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Broken chiral symmetry in sliding carbon nanotubes

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Dynamical Chiral Symmetry Breaking: from nano-sliding to nano-rotation

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Outline

Sliding nano-friction: experiment, theory

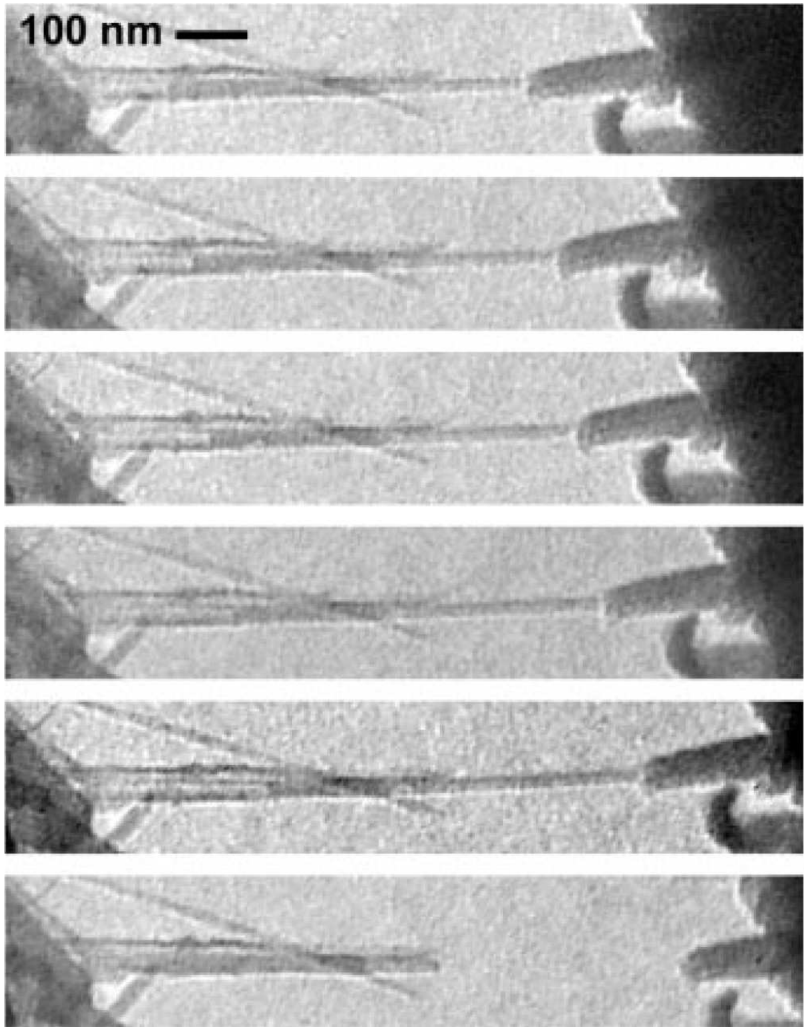
Intertube interaction: size effect, atomic potential

→ Frictional peaks and speed plateaus

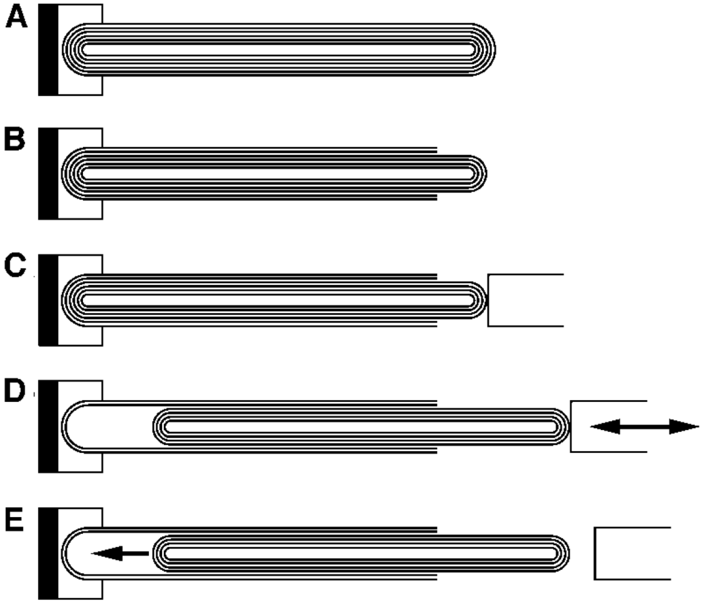
→ Dynamical chiral symmetry breaking: simulation, theory

Why interesting? A way to rotate in nano-scale

Sliding nano-friction between CNTs



Cumings and Zettl, Science **289**, 602 (2000)

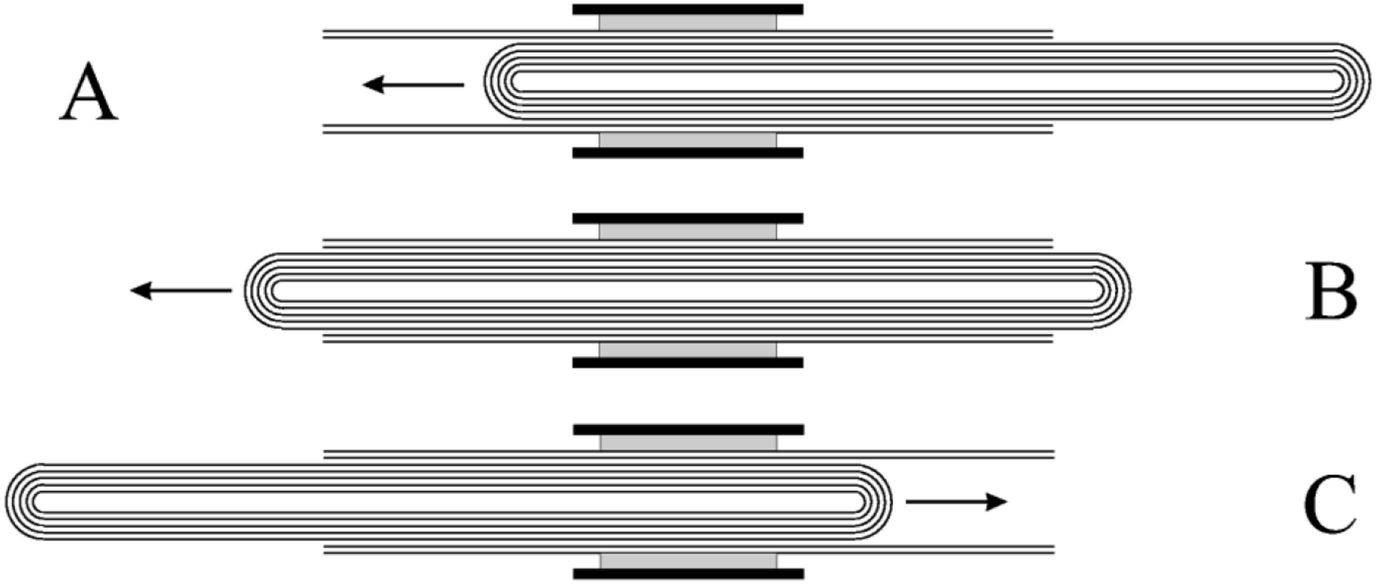


1) Retraction force (total): 9 nN

2) Static friction force: < 0.024 pN/atom (sheer stress 6.6 bar)

3) Dynamics friction: < 0.015 pN/atom (sheer stress 4.3 bar)

