Sliding prevention in super-strong self-collapsed nanotube cables (and graphene nanoscrolls)

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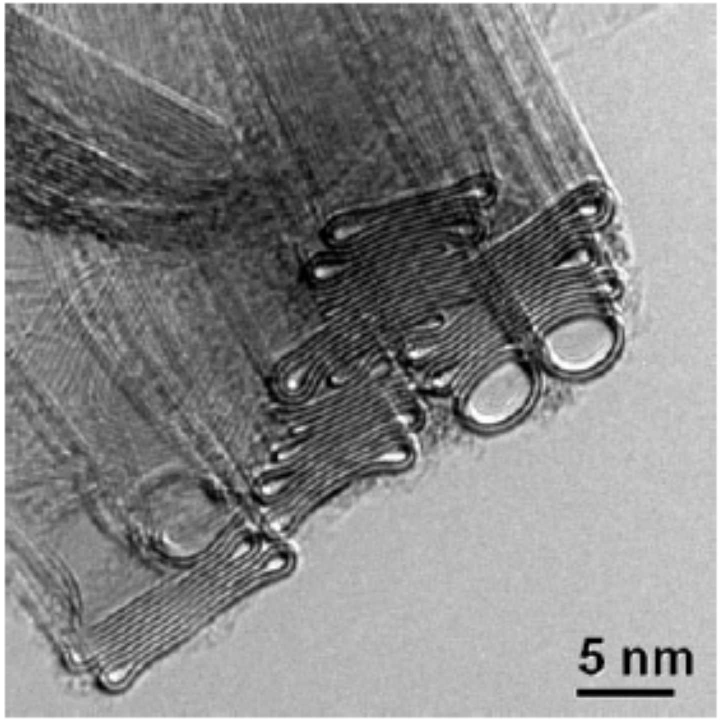
TRIESTE, TRENDS IN NANOTRIBOLOGY 2011

Self-collapsed nanotubes in a bundle



Experimental evidence:
Motta et al., Advanced Materials, 2007

Theory:

Journal of the Mechanics and Physics of Solids 58 (2010) 1397–1410

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

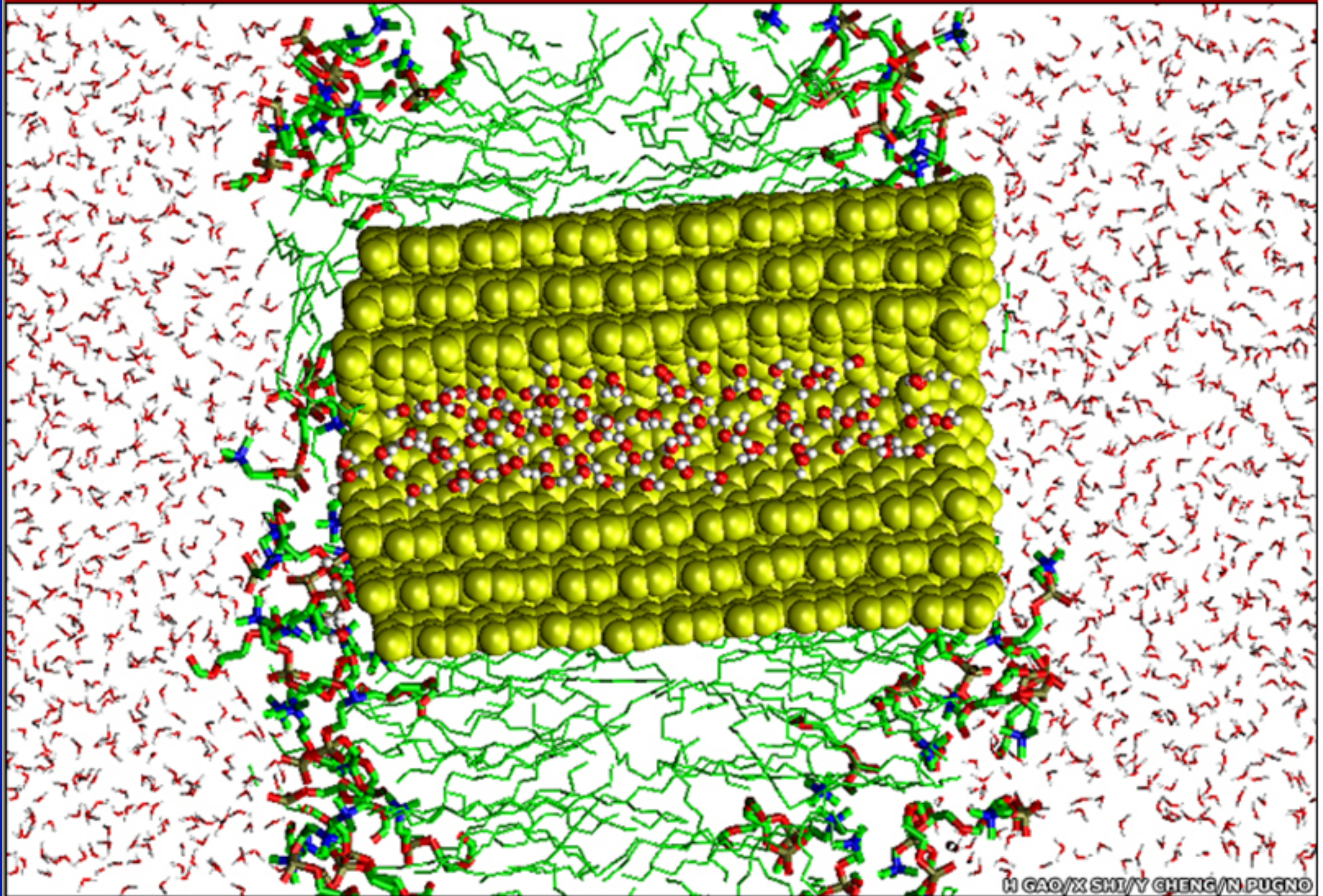
ELSEVIER

The design of self-collapsed super-strong nanotube bundles

Nicola Maria Pugno [a,b,c,*]

Graphene nanoscrolls

BBC NEWS



Graphene, a promising nanomaterial for future electronics, can be rolled up into "nanoscrolls", shown here in cross section in yellow. Simulations reported in the journal Small show these scrolls can be controlled using a tiny voltage to direct the flow of water or even drugs across cell membranes.

