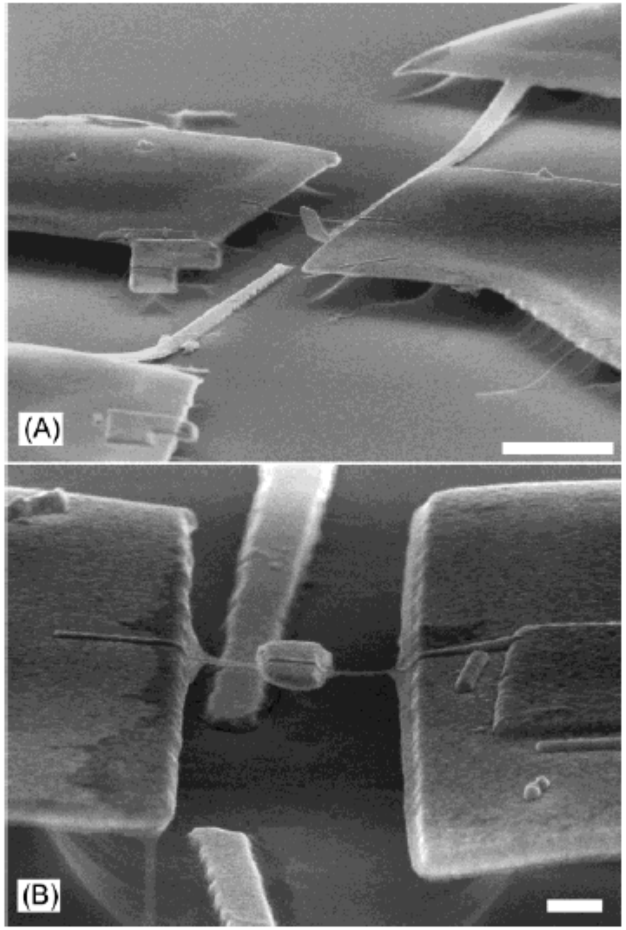
Mechanics of thick MWCNTs

I. Arias and M. Arroyo, Size-dependent nonlinear elastic scaling of multiwalled carbon nanotubes, *Physical Review Letters*, 100:085503 (2008).

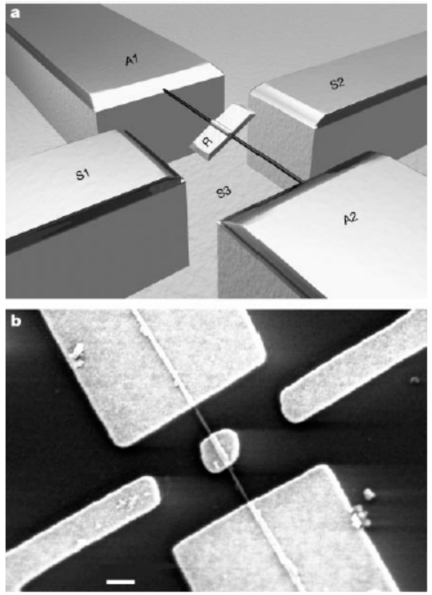
Mechanics of thick MWCNTs

Thick MWCNTs are central in a number of nanodevices and materials

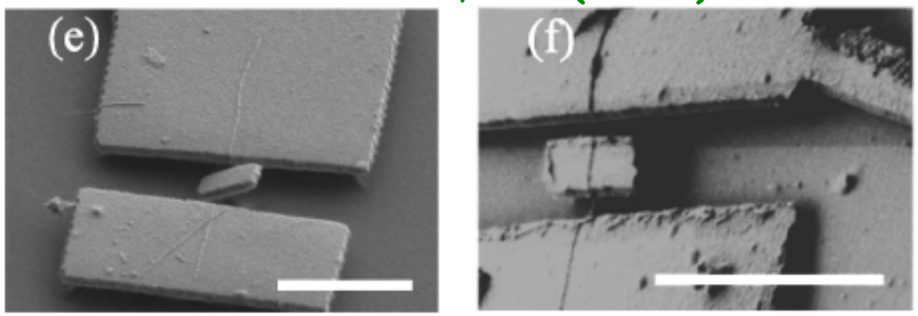
Bournlon et al, Nanoletters (2004)



Fennimore et al, Nature (2003)

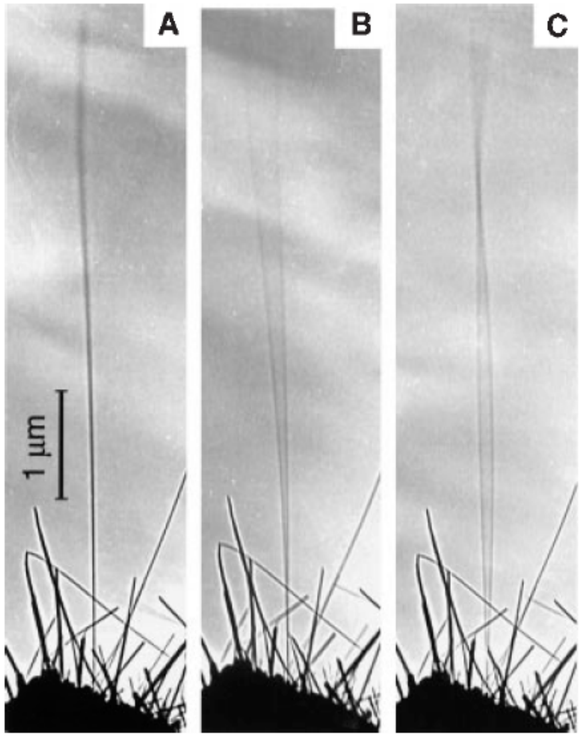


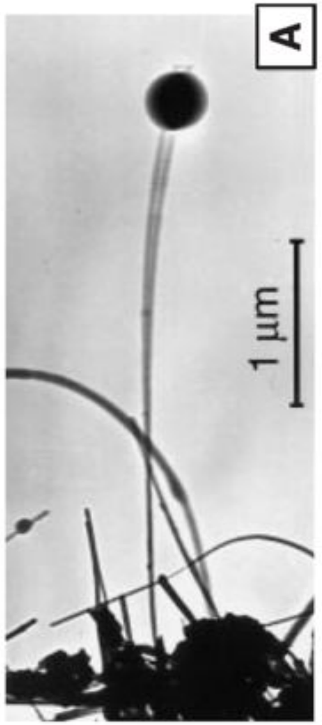
Williams et al, PRL (2003)