Sliding nano-friction between CNTs

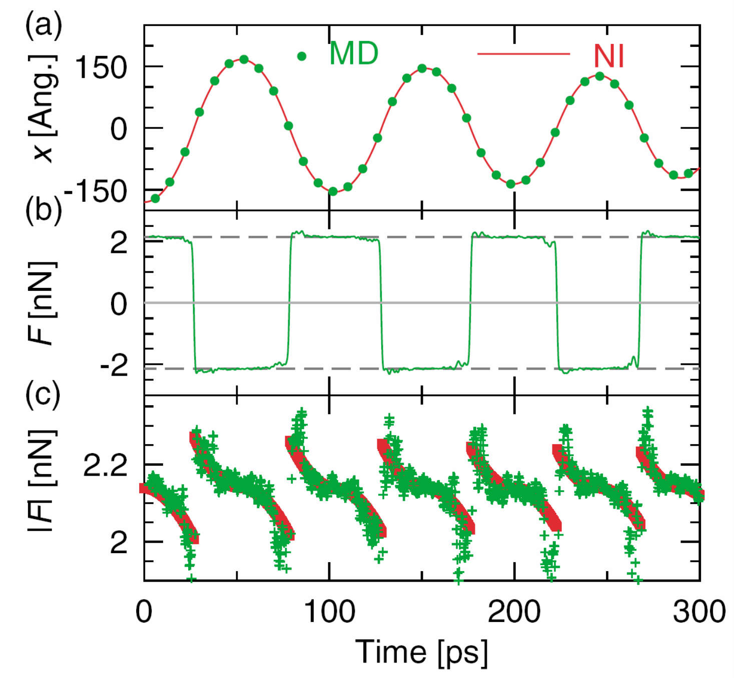


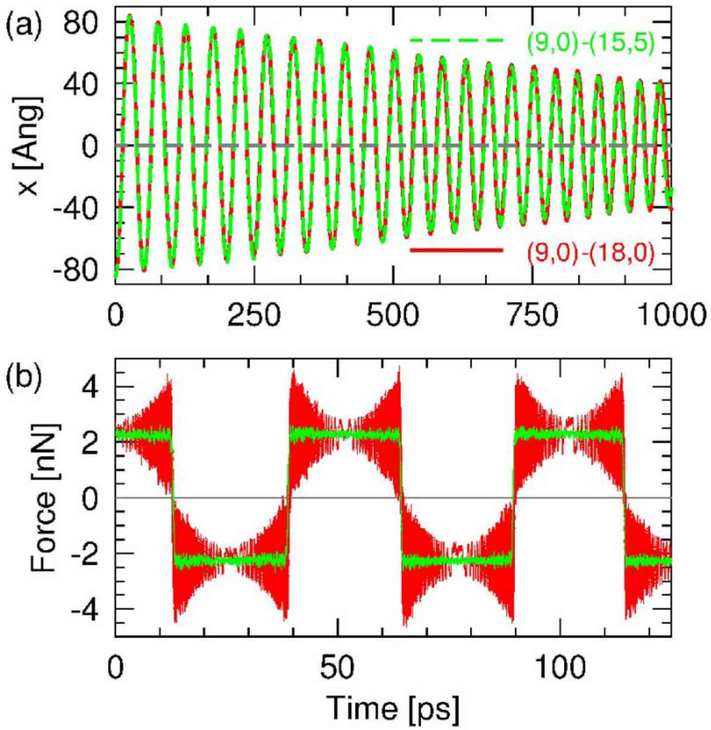
Nanotubes as gigahertz oscillators

Interactions: capped termination – open termination

Zheng and Jiang, Phys. Rev. Lett. **88**, 045503 (2002)

Sliding nano-friction between CNTs





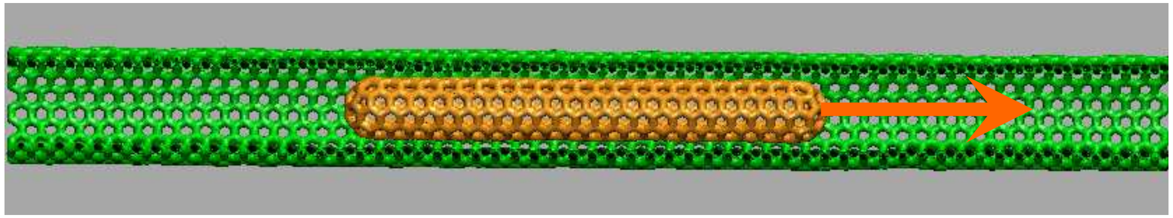
20 nm (5,5)-(16,2), 10 nm (9,0)-(18,0), and 10 nm (9,0)-(15,5)

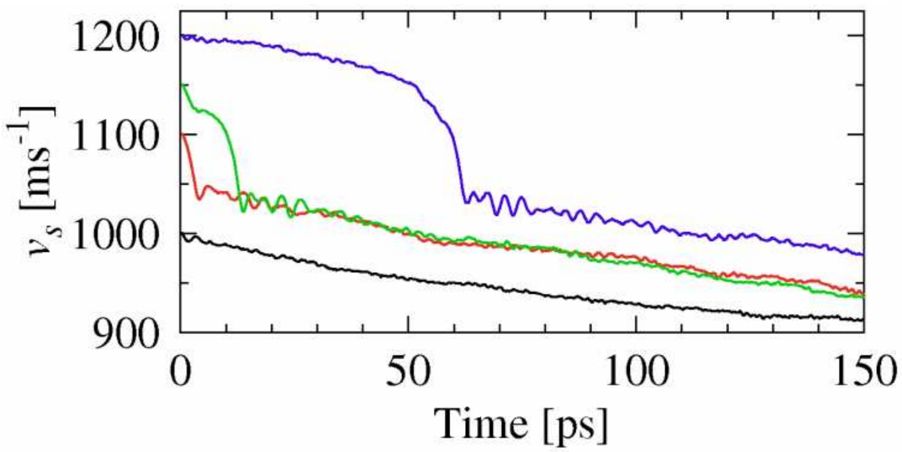
Lennard-Jones interaction between tubes

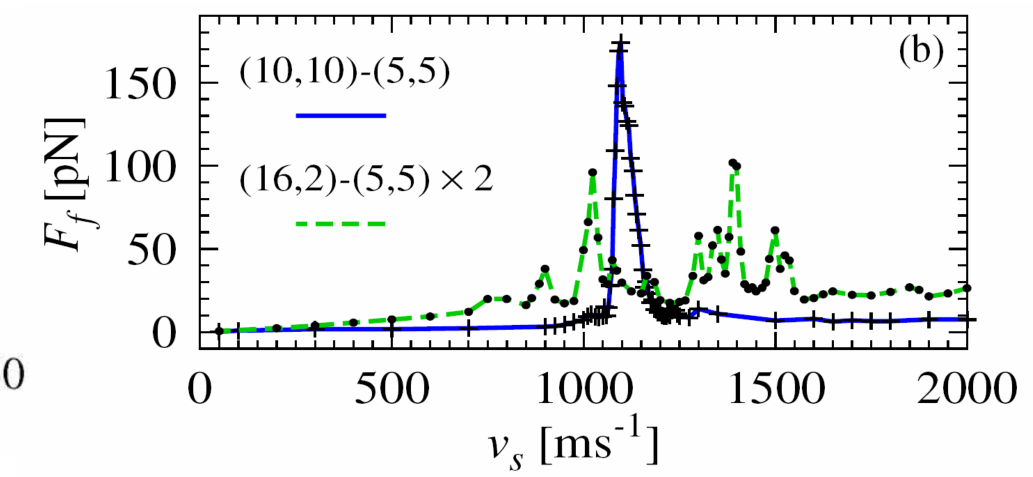
Primary source of friction comes from the tube ends

Tangney et al., Phys. Rev. Lett. **93**, 065503 (2004)

Sliding nano-friction between CNTs







Giant wave-drag intertube friction ← **phonon excitations**

matching between washboard freq. and group velocity of phonon

Interactions come from terminations

Tangney et al., Phys. Rev. Lett. **97**, 195901 (2006)

Outstanding issues

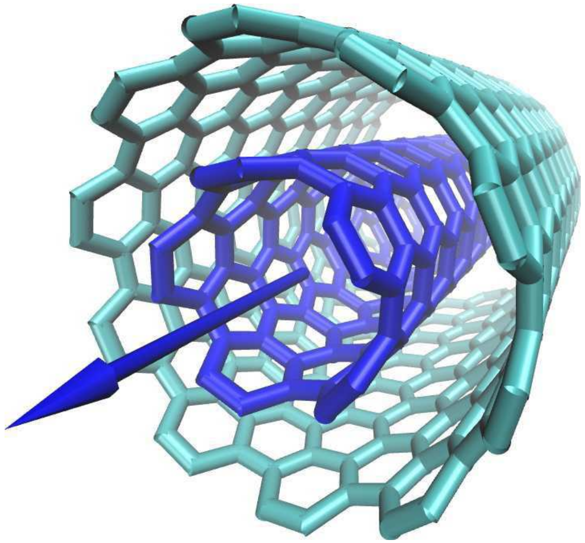
What about friction from nanotube **body** rather than from **terminations**?