Buckling pressure: theory

$$p_C = \frac{3N^{\alpha}D}{R^3}$$

Buckling pressure of long cylindrical shells

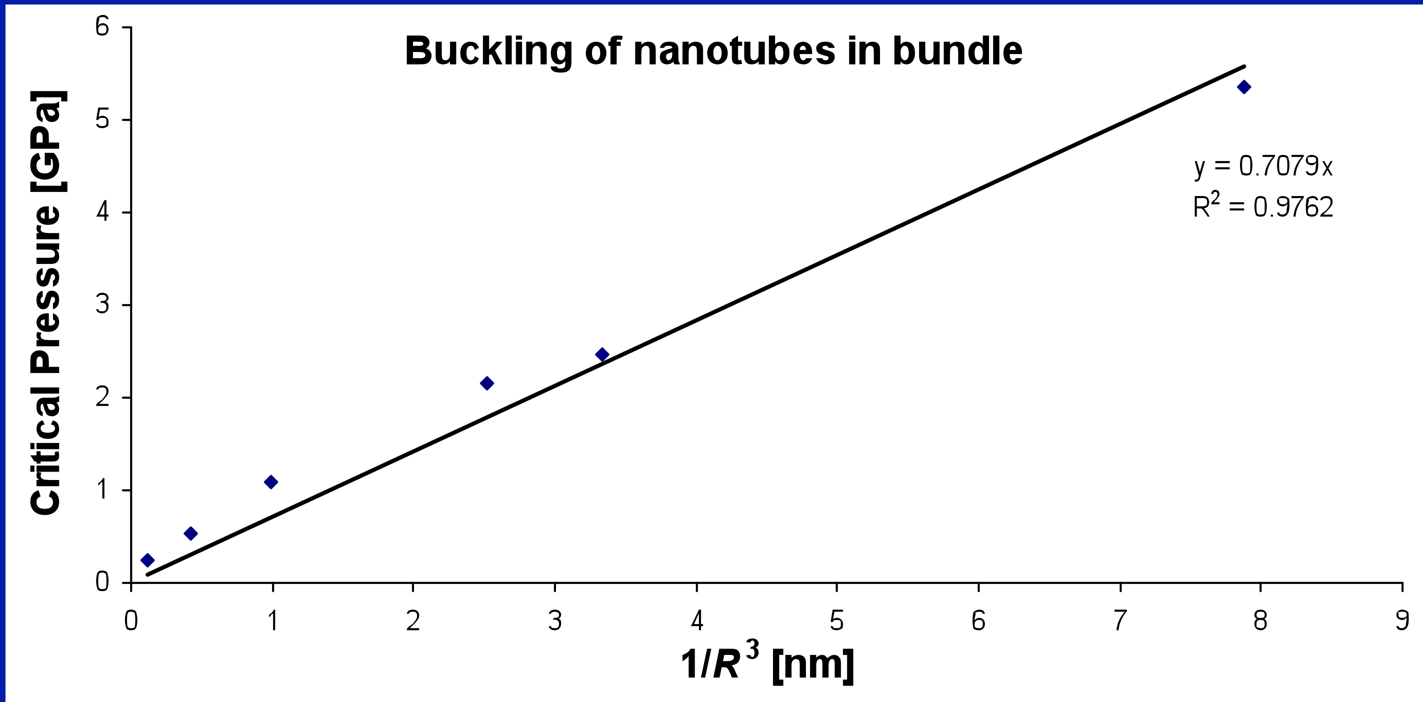
$$p = \frac{\gamma}{R}$$

Pressure around a cylindrical cavity in a "liquid-like" materal: interaction between the nanotubes

$$p_C = \frac{3N^{\alpha}D}{R^3} - \frac{\gamma}{R}$$

Buckling pressure of nanotubes in a bundle

Buckling pressure: theory vs MD



Theory vs MD (MD by Elliot et al., Physical Review Letters, 2004)

Self-collapse: theory

$$p_C = 0$$

Self-collapse condition

$$R \geq R_C^{(N)} = \sqrt{\frac{3N^\alpha D}{\gamma}} = \sqrt{6}R_0^{(N)}$$

Self-collapse radius

$$D = 0.11\,\mathrm{nN}\cdot\mathrm{nm}$$

$$\gamma = 0.18\,\mathrm{N/m}$$

$$\alpha \approx 2$$

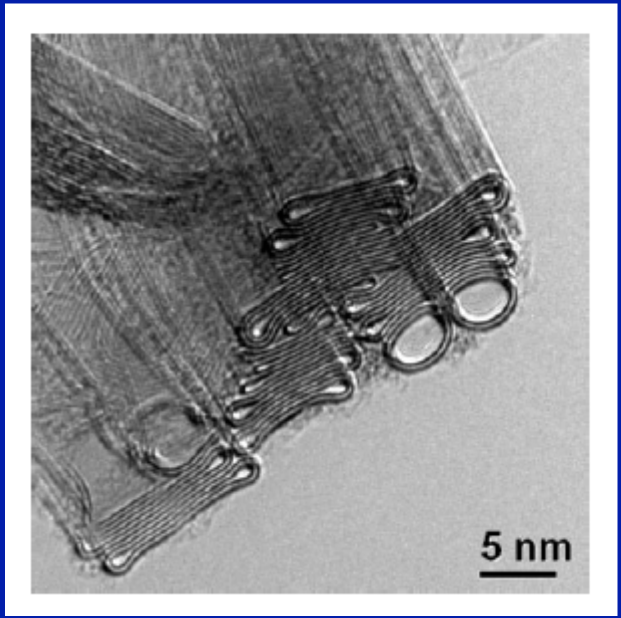
$$2R_C^{(1)} \approx 2.7\,\mathrm{nm}$$

$$2R_C^{(2)} \approx 5.4\,\mathrm{nm}$$

$$2R_C^{(3)} \approx 8.1\,\mathrm{nm}$$

Self-collapse: theory vs experiments

Nanotube number	Number N of walls	Diameter of the internal wall [nm]	Collapsed (Y/N) Exp. & Theo.
1	1	4.6	Y
2	1	4.7	Y
3	1	4.8	Y
4	1	5.2	Y
5	1	5.7	Y
6	2	4.2	N
7	2	4.6	N
8	2	4.7	N
9	2	6.2	Y
10	2	6.5	Y
11	2	6.8	Y
12	2	6.8	Y
13	2	7.9	Y
14	2	8.3	Y
15	2	8.3	Y
16	2	8.4	Y
17	3	14.0	Y



Sliding failure

$$\mathrm{d}\Phi - F\mathrm{d}u - 2\gamma\left(P_C + P_{vdW}\right)\mathrm{d}z = 0$$

Fracture Mechanics

$$\sigma_C = 2\cos\beta\sqrt{E\gamma\frac{P}{S}}$$

Predicted bundle strength

$$\sigma_C^{(theo,N)} = 2\sqrt{\frac{E\gamma}{Nt}}$$

Maximum strength

$$\sigma_C^{(\max)} = \sigma_C^{(theo,1)} = 48.5\mathrm{GPa}$$

$$\sigma_C^{(theo,2)} = 34.3\mathrm{GPa}$$

$$\sigma_C^{(theo,3)} = 28.0\mathrm{GPa}$$

Strength increment due to the self-collapse

$$\frac{\sigma_C^{(0)}}{\sigma_C^{(O)}} = \sqrt{\frac{2\pi R + P_{vdW}}{2\pi R\left(1 - \frac{1}{R}\sqrt{\frac{N^{\alpha} D}{2\gamma}}\right) + P_{vdW}}}$$

Strength self-collapsed/strength not self-collapsed

$$R \geq R_C^{(N)} = \sqrt{\frac{3N^{\alpha} D}{\gamma}}$$

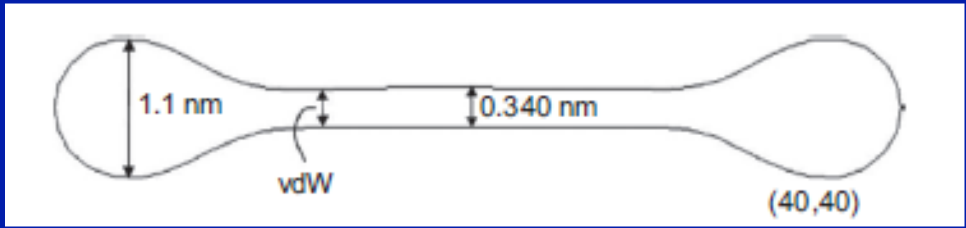
Self-collapsed radius

$$\left.\frac{\sigma_C^{(0)}}{\sigma_C^{(O)}}\right|_{\max} = \sqrt{\frac{1}{1 - \frac{1}{\sqrt{6}}}} \approx 1.30$$