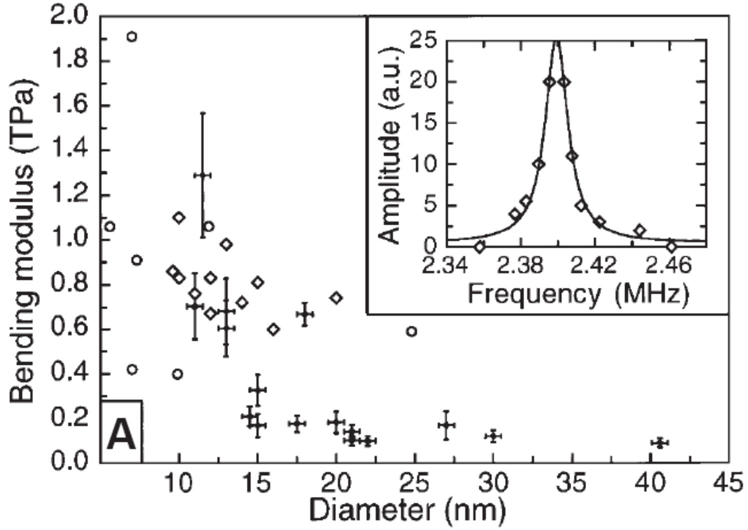


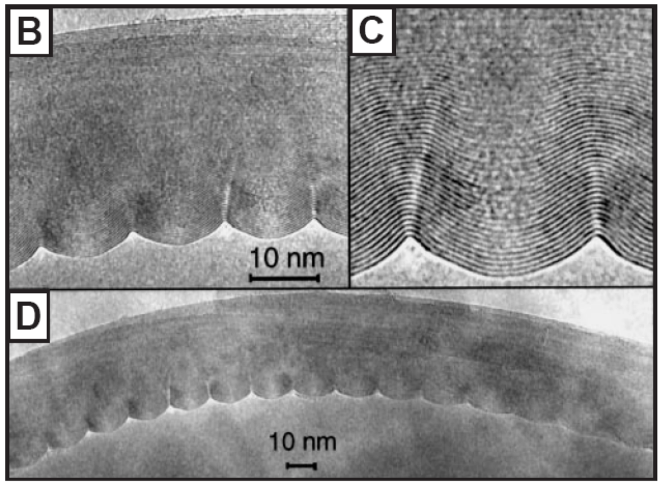
Mechanics of thick MWCNTs

Thick MWCNTs are central in a number of nanodevices and materials









$$\nu_j = \frac{\beta_j^2}{8\pi} \frac{1}{L^2} \sqrt{(D^2 + D_i^2)} \sqrt{\frac{E_b}{\rho}}$$

Poncharal et al, *Science* (1999)

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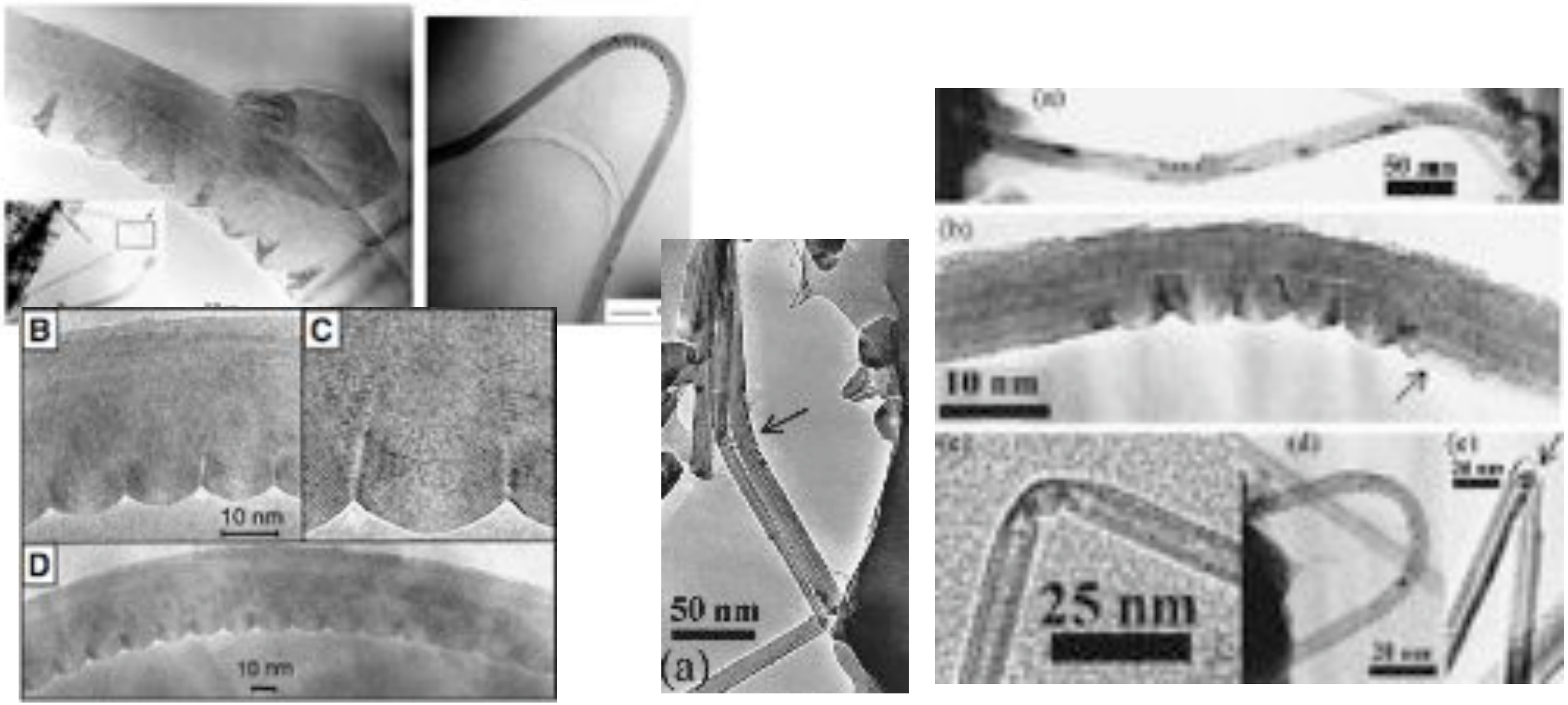
Mechanics of thick MWCNTs

- In analyzing experiments, and modeling devices and materials, thick MWCNTs are usually modeled as ***linear elastic beams***…



- Reliable simulations of these multi-milion atom systems are prohibitive, simplified unrealistic models instead

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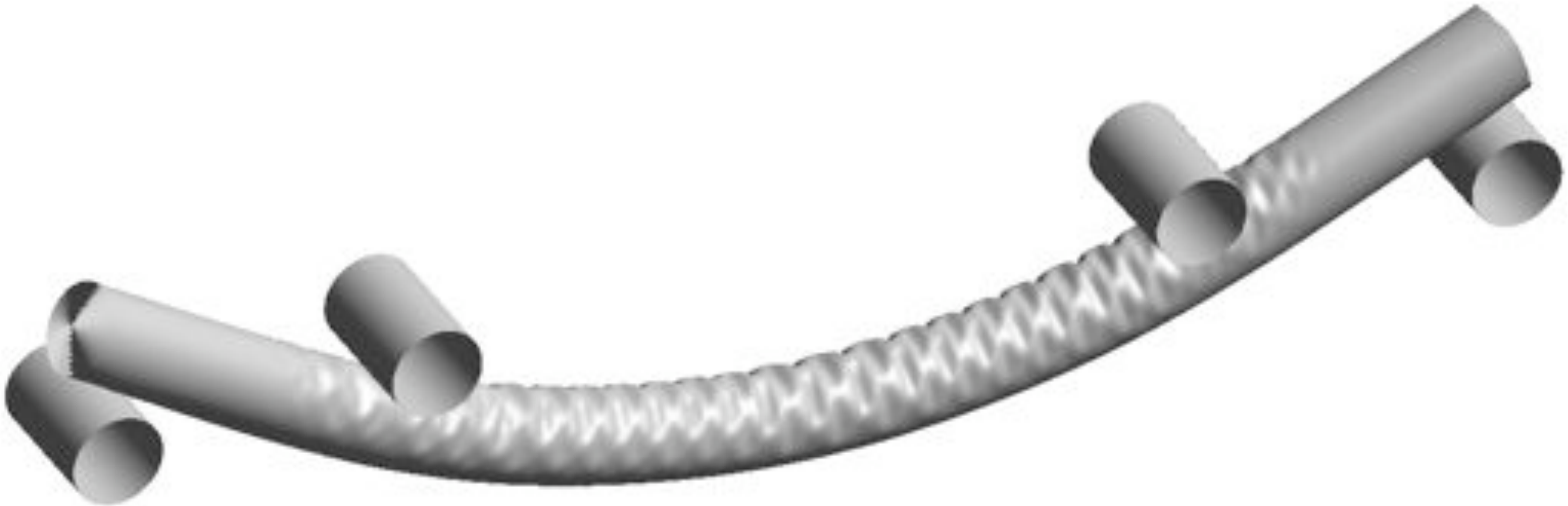
Mechanics of thick MWCNTs