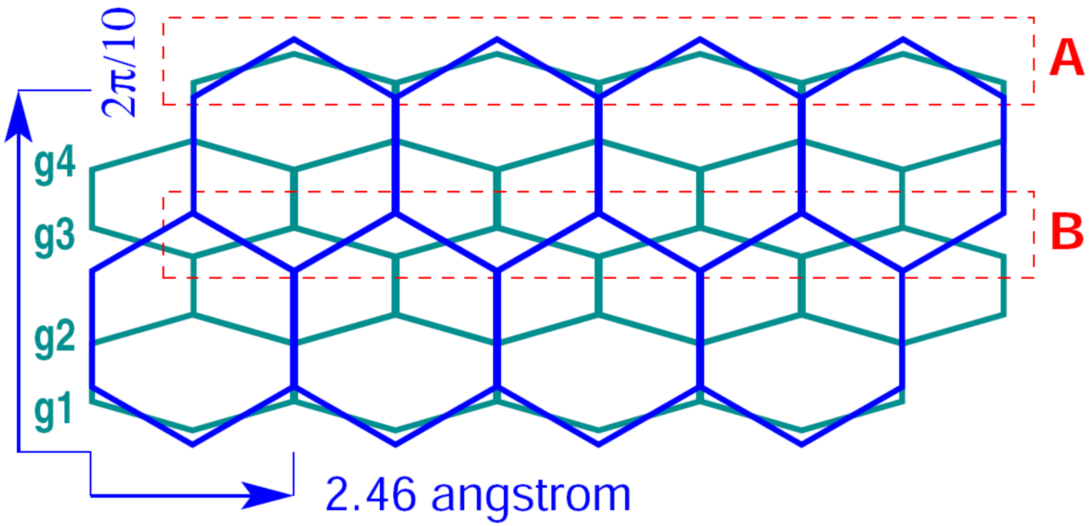
Is **corrugation** (energy variation in sliding) well described?

Apply **force** to get sliding **velocity**, not the opposite?