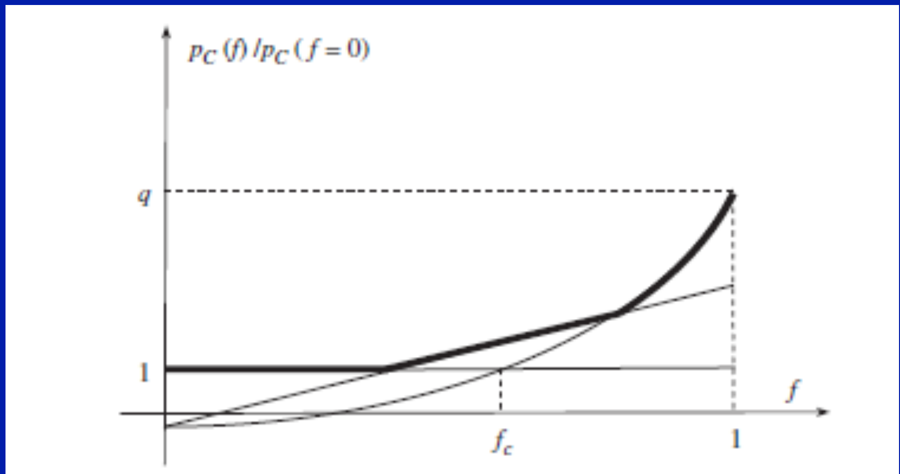
Maximum ratio

Strength increment up to 30%

Other related calculations



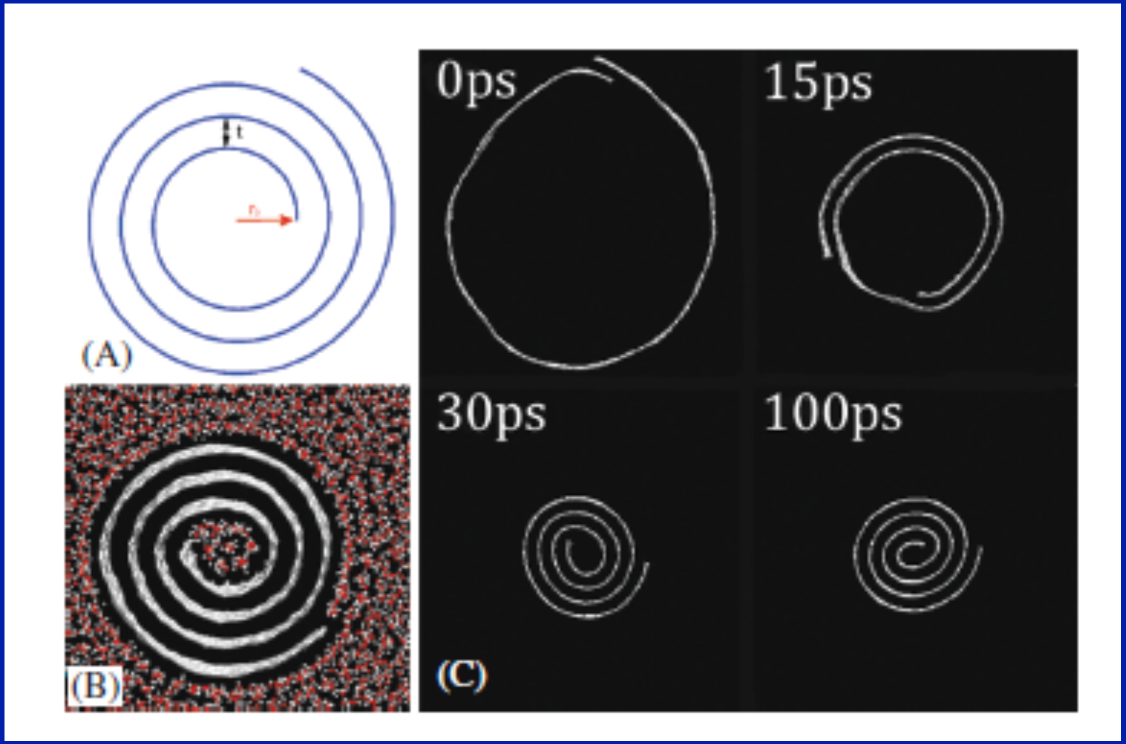
Dog-bone configurations



Peapods:
fullerens in a nanotube

Critical buckling pressure
vs fullerene (linear fractional)
content

Graphene nanoscrolls



Work performed
in collaboration
with the H. Gao' group
(LAMMPS MD simulations)

Self-rolling of graphene nanoribbons due to the competition between surface (vdW), initially prevailing, and elastic (bending), finally prevailing, energies: formation of nanoscrolls (SEE MOVIE)

Geometry

$$r = r_0 + \frac{t}{2\pi}\vartheta$$

Geometry

$$B \approx \int_0^{2\pi N} \left(r_0 + \frac{t}{2\pi}\vartheta \right) \mathrm{d}\vartheta = 2\pi r_0 N + \pi t N^2$$

Length

$$B = \frac{\pi}{t}(R^2 - r_0^2)$$

Constant length: one degree of freedom,
e.g. the core radius

$$\frac{\mathrm{d}N}{\mathrm{d}r_0} = -\frac{N}{R},$$

$$\frac{\mathrm{d}R}{\mathrm{d}r_0} = 1 + \frac{\mathrm{d}N}{\mathrm{d}r_0}t = 1 - \frac{Nt}{R} = \frac{r_0}{R}.$$

Elastic bending energy

$$\frac{\mathrm{d}W}{\mathrm{d}A}(r) = \frac{D}{2}\frac{1}{r^2}$$

Bending energy per unit area

$$W = \frac{\pi DL}{t}\ln\left(\frac{R}{r_0}\right)$$

Stored bending energy

$$\mathrm{d}W = \frac{\pi DL}{t}\left(\frac{\mathrm{d}R}{R} - \frac{\mathrm{d}r_0}{r_0}\right)$$

Change in bending energy

Energy minimization

$$dW = -\frac{\pi D L}{t}\frac{R^2 - r_0^2}{R^2}\frac{dr_0}{r_0}$$

Bending energy

$$d\Gamma = 2\pi\gamma L(dr_0 + dR) = 2\pi\gamma L\left(1 + \frac{r_0}{R}\right)dr_0$$