The method proposed in Arroyo & Belytschko, *IJNME* (2004) allows for realistic simulations by reducing the number of dofs by two orders of magnitude, which still require high-performance computing facilities



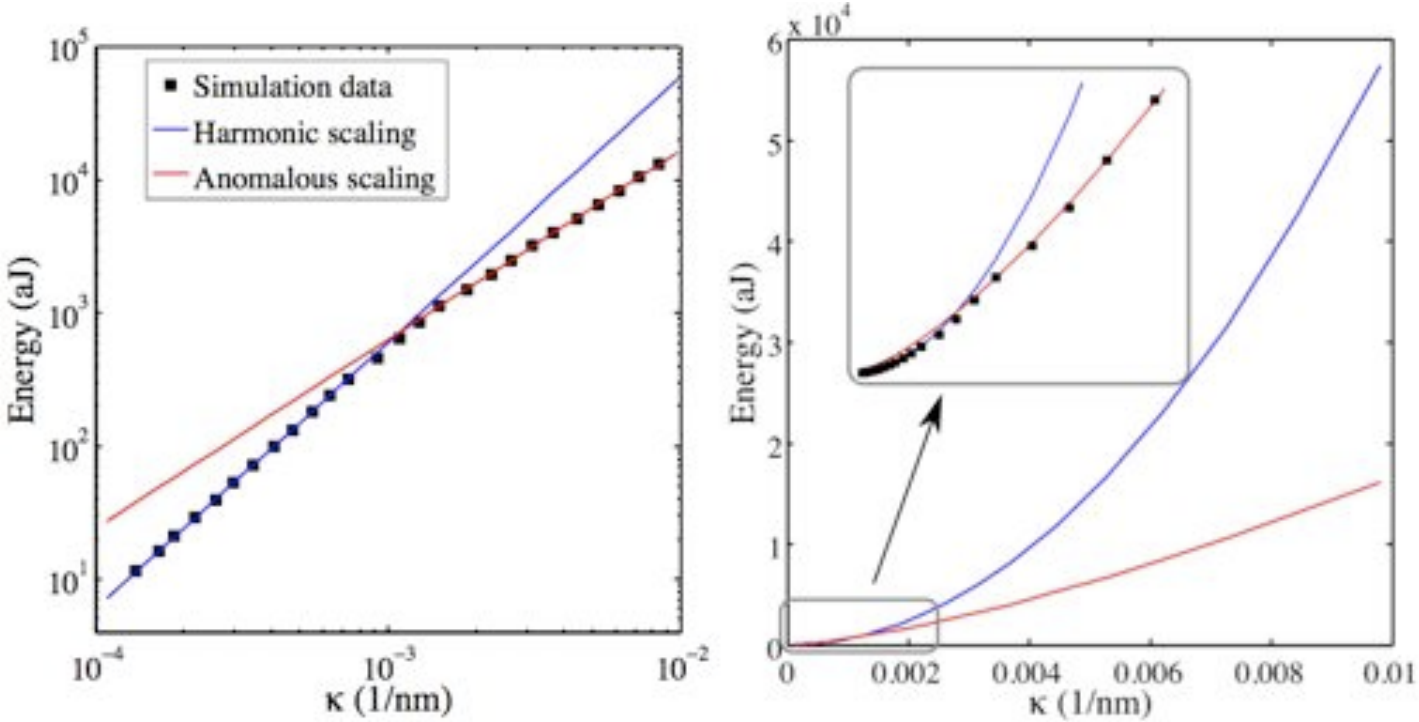
40-walled CNT 0.5 microns long: system containing nominally 31 million atoms is modeled with 400 000 FE nodes and computed on 512 processors

Mechanics of thick MWCNTs

Energy vs curvature relation has two regimes, **it is a composite power law** (Arroyo & Belytschko, *PRL* 2003);

- The **harmonic regime** in which E ~ curvature^2
- An **anomalous elastic** regime with E ~ curvature^a and $1<a<2$ for larger deformations, result of interplay of membrane, bending and vdW forces

This behavior is reversible with no significant hysteresis



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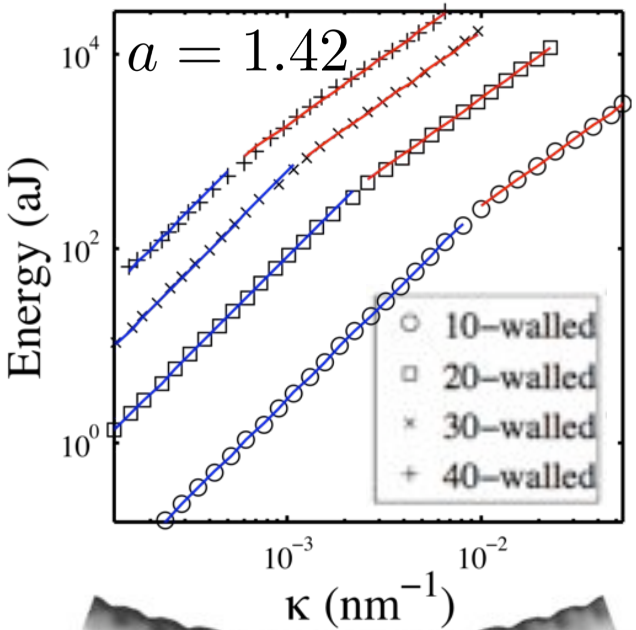
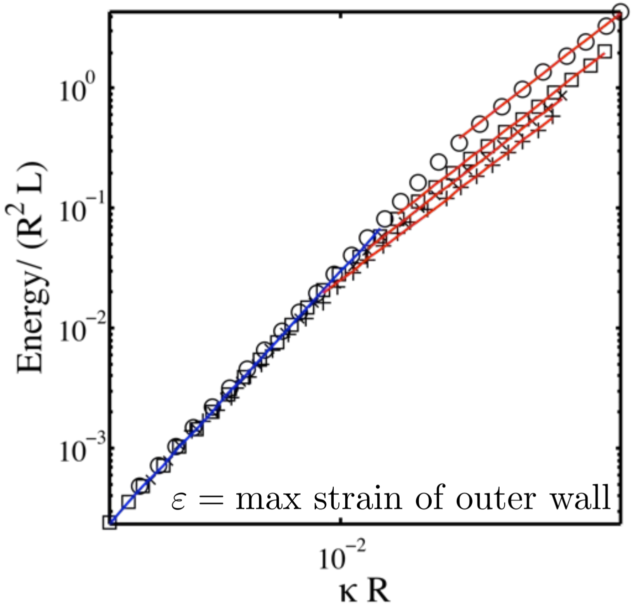
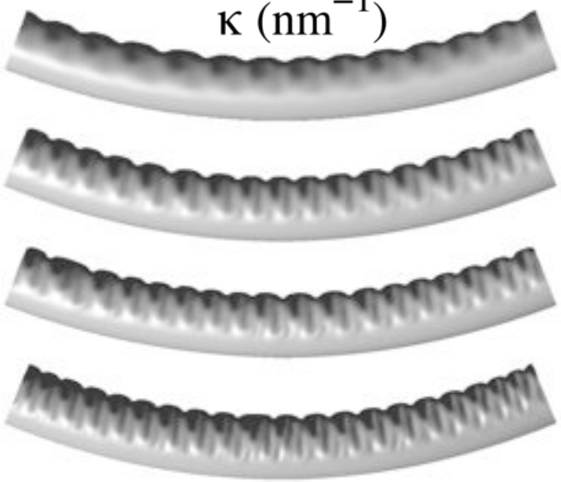
Mechanics of thick MWCNTs