Intertube interaction

Unrolled (5,5)-(10,10) CNT

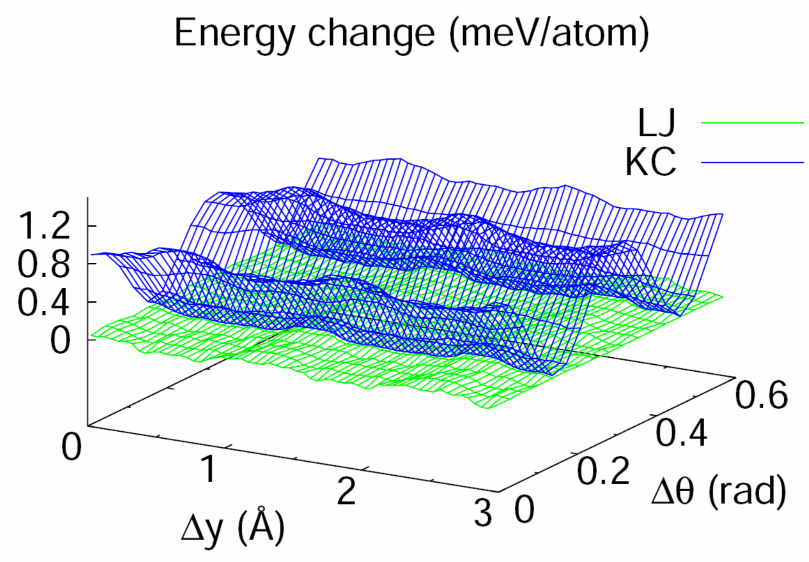


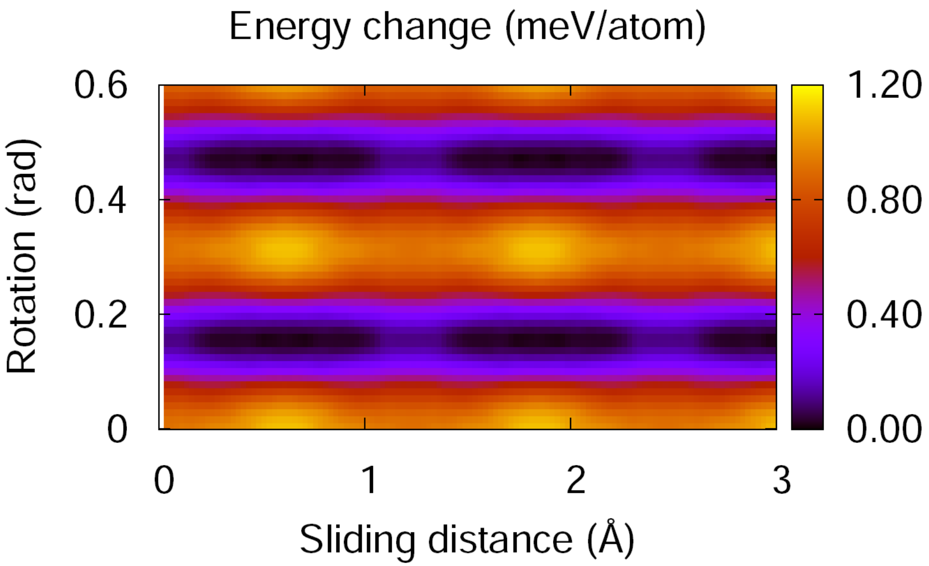


washboard frequency: $\omega = 2\pi\, v / a$

Intertube interaction

Potential: Lennard-Jones vs Kolmogorov-Crespi



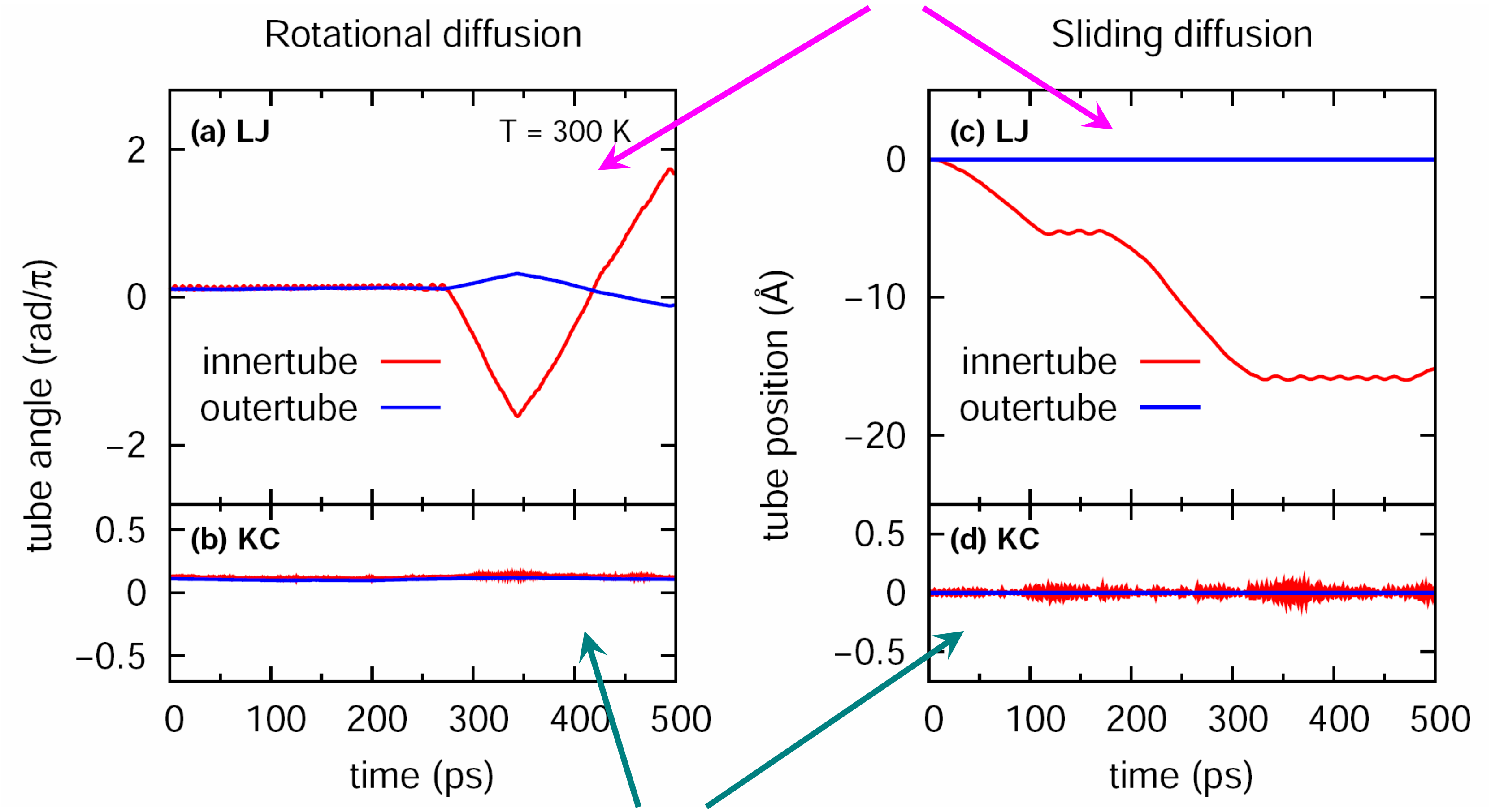


KC intertube energy

Intertube interaction

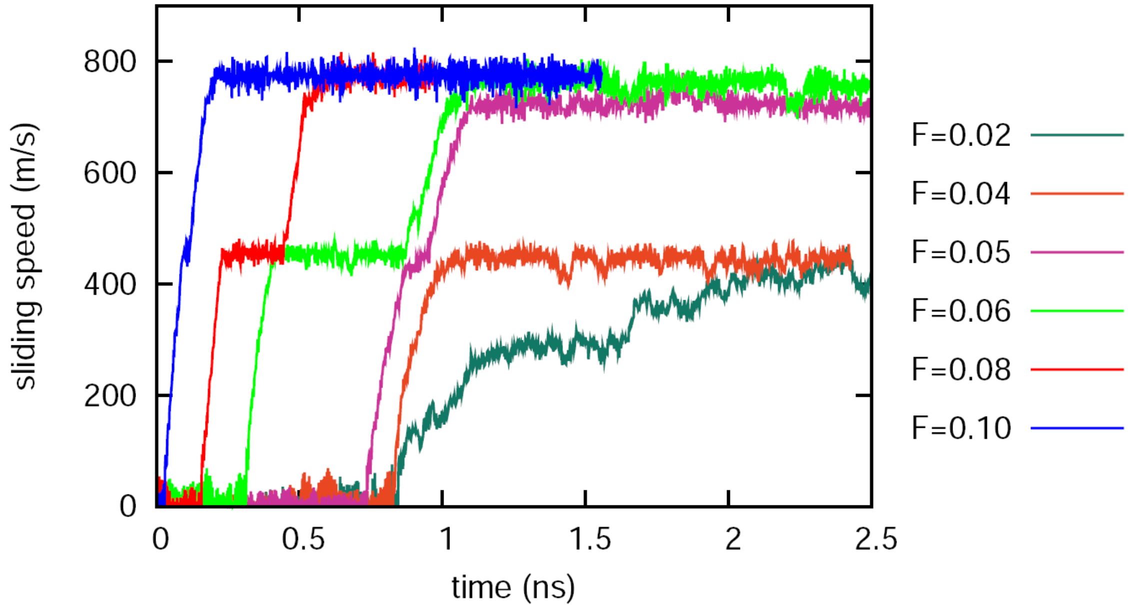
Finite size effect: innertube diffusion

LJ: diffusion (both sliding and rotation)



KC: no diffusion (either sliding or rotation)

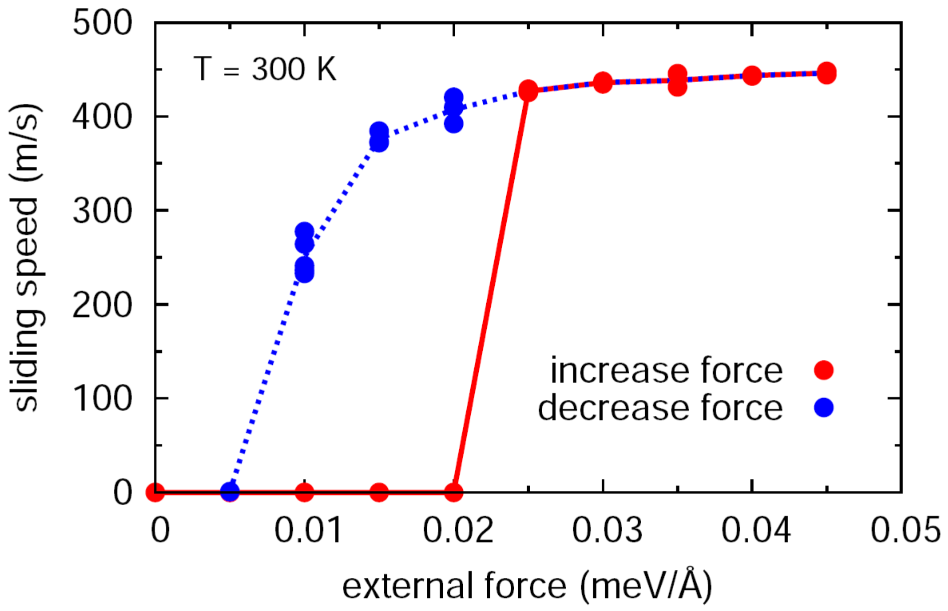
Pulling innertube → speed plateaus



Outertube: fixed to move

Innertube: pulled under force F on each atom

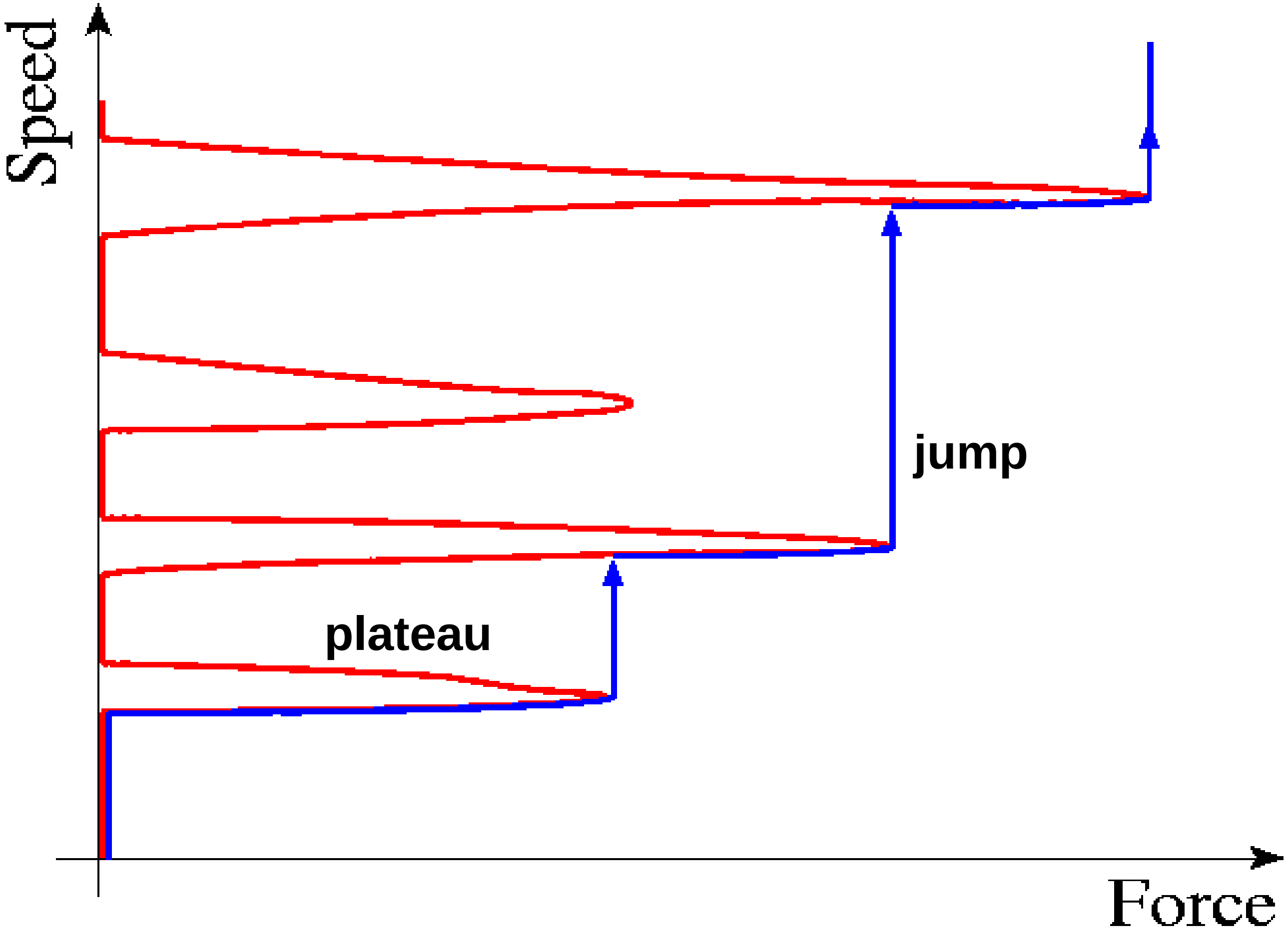
speed goes up by **jumping between plateaus**



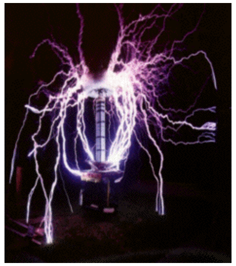
Depinning force (static force): possible way for experiment to measure the intertube potential