Surface energy

$$\frac{dE_{tot}}{dr_0} = \frac{dW}{dr_0} + \frac{d\Gamma}{dr_0}$$

Total energy

Equilibrium can be calculated imposing dE=0

Equilibrium core radius

$$\frac{2\gamma t}{D} = \frac{1}{r_0} - \frac{1}{\sqrt{(Bt/\pi) + r_0^2}}$$

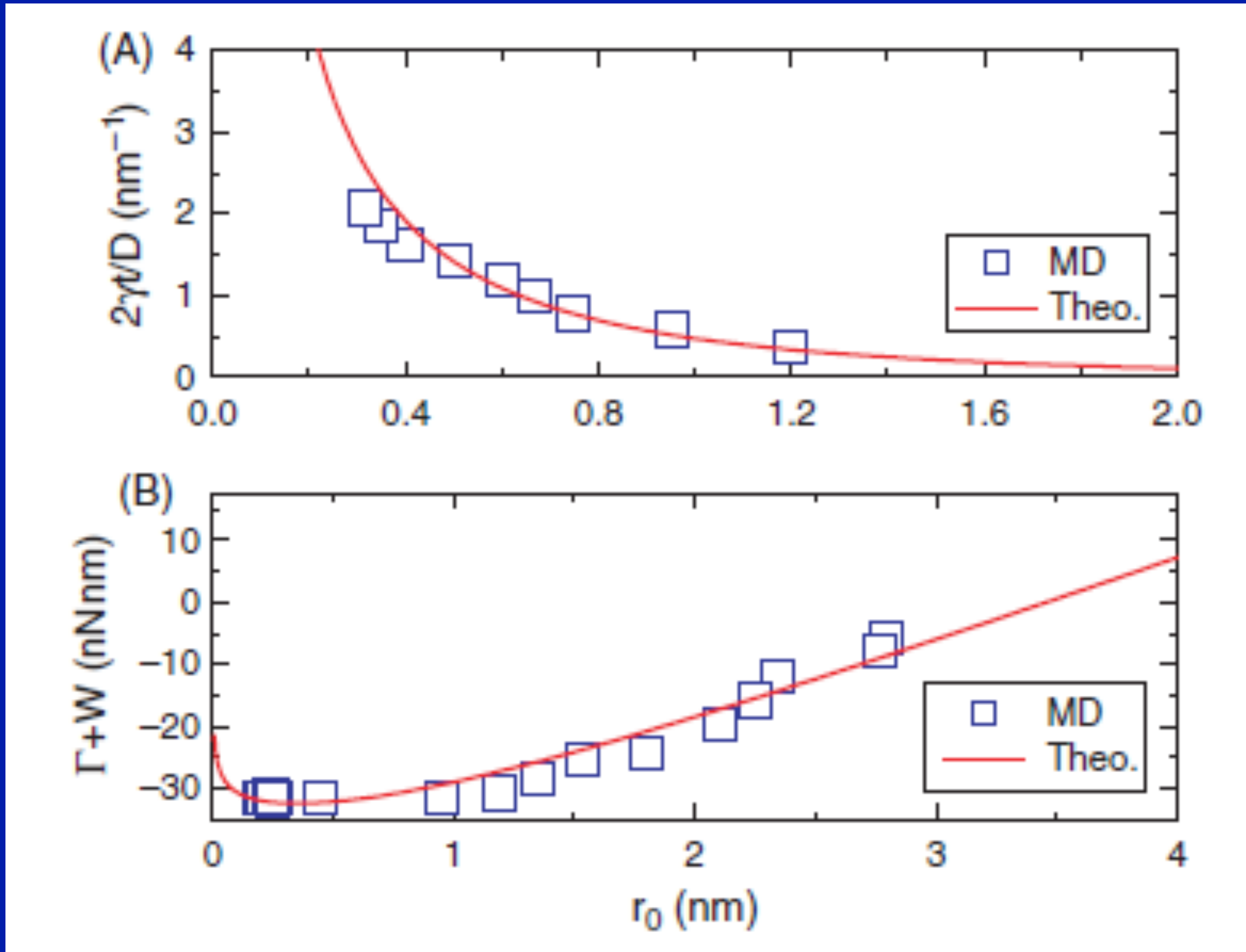
Equilibrium

Theo/MD comparison	r_0 (nm)		R (nm)	
	MD	Theo.	MD	Theo.
Zigzag$^{(v)a}$	0.32	0.37	1.50	1.65
Armchair$^{(v)}$	0.25	0.36	1.42	1.64
Chiral$^{(v)}$	0.23	0.33	1.56	1.61
Zigzag$^{(w)}$	0.60	0.59	1.59	1.7
Armchair$^{(w)}$	0.61	0.56	1.60	1.68
Chiral$^{(w)}$	0.68	0.79	1.67	1.73
Zigzag$^{(v,\ half\,vdW)b}$	0.67	0.63	1.76	1.73

[a](v) means in vacuum and (w) means in water, [b]50% reduction in van der Waals interaction.

Close agreement with MD simulations

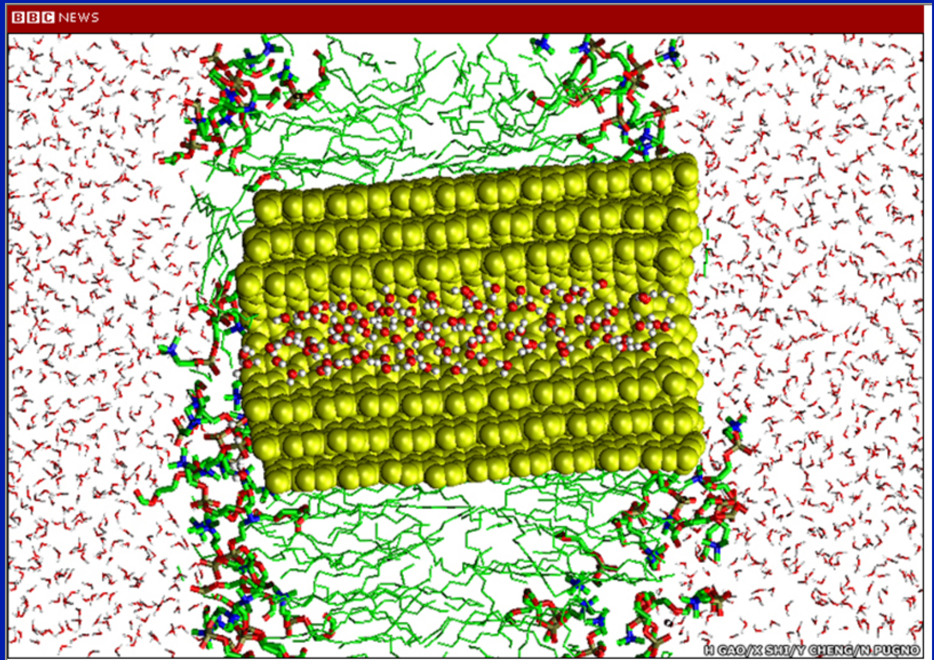
Theory vs MD



No best fit

J. Comput. Theor. Nanosci. 2010, Vol. 7, No. 3

Nano-channels



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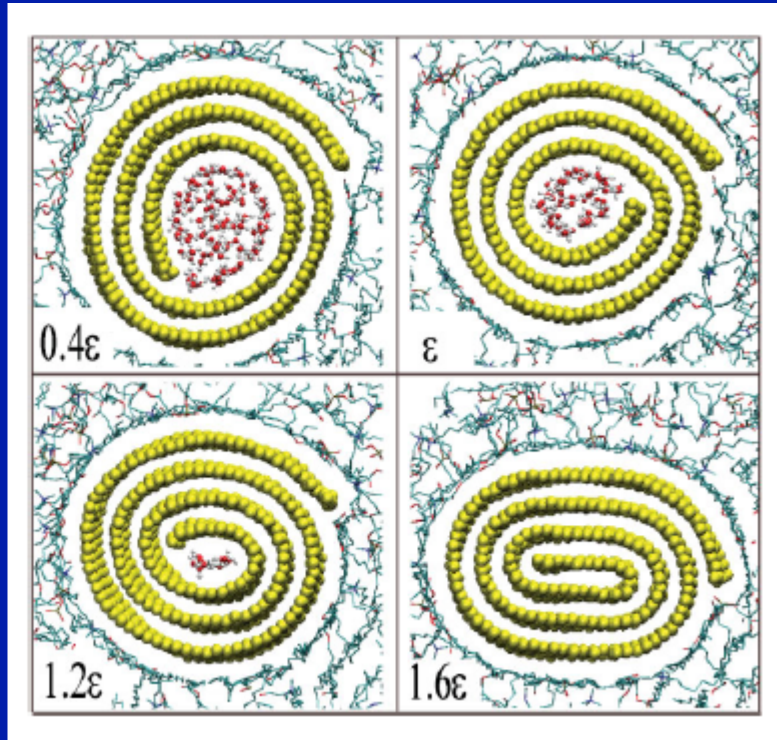


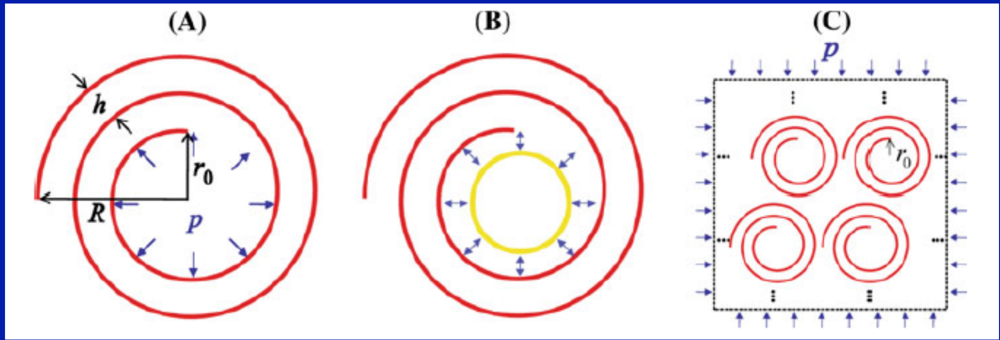
$$\gamma_{\text{dipole}} = \frac{1}{2\pi L}\,\frac{d\Phi_{\text{dipole}}}{d(r_0 + R)}$$