The anharmonic exponent does not depend on the MWCNT diameter
The usual non-dimensional scaling collapses only the harmonic response.

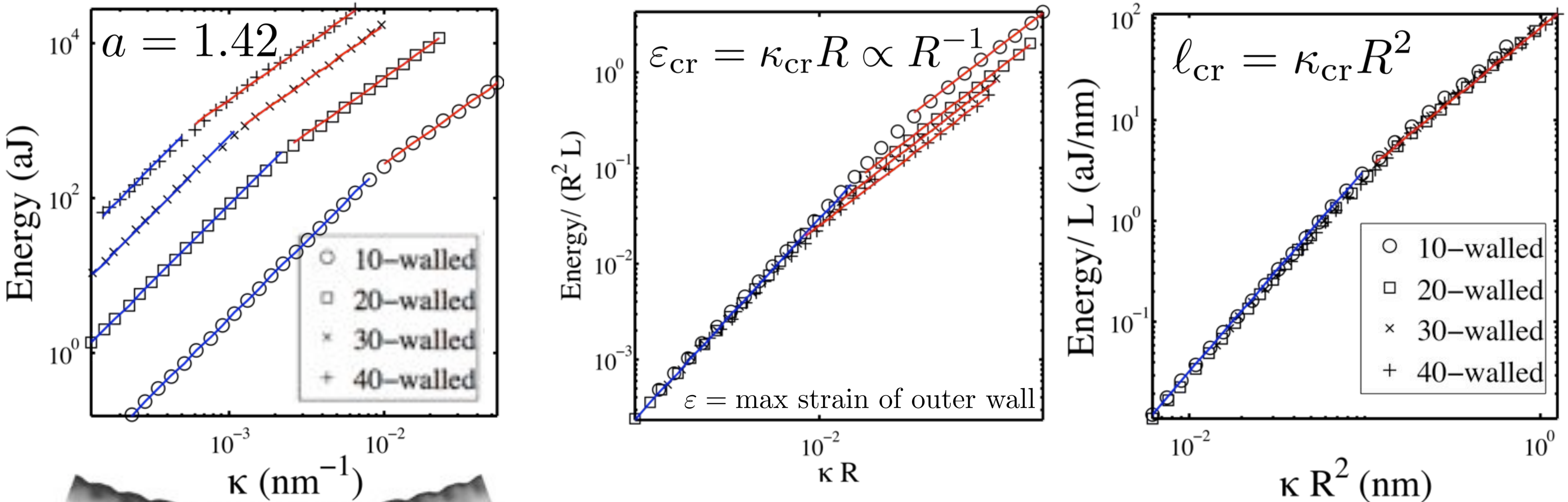


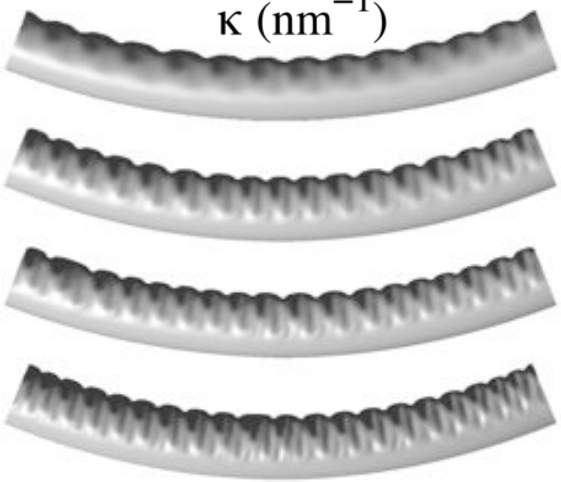




Mechanics of thick MWCNTs

Universal bending law: upon appropriate scaling we find data collapse for all the tested tubes. The law is characterized by three parameters.





Size effect. the rescaling introduces a critical lengthscale ℓ_{cr}: thicker tubes ripple earlier

$$w(\kappa) = \pi Y_s/(8t) \begin{cases} (\kappa R^2)^2 & \text{for } |\kappa R^2| \leq \ell_{cr} \\ \ell_{cr}^{2-a} |\kappa R^2|^a & \text{for } |\kappa R^2| > \ell_{cr} \end{cases}$$