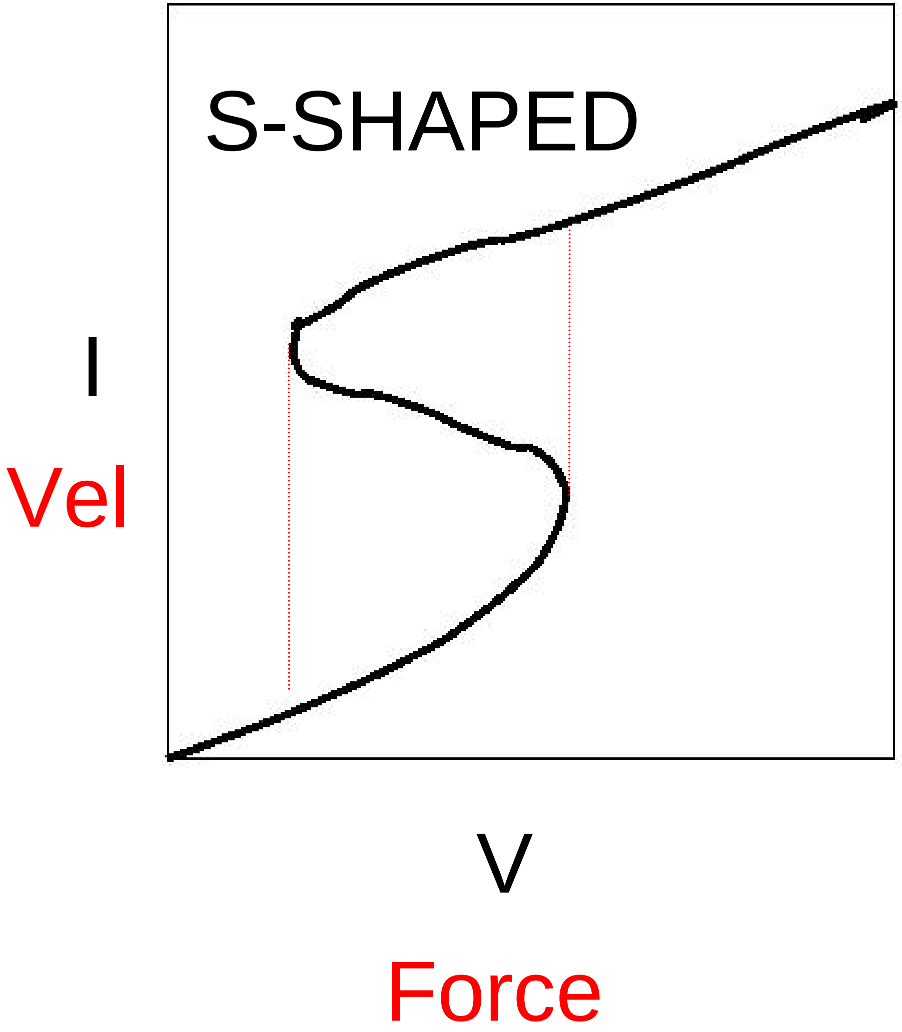
0.02 meV/angstrom = 0.032 pN

Pulling innertube: negative differential friction

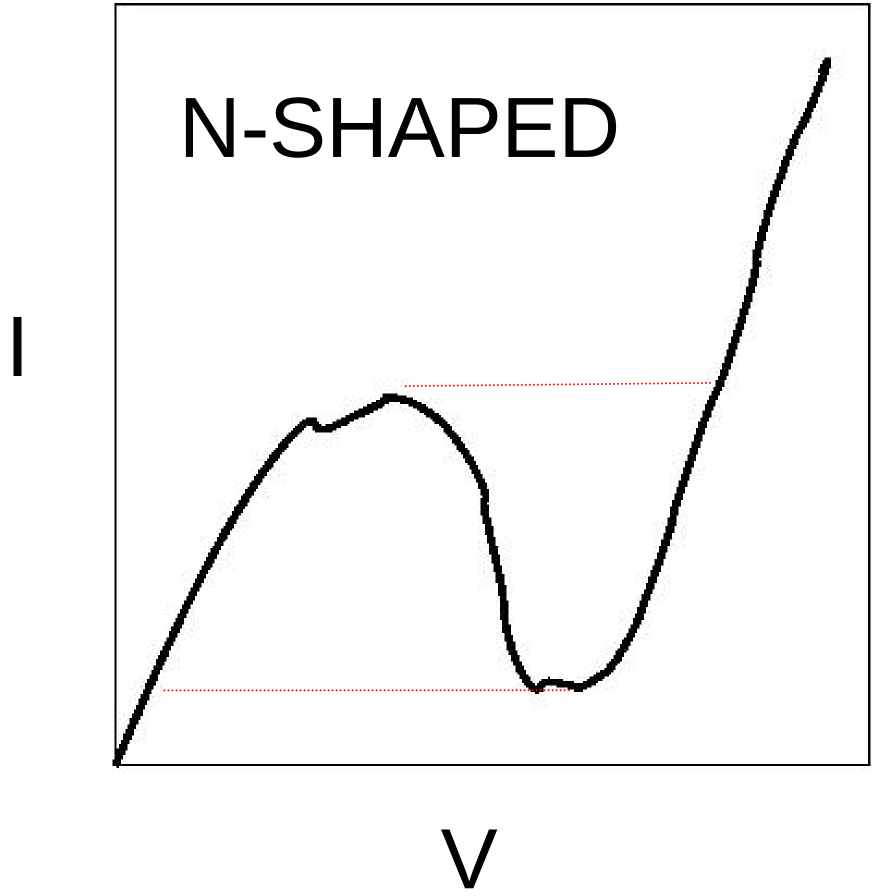


Ex.: GAS DISCHARGE





Ex.: GUNN EFFECT OSCILLATOR (GaAs)



Pulling innertube: Conclusion

→ **Bulk** nanotube friction important

→ When apply **force** and not velocity

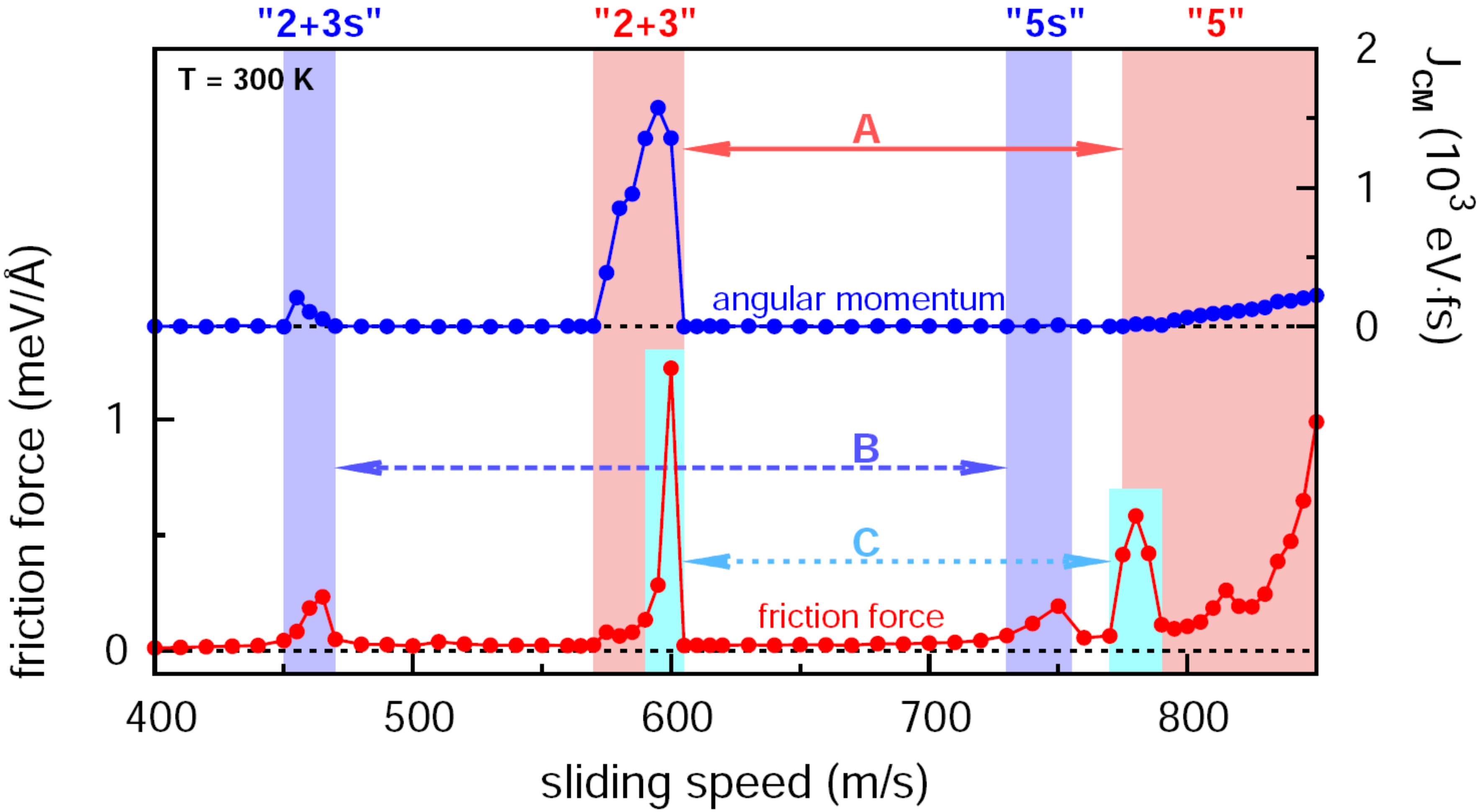
  ➔ velocity **plateaus** and **jumps**

→ S-shaped **negative differential friction**

→ Underlying mechanism: **dynamical chiral symmetry breaking** due to nonlinear excitation of outertube "pseudorotational" modes