$$\gamma_{\text{eff}} = \gamma_{\text{vdW}} + \gamma_{\text{dipole}}$$

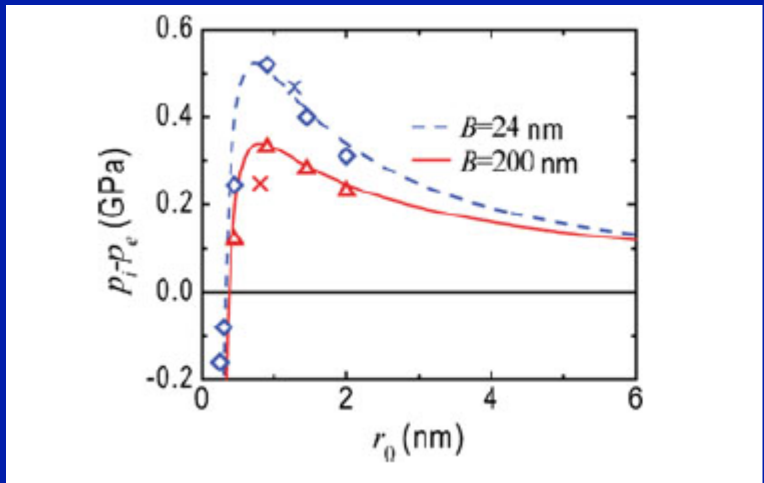
small 2010, 6, No. 6, 739–744

By applying an electrical field we can tune the effective surface energy and the core radius and thus we can control the fluid (here water) flow

Energy storage: modeling



Pressure inside the nanoscroll: new energy term in the equilibrium equation



Gigapascals are required to open (in an explosive way, i.e. the process is unstable) the nanoscroll.

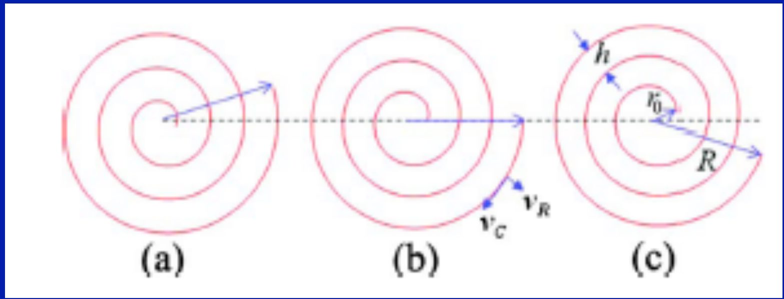
$$\mathrm{d}\Phi = -p_i 2\pi L r_0 \mathrm{d}r_0 + p_e 2\pi L R \mathrm{d}R = -2\pi L r_0 \mathrm{d}r_0 p,$$

$$\frac{\mathrm{d}E}{\mathrm{d}r_0} = \frac{\mathrm{d}W}{\mathrm{d}r_0} + \frac{\mathrm{d}\Gamma}{\mathrm{d}r_0} + \frac{\mathrm{d}\Phi}{\mathrm{d}r_0}.$$

Int J Fract
DOI 10.1007/s10704-010-9545-y

Published online: 12 October 2010

Nano-oscillators: modeling



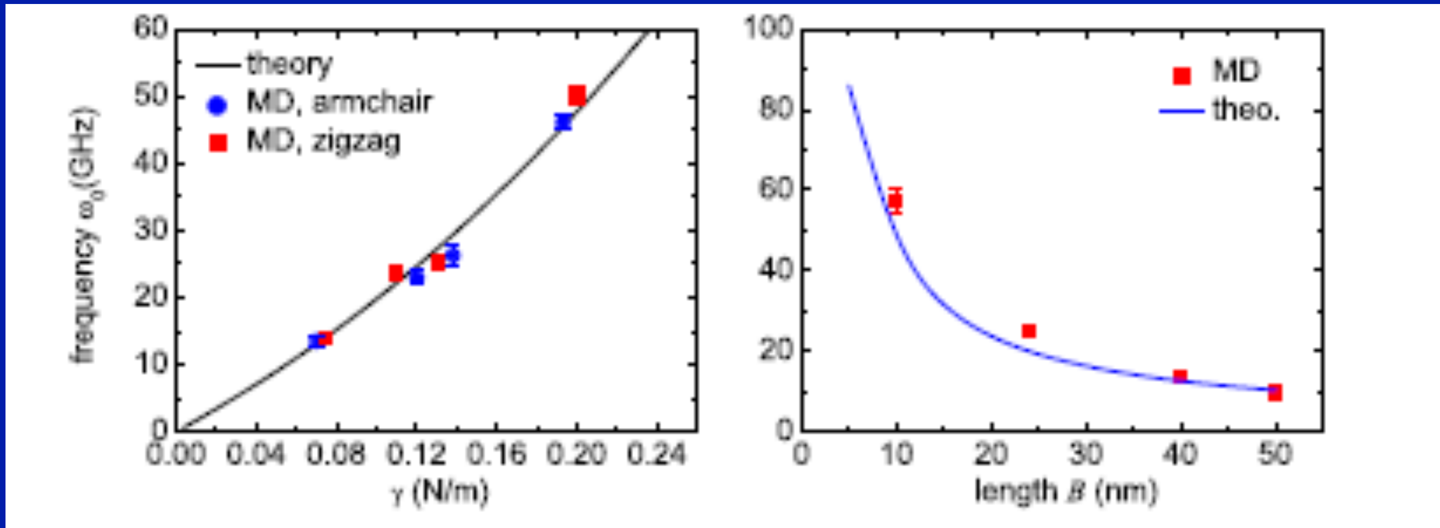
Lagrange Equation
and breathing motion

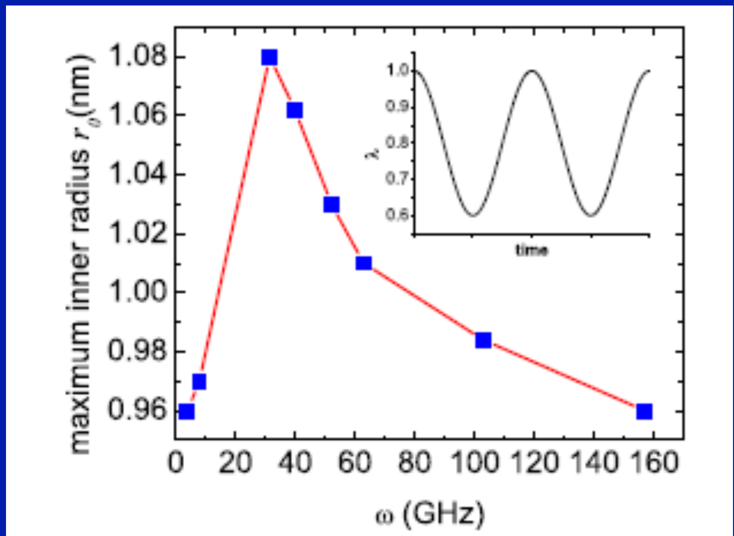
$$\frac{\pi D L}{h}\left(1-\frac{r_0^2}{Bh/\pi + r_0^2}\right)\frac{1}{r_0} - 2\pi\gamma L\left(1+\frac{r_0}{\sqrt{Bh/\pi + r_0^2}}\right)$$
$$+ 2\pi r_0 L p - \frac{4\pi^2 M}{h^2}\left(r_0\dot{r}_0^2 + r_0^2 \ddot{r}_0\right) - C\dot{r}_0 = 0$$

Natural frequency of the
system can be deduced

$$\omega_0 = \sqrt{\frac{\pi D}{4\rho B^3 h^2}\left[\frac{\alpha^3(\alpha+3)}{(1+\alpha)^2} + 2\frac{\gamma}{D}\sqrt{\frac{Bh^3}{\pi}}\frac{\alpha^2\sqrt{\alpha}}{(1+\alpha)^{3/2}} - 2\frac{Bh^2 p}{\pi D}\alpha\right]}$$