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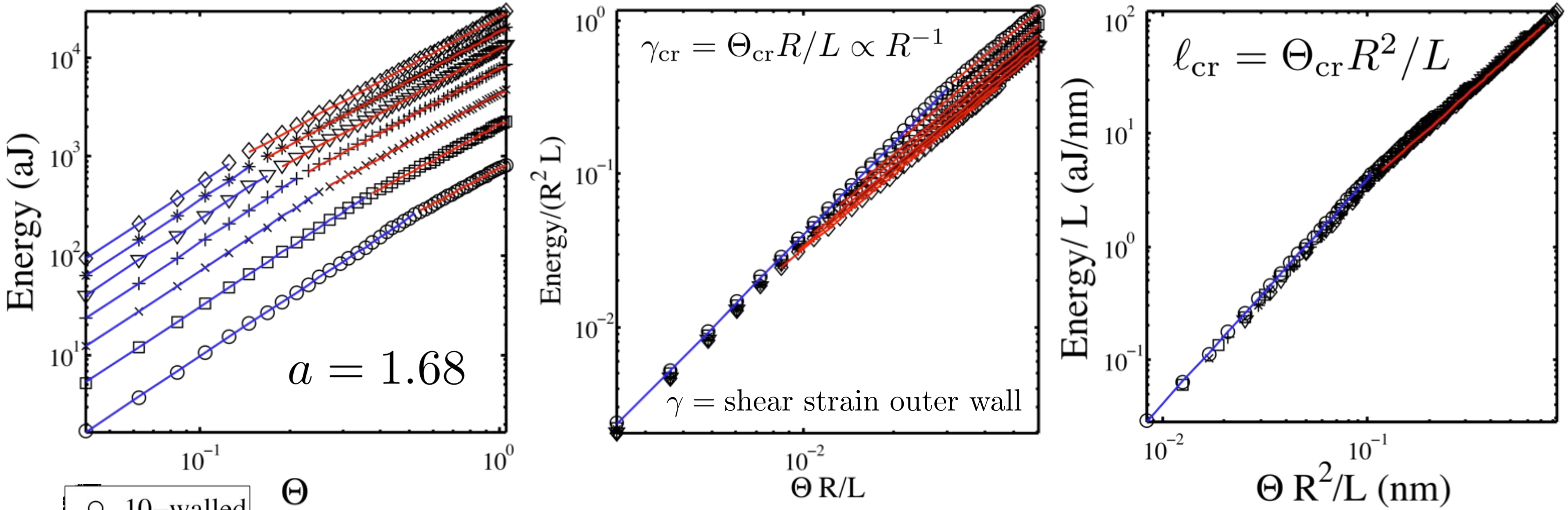
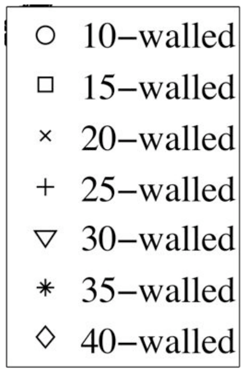
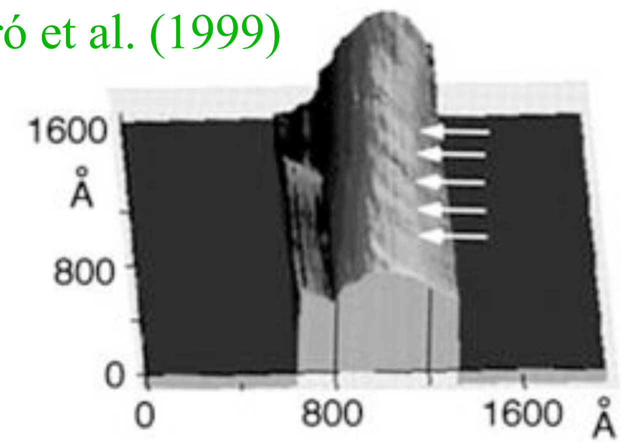
Mechanics of thick MWCNTs

MWCNTs in torsion exhibit a **universal law** upon appropriate scaling with a **strong size-effect** (the scaling introduces a lengthscale).





Forró et al. (1999)



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Mechanics of thick MWCNTs

Both for torsion and bending, we find $\ell_{cr} \sim 0.1 \text{ nm}$

	Prediction based on measurements	Actual observations
45-walled in bending [1]	$R^2\kappa = 0.6 \text{ nm} > \ell_{cr}$	TEM image of rippled tube
45-walled in bending [1]	$R^2\kappa = 0.2 \text{ nm} > \ell_{cr}$	Indirect evidence of nonlinearity and softening
12-walled in bending [1]	$R^2\kappa = 0.05 \text{ nm} < \ell_{cr}$	TEM image of smoothly bent tube
18 to 50-walled in torsion [2]	$R\gamma = 0.12 \text{ nm} > \ell_{cr}$	Indirect evidence of nonlinearity

[1] Poncharal et al, *Science* (1999)
[2] Papadakis et al, *Phys. Rev. Lett.* (2004)

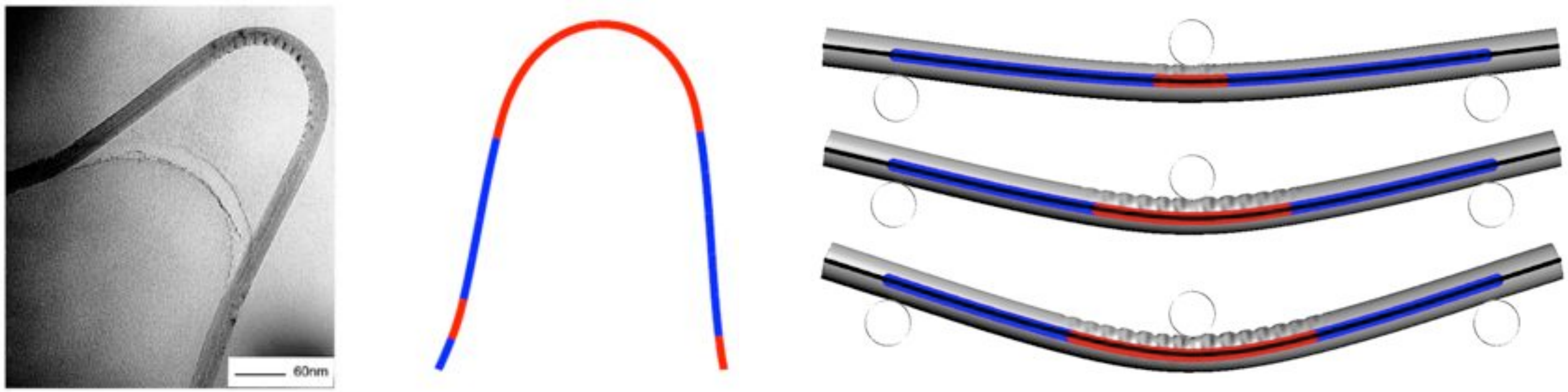
From experiments by Wong et al., *Science* (1997) $\ell_{cr} \sim 0.18 \text{ nm}$

Multiple-scale analysis

Continuum surface models from atomistic models Arroyo & Belytschko, JMPS (2002)

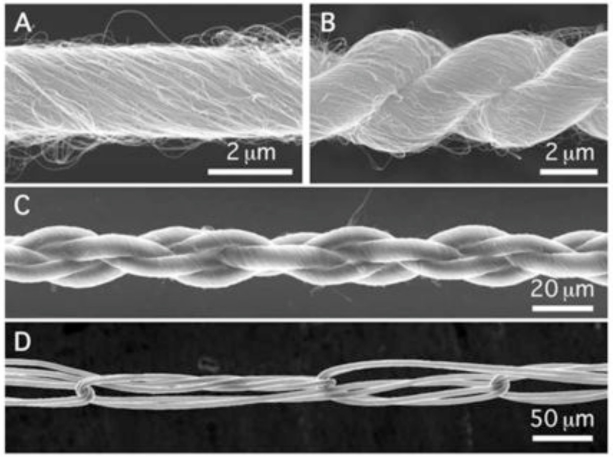
Mechanics of thick multiwalled CNTs through scaling laws

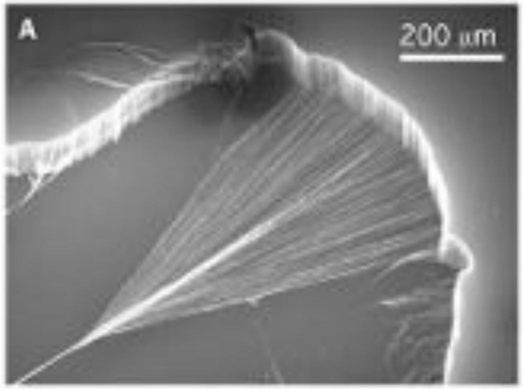
Mesoscopic models, phase-transforming elastica