Zhang, Tartaglino, Santoro, Tosatti. Surface Science **601**, 3693 (2007)

Sliding innertube



Frictional peaks with **nonzero angular momentum**

Sliding innertube

Angular momentum analysis

$$J = J_{\mathrm{CM}} + J_{\mathrm{pseudo}}$$

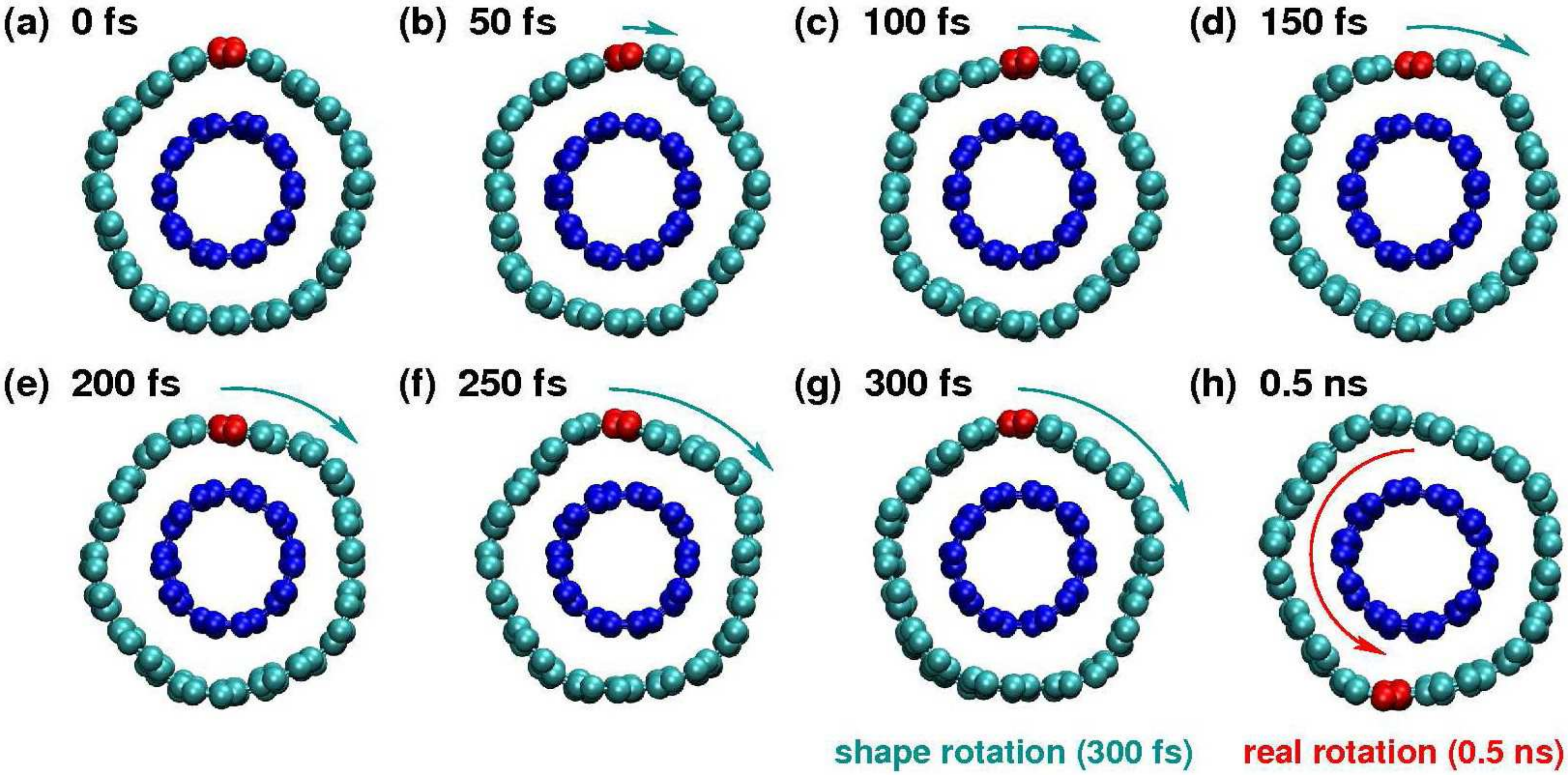
$$J_{\mathrm{CM}} = \sum_i m_i[\vec{r}_i \times (\vec{\omega} \times \vec{r}_i)]_y$$ **Rigid body rotation**

$$J_{\mathrm{pseudo}} = \sum_i m_i(\vec{r}_i \times \dot{\vec{r}}_i)_y$$ **Shape rotation (pseudo-rotation)**

Generally, $J_{CM} = - J_{pseudo} = 0$ (total J = 0 and conserved)

At frictional peaks, $J_{pseudo} \neq 0 \rightarrow J_{CM} = - J_{pseudo} \neq 0 \rightarrow$
overall rigid rotation and **counterwise pseudo-rotation**