Nano-oscillators: Theory vs MD

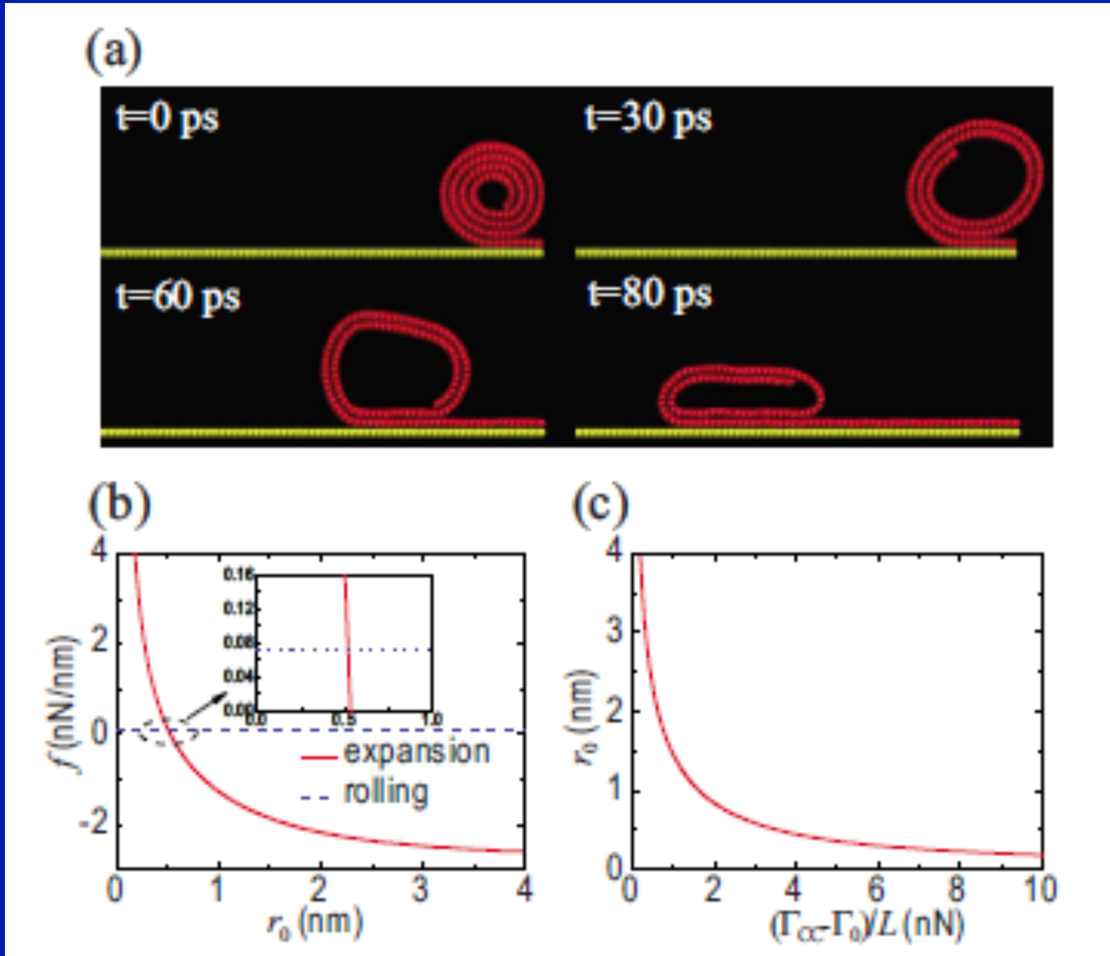




APPLIED PHYSICS LETTERS **95**, 163113 (2009)

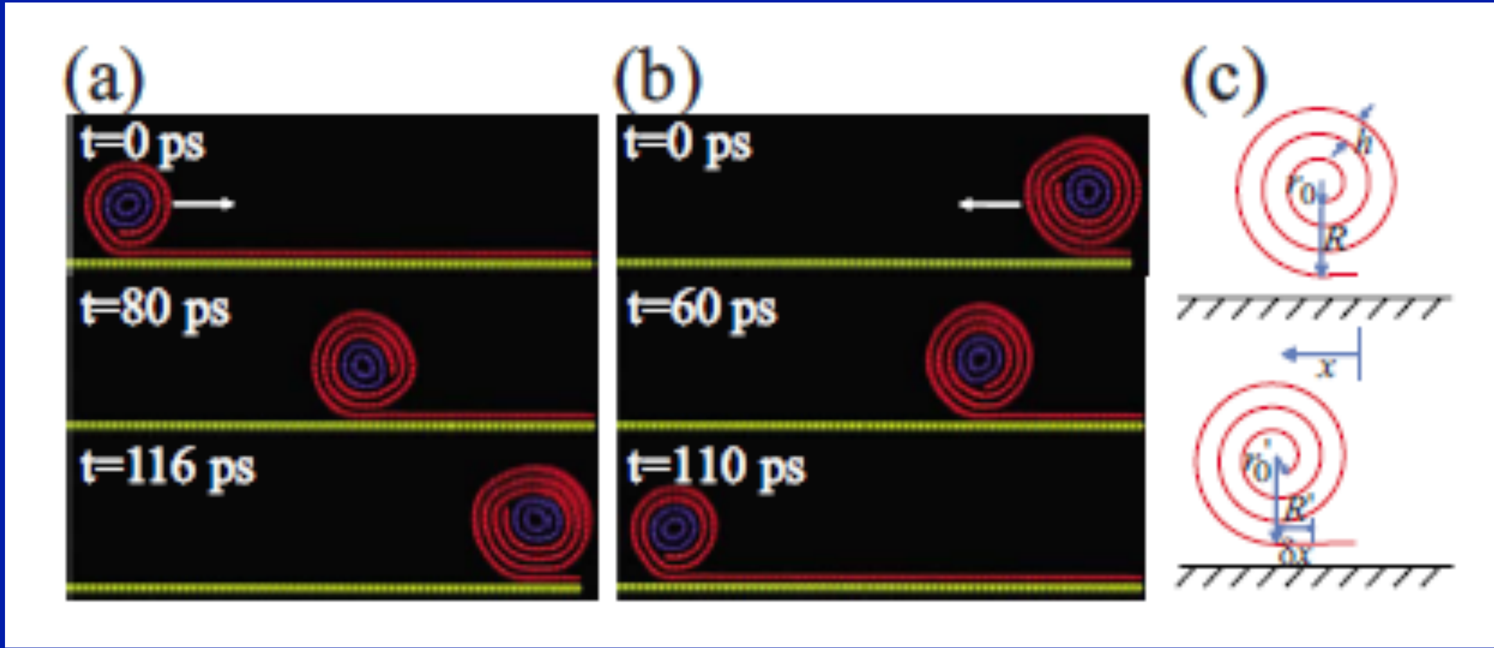
We can open the nanoscroll under resonance!
Smart nanovectors.

Nano-motors: the first tentative



But expansion prevails over rolling:
we fixed the core radius inserting a CNT...