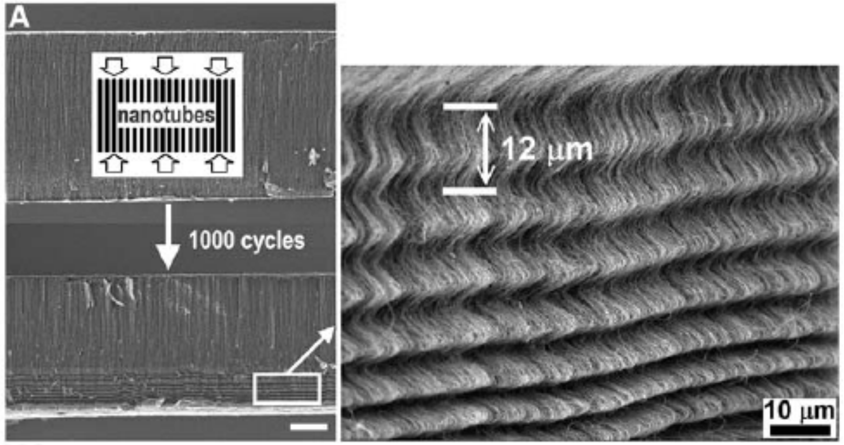
Mesoscopic model for thick MWCNTs

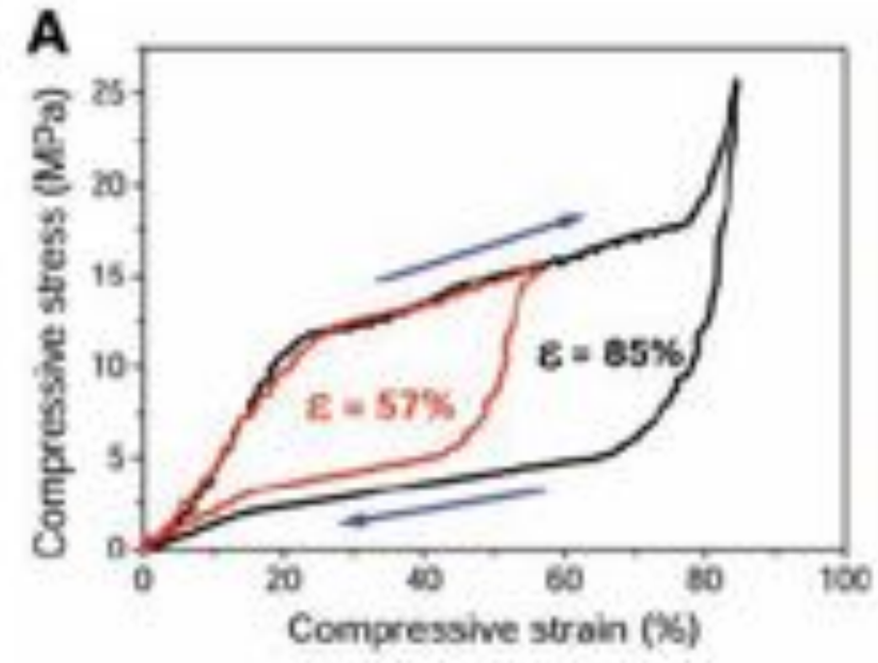
Textile technology
Zhang et al, Science (2004)





Supercompressible foam-like MWCNT films
Cao et al, Science (2005)





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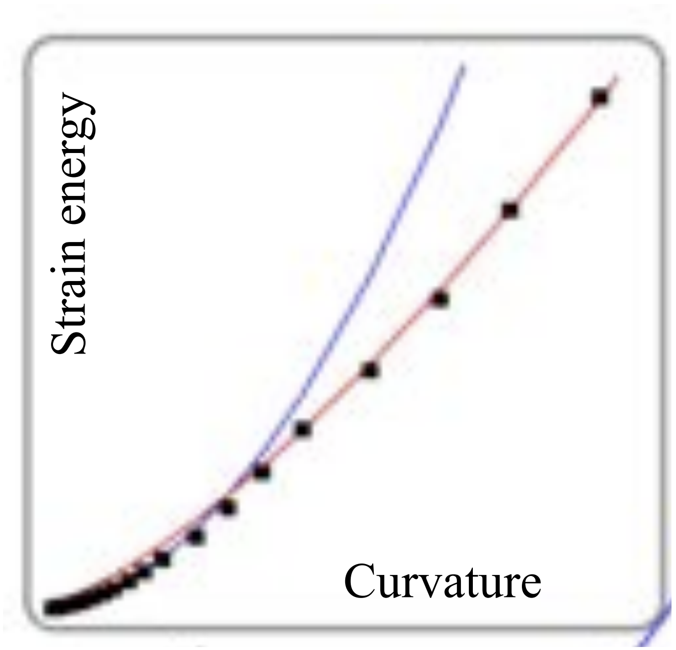
Mesoscopic model for thick MWCNTs

We have seen that for uniform bending, the strain energy per unit length follows

$$w(\kappa) = \min\left\{\frac{1}{2}B\kappa^2; C\kappa^a\right\}$$



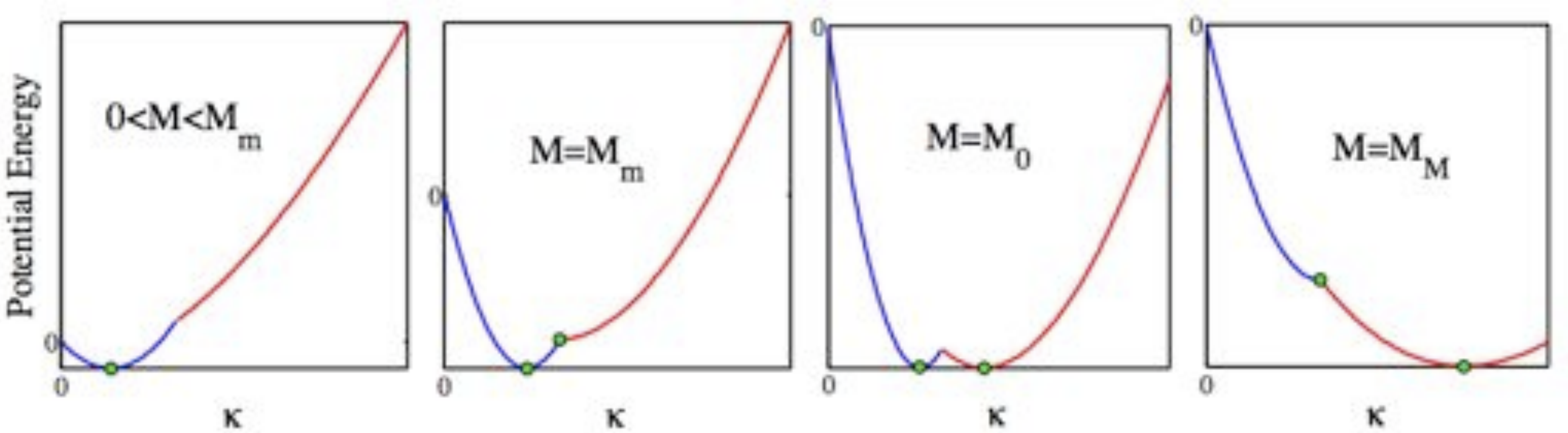
We can understand this as constitutive material response for a nonlinear beam?