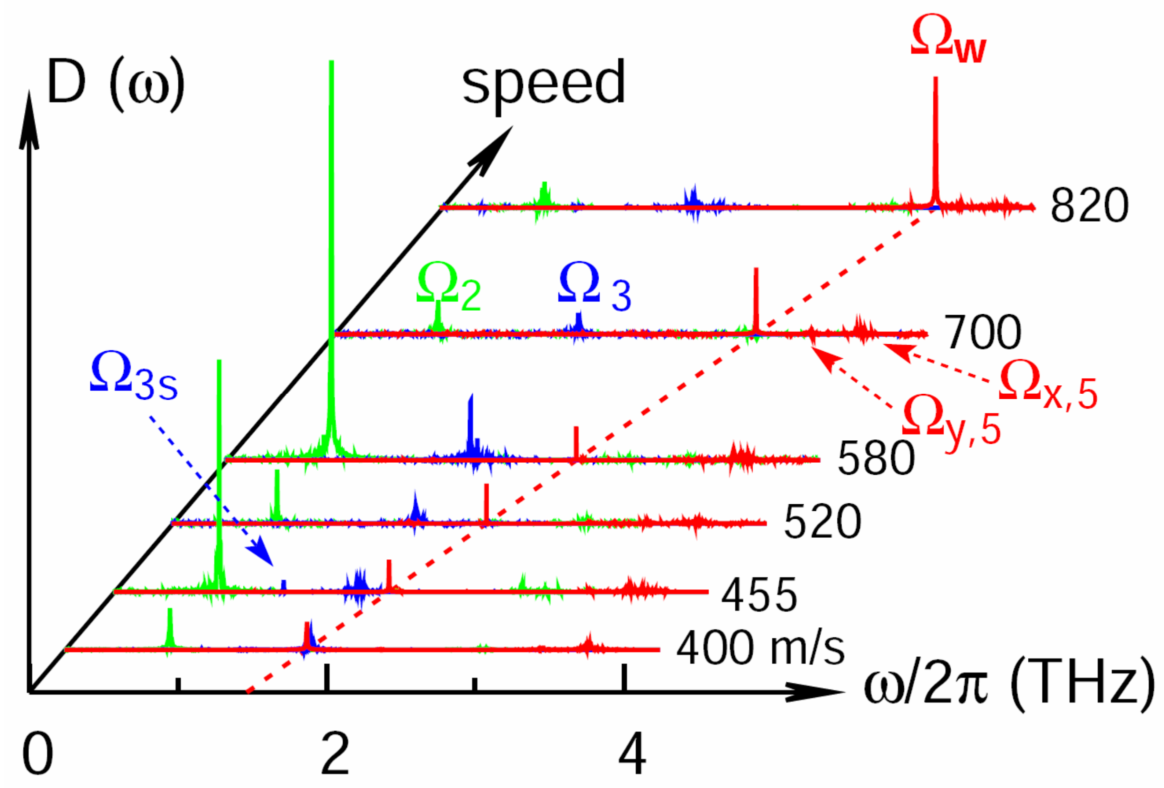
Sliding innertube



(**washboard**) *v* = 820 m/s → one period of 300 fs

“*n* = 5” excitation: breathing phonon quantized by 5

Sliding innertube



Fourier spectra on outertube radial vibrations

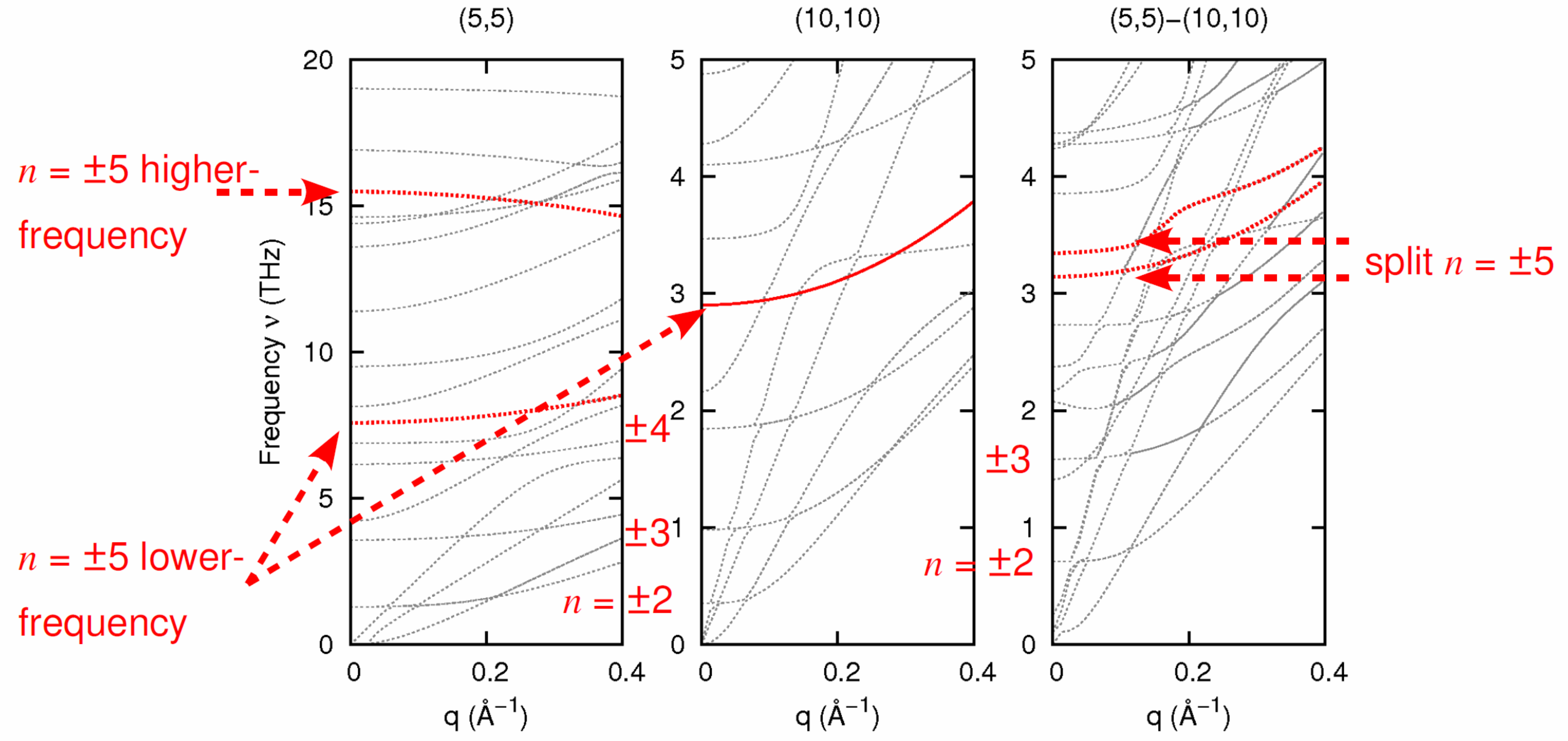
Possible phonon resonant excitations:

1) "$n = 5$": $v = 820$ m/s
2) "2 + 3 = 5": $v = 580$ m/s
3) "2 + 3s = 5": $v = 455$ m/s

Other velocities:

"$n = 5$" always exists due to washboard in case of (5,5)@(10,10)

Sliding innertube



Resonant conditions:

- → Frequency: washboard 1) equal n=5 normal frequencies or 2) equal sum of n=2 and n=3 frequencies
- → Symmetry: washboard with symmetry 5 1) matches n=5 or 2) matches 2+3

Sliding innertube: theory

based on Suzuura-Ando model

Suzuura and Ando, Phys. Rev. B 65:235412, 2002

$$K[\boldsymbol{u}] = L_y \int_0^{2\pi R} dx\, \tilde{K}$$

$$U[\boldsymbol{u}] = L_y \int_0^{2\pi R} dx\, (\tilde{U}_2 + \tilde{U}_3 + \tilde{U}_4 + \tilde{U}_c)$$

$$\tilde{K} = \frac{M}{2}\left(\dot{u}_x^2 + \dot{u}_z^2\right)$$

kinetic energy density

$$\tilde{U}_2 = \frac{\alpha}{2}\left(\frac{\partial u_x}{\partial x} + \frac{u_z}{R}\right)^2$$

quadratic potential

$$\tilde{U}_3 = \frac{\alpha}{2}\left(\frac{\partial u_x}{\partial x} + \frac{u_z}{R}\right)\left(\frac{\partial u_z}{\partial x} - \frac{u_x}{R}\right)^2$$

third-order potential (new)

$$\tilde{U}_4 = \frac{\alpha}{8}\left(\frac{\partial u_z}{\partial x} - \frac{u_x}{R}\right)^4$$

fourth-order potential (new)

$$\tilde{U}_c = \frac{a^2 C}{2}\left(\frac{\partial^2 u_z}{\partial x^2} + \frac{u_z}{R^2}\right)^2$$

curvature potential for CNT

$$\boldsymbol{u}(\theta, t) = \boldsymbol{u}_0(t) + \sum_{n>0}\left(\boldsymbol{u}_n(t) e^{in\theta} + c.c.\right)$$

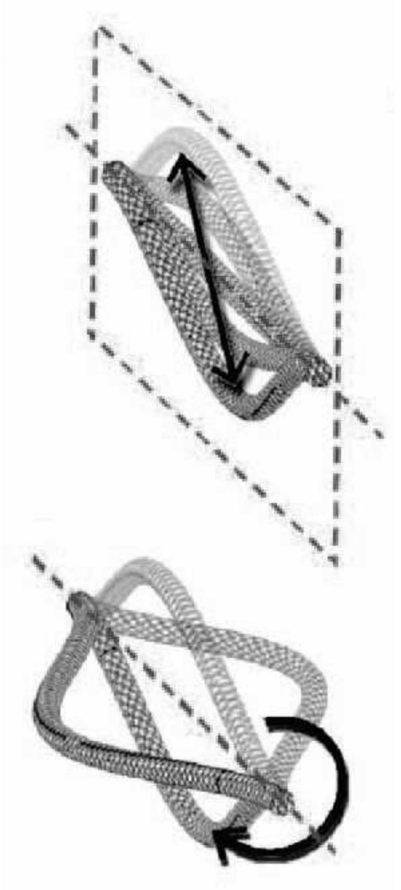
$$\boldsymbol{u}_n(t) = \boldsymbol{u}_{n,+} e^{i\Omega_n t} + \boldsymbol{u}_{n,-} e^{-i\Omega_n t}$$

displacement is summation of all phonons with quantization number *n*

“n = 5” excitation

Similar to instability of vibrating string, such as jump ropes, guitar string

$$\begin{aligned}\ddot{X} &= -[\omega_{k,T}^2 + K(|X|^2 + |Y|^2)]X + F\cos(\Omega t)\\ \ddot{Y} &= -[\omega_{k,T}^2 + K(|X|^2 + |Y|^2)]Y\end{aligned}$$



Forcing in X plane, rope vibrates also in X plane, if $K = 0$

Forcing in X plane, rope rotates (Y being excited), if $K \neq 0$ and Ω is beyong a critical value