Nano-motors: modeling



$$\frac{f}{L} = -\frac{1}{L}\frac{\delta V}{\delta x} = \gamma_{CS} - \gamma_{CC} + \frac{D}{2\left[(B-x)h/\pi + r_0^2\right]}.$$

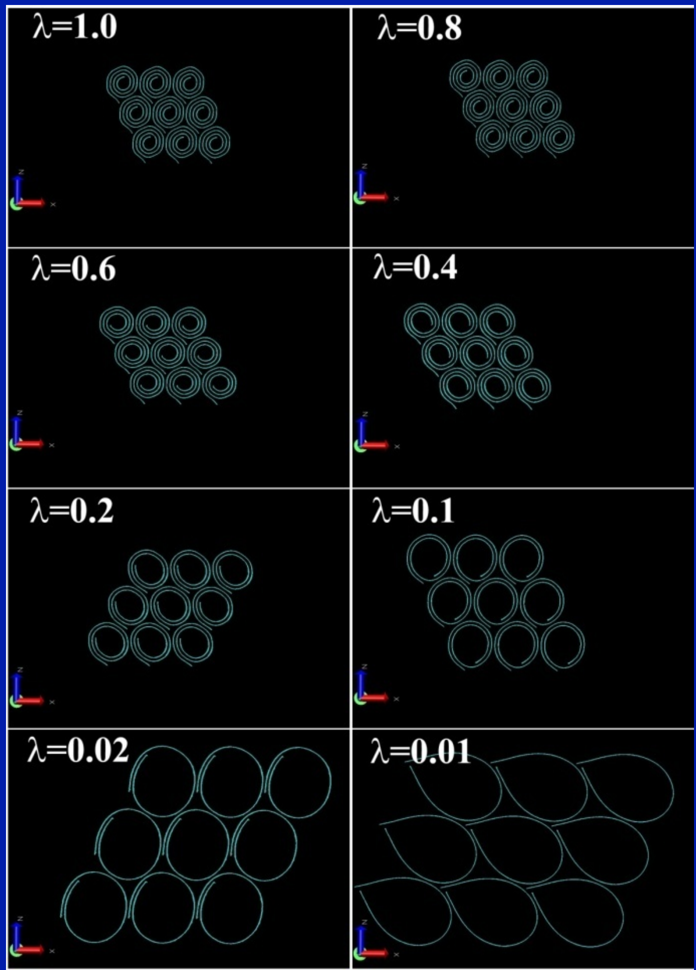
APPLIED PHYSICS LETTERS **96**, 053115 (2010)

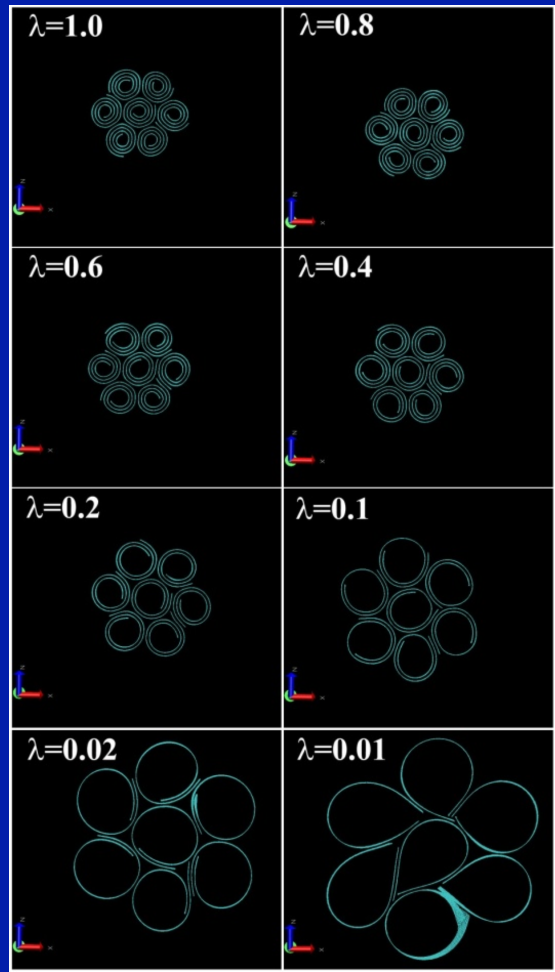
$$6\left[\rho(B-x) + M_0/L\right]\ddot{x} - 3\rho\dot{x}^2 + 4(\gamma_{CC} - \gamma_{CS}) - 2D/\left[(B-x)h/\pi + r_0^2\right] = 0.$$

Net (positive or negative) driving force
and Lagrange equation

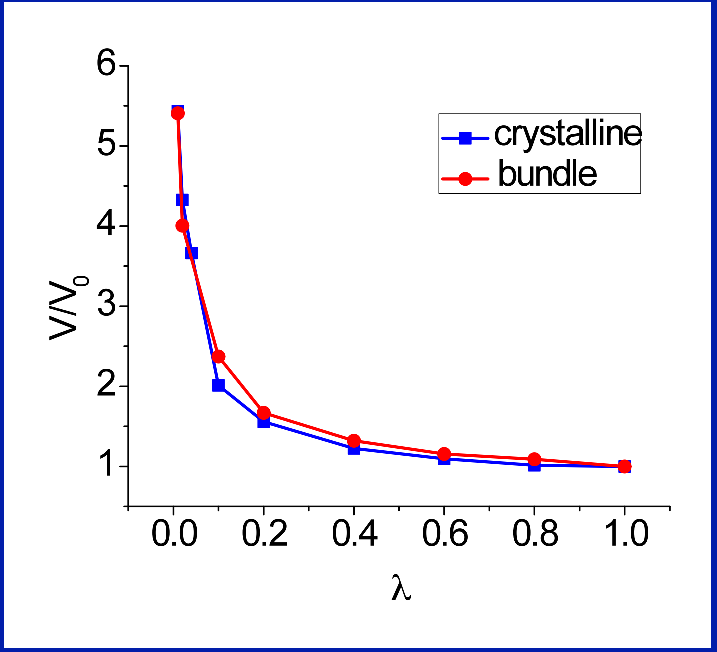
Nanoscroll crystals

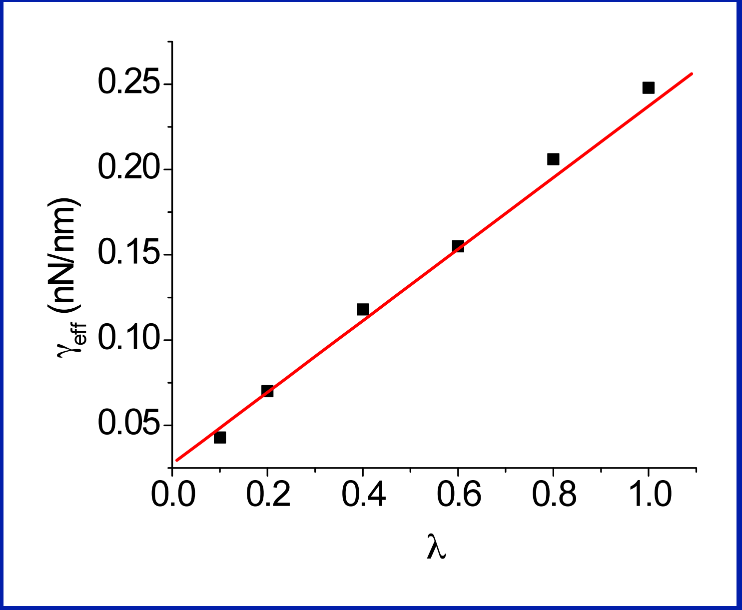
Theory and MD (still to be submitted,
similar to the previously discussed one for nanotube bundle/crystals)