M. Arroyo and I. Arias, *J. Mech. Phys. Solids* (2008).

Mesoscopic model for thick MWCNTs

Non-convex energy leads to phase mixtures, a high strain phase (rippled) and a low-strain phase (smoothly bent) *(Abeyaratne&Knowles, 2006)*,

$$P(\kappa, M) = \min\left\{\frac{1}{2}B\kappa^2; C\kappa^a\right\} - M\kappa$$



M. Arroyo and I. Arias, *J. Mech. Phys. Solids* (2008).

Mesoscopic model for thick MWCNTs

Three point bending of a 280 nm long 20-walled CNT

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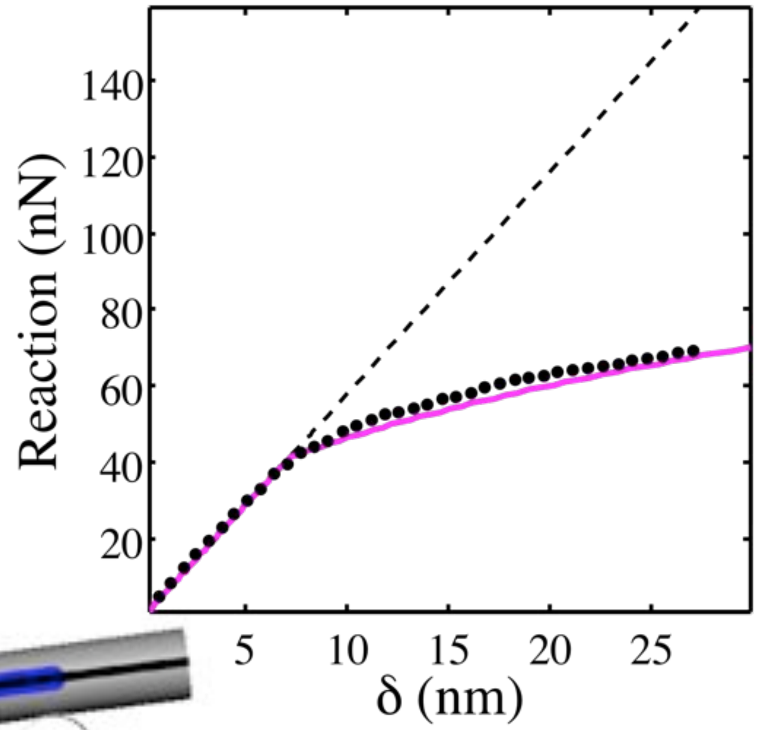
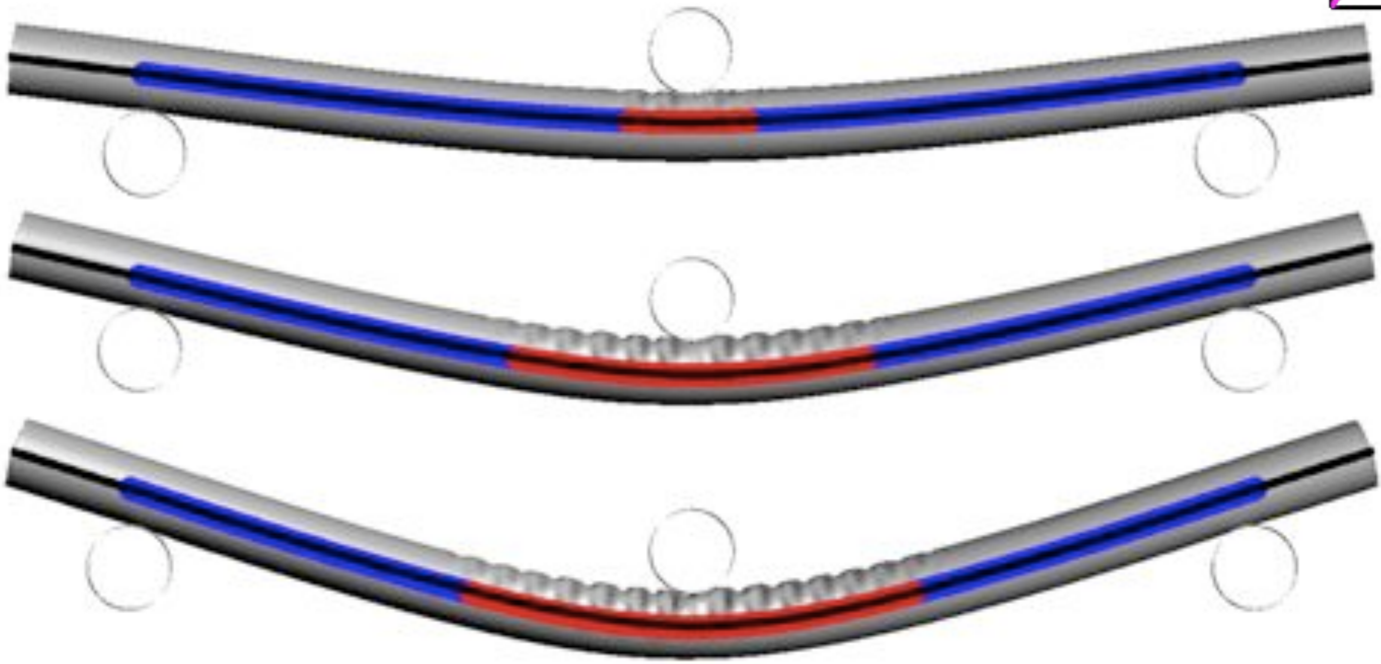
Mesoscopic model for thick MWCNTs

Validation of the model solved analytically against 3D simulations for 20-walled tube (1/2 million dofs)

Actual force is less than half the force with harmonic beam





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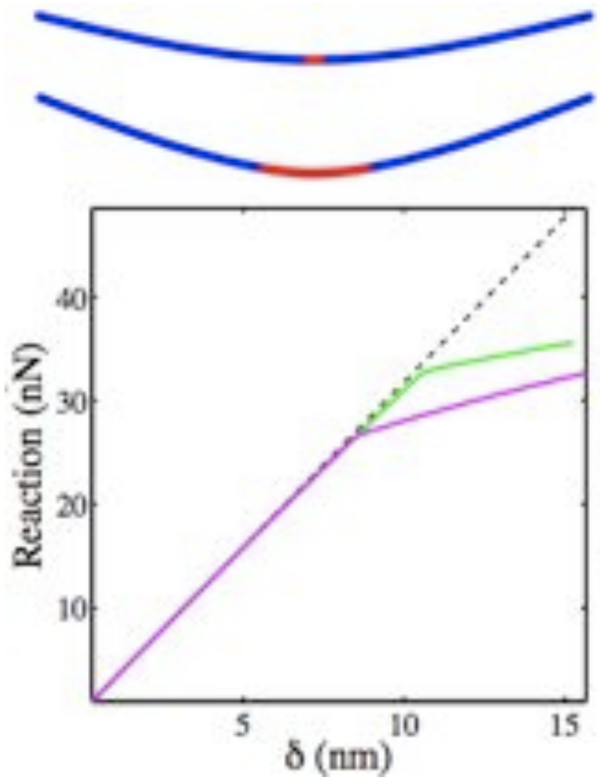
Mesoscopic model for thick MWCNTs