“*n* = 5” excitation

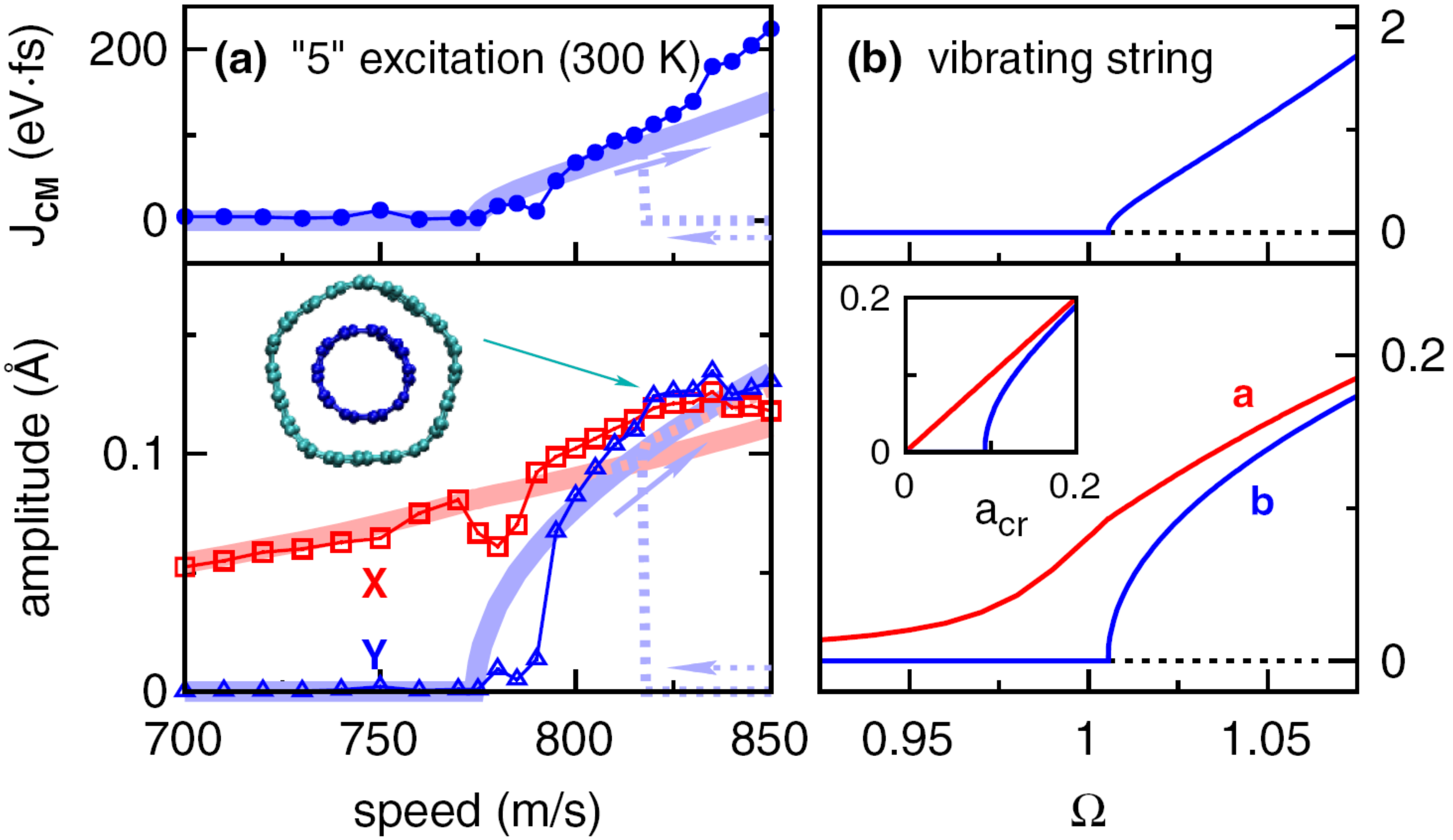
nanotube “*n* = 5”

$$\begin{aligned}\ddot{X} &= -[\omega_5^2 + Q + (P/4)(|X|^2 + |Y|^2)]X + 4F\cos(\Omega_w t)\\ \ddot{Y} &= -[\omega_5^2 - Q + (P/4)(|X|^2 + |Y|^2)]Y\end{aligned}$$

Nonlinearity *P* (*K* in string case) account for increase of frequency, comes from fourth-order energy terms

Q is Umklapp in nanotube (due to 10-chain structure of innertube) that: phonon n = 5 → n = - 5

“*n* = 5” excitation



“2 + 3 = 5” excitation

$$\ddot{u}_{z,5} = -\gamma\dot{u}_{z,5} - Qu^{*}_{z,5} - \left(\omega_5^2 + \sum_{m=2,3,5} B_m |u_{z,m}|^2\right)u_{z,5}$$

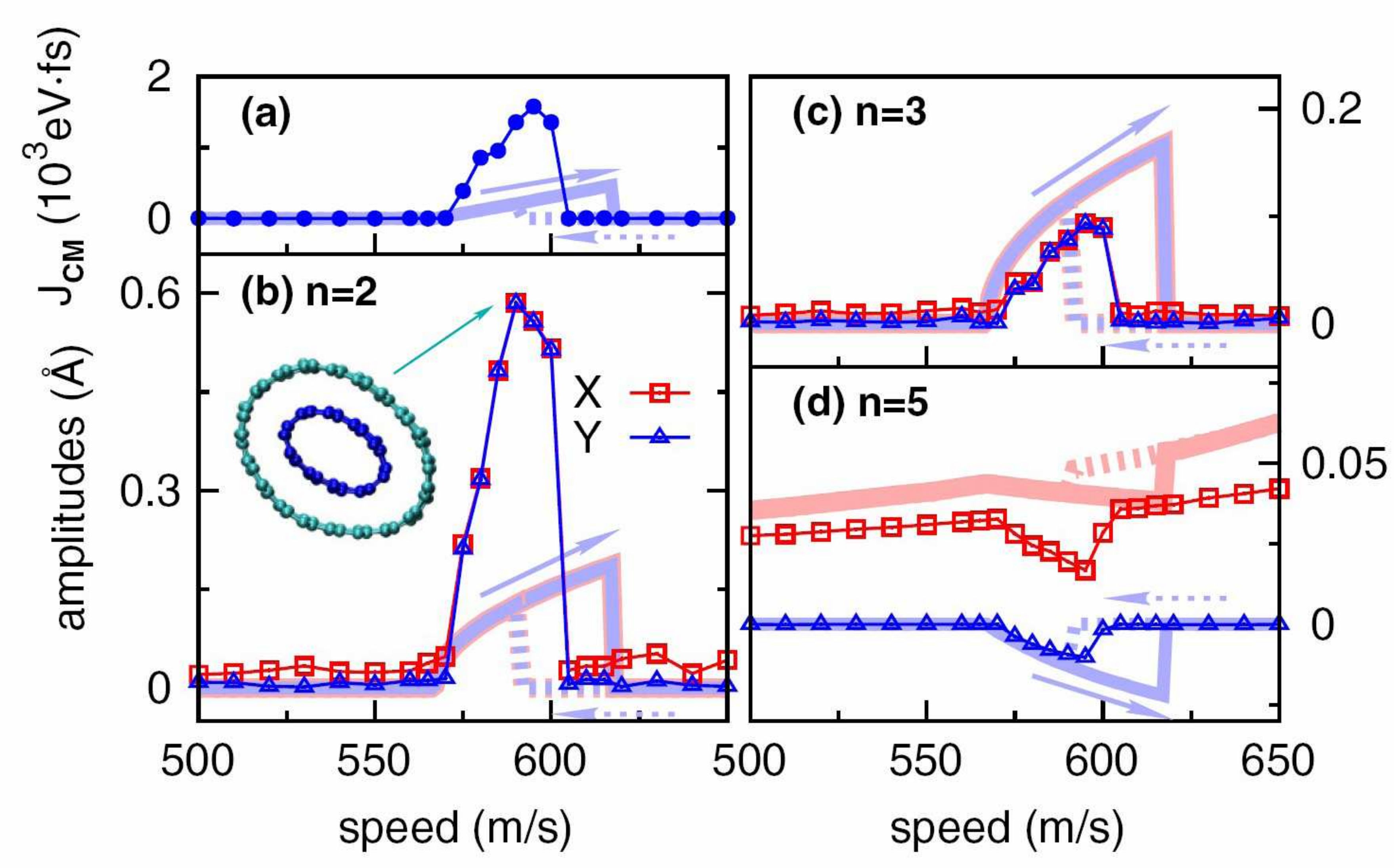
$$- A^{\mathrm{dir}} u_{z,2} u_{z,3} + A^{\mathrm{umkl}} u^{*}_{z,2} u^{*}_{z,3} + 2F\cos(\Omega_w t),$$

Coupling of three phonon modes through third-order nonlinearities:

A^{dir}: 2 + 3 = 5

A^{umkl}: 2 + 3 = 5 → - 5

“2 + 3 = 5” excitation