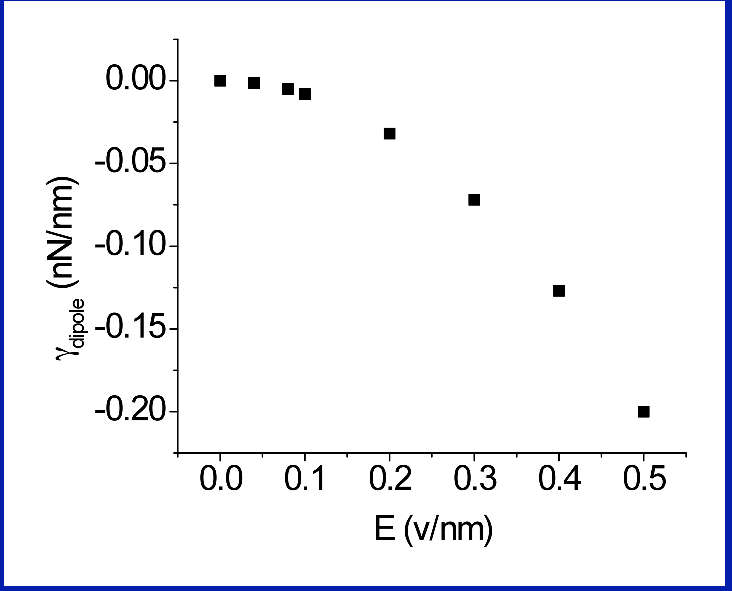


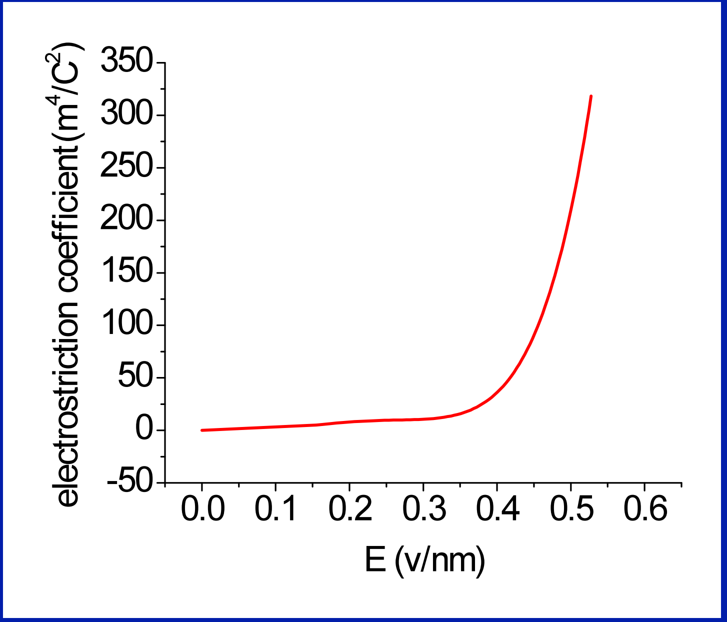


Gigantic electro-striction









Thanks

I thank:

the European Research Council (ERC Starting Grant 2011 on “Bio-inspired hierarchical super nanomaterials) for support;

the conference organizers for the invitation;

and you for your attention!

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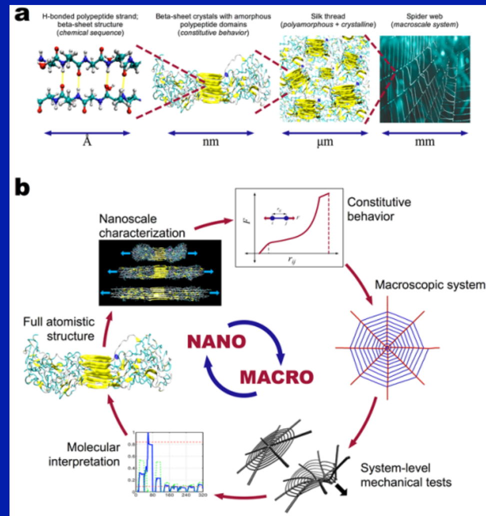
Spider silk and bio-inspired super-tough fibers

NANO LETTERS
pubs.acs.org/NanoLett

Molecular and Nanostructural Mechanisms of Deformation, Strength and Toughness of Spider Silk Fibrils

Andrea Nova,[†,∥] Sinan Keten,[†] Nicola M. Pugno,[†,⊥,#,∇] Alberto Redaelli,[∥] and Markus J. Buehler*[,†,‡,§,⊥]

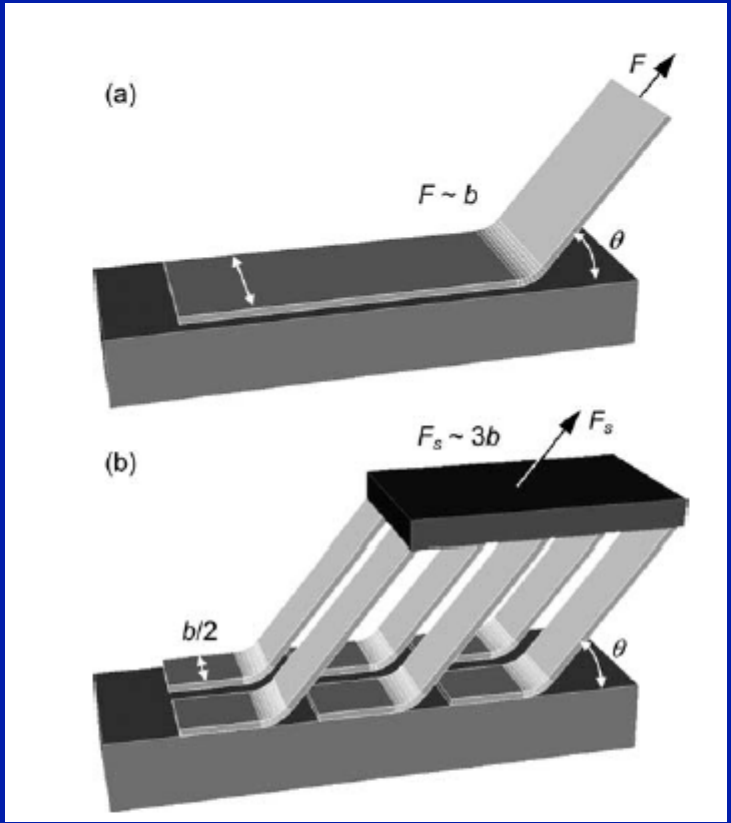


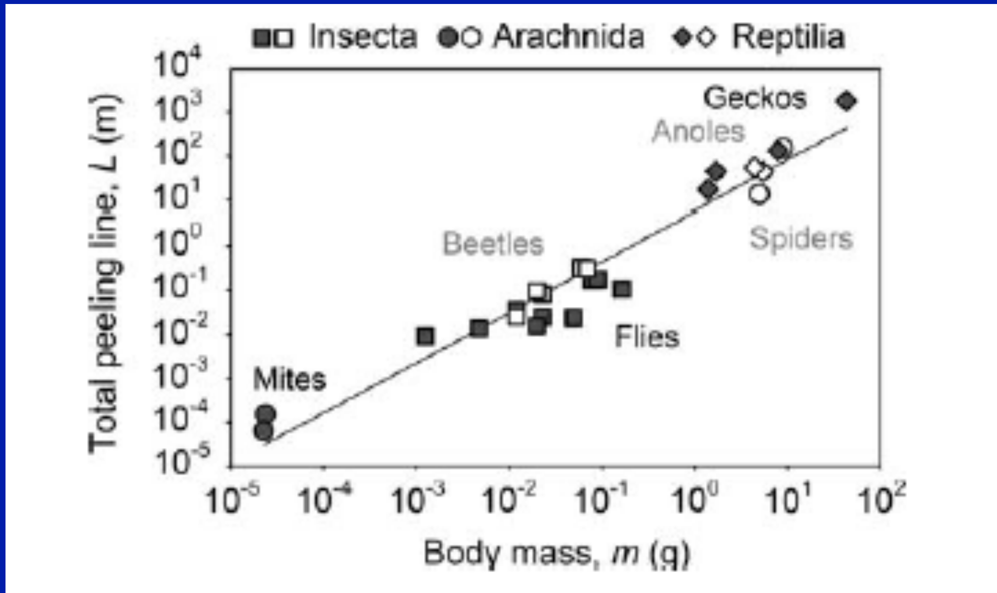
PHYSICAL REVIEW E **82**, 056103 (2010)

Hierarchical simulations for the design of supertough nanofibers inspired by spider silk

Federico Bosia,[1,*] Markus J. Buehler,[2,3,†] and Nicola M. Pugno[2,3,4,5,‡]

Km-long crack front in geckos





Experiments on several insects, spiders and lizards (from S. N. Gorb, M. Varenberg, N. M. Pugno, Soft Matters, 2010) Peeling line proportional to mass supports our model