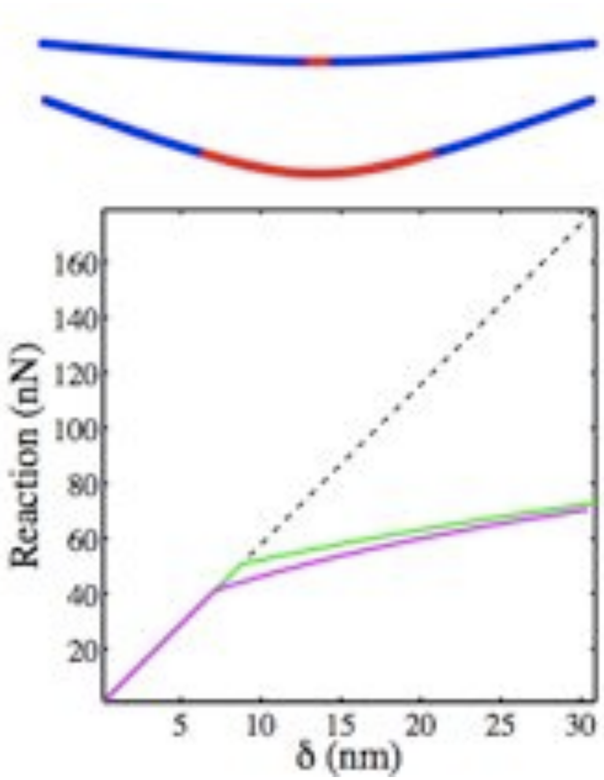
Size effect: *"Thicker tubes ripple earlier and appear softer"*

10-walled CNT 140 nm long



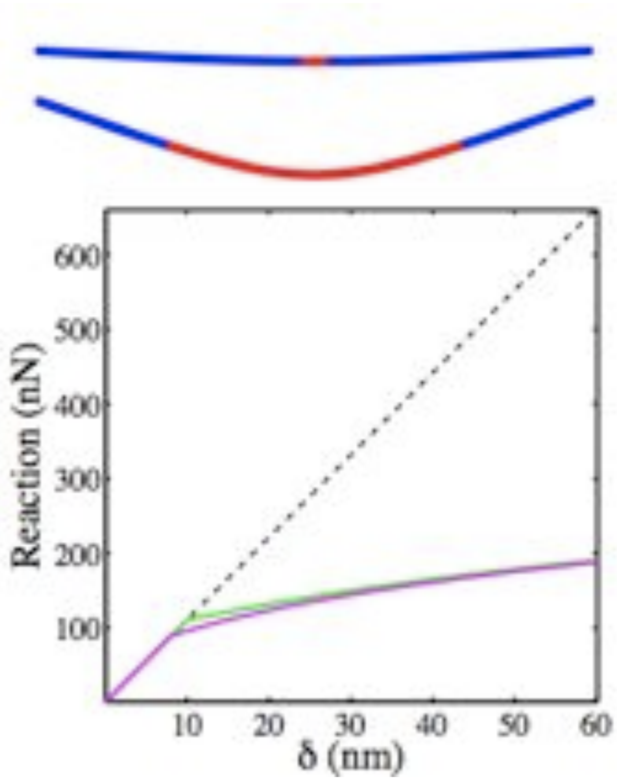
66% of elastic load

20-walled CNT 280 nm long



40% of elastic load

40-walled CNT 560 nm long

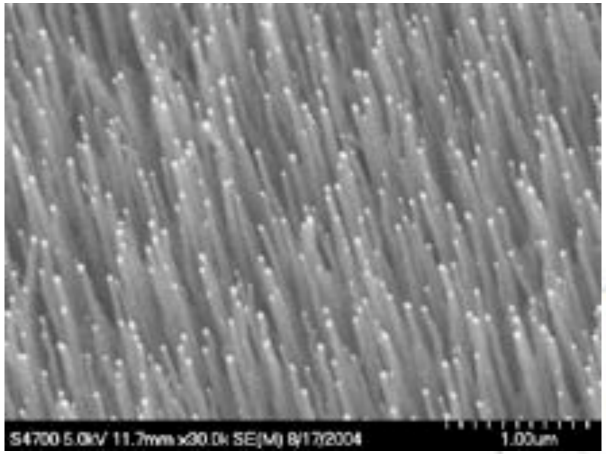


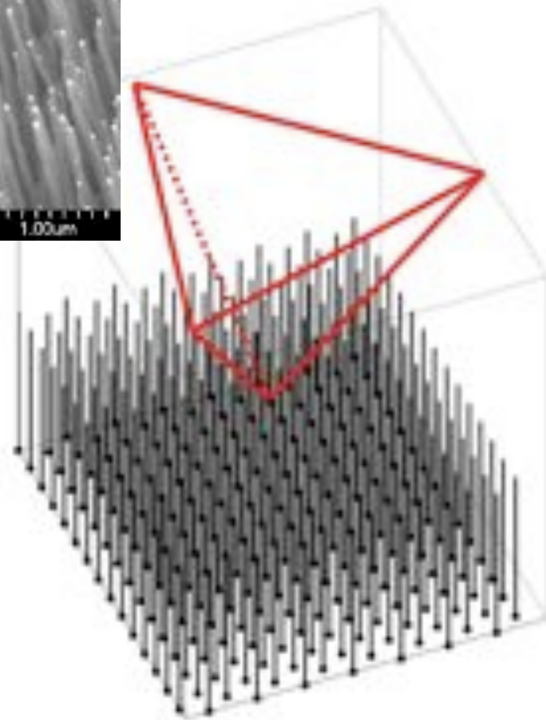
28% of elastic load

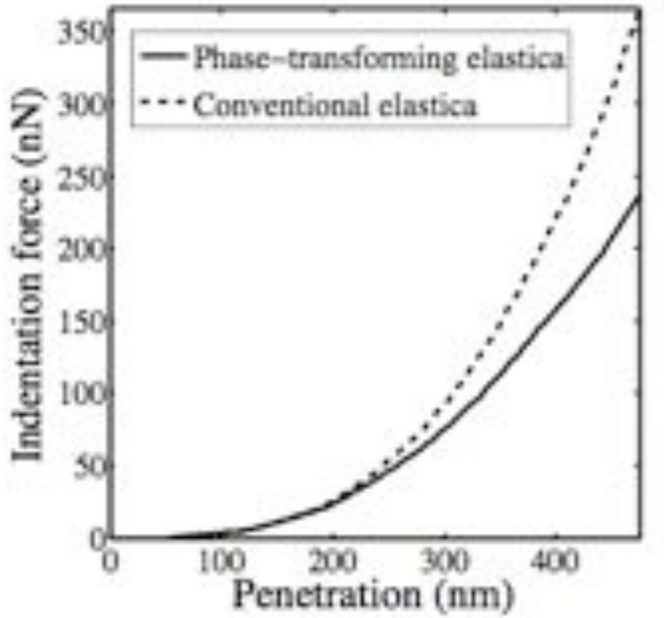
Mesoscopic model for thick MWCNTs

Nano-indentation of forests of vertically aligned MWCNTs forests, following the succesive contact model of Qi et al, *JMPS* (2003)

(40-walled 500 micon long tubes, density 200 MWCNTs/square micron)







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Summary

- We have presented a multiple-scale modelling and simulation study of MWCNTs, from atomistic interactions up to engineering scales.
- MWCNTs are prone to rippling, both in bending and torsion.
- A universal scaling law (a composite power law) has been identified, which results in **strong size effect:** ***thicker tubes are softer***.
- The super-stiff response of MWCNTs is lost for thick tubes undergoing moderate deformation subject to other than pure tension.
- MWCNTs exhibit mixtures of rippled and smoothly bend regions, as a consequence of the non-convexity of the strain energy.
- The structural behavior is strongly hysteretic, with high energy dissipation in deformation cycles: tough energy-absorbing materials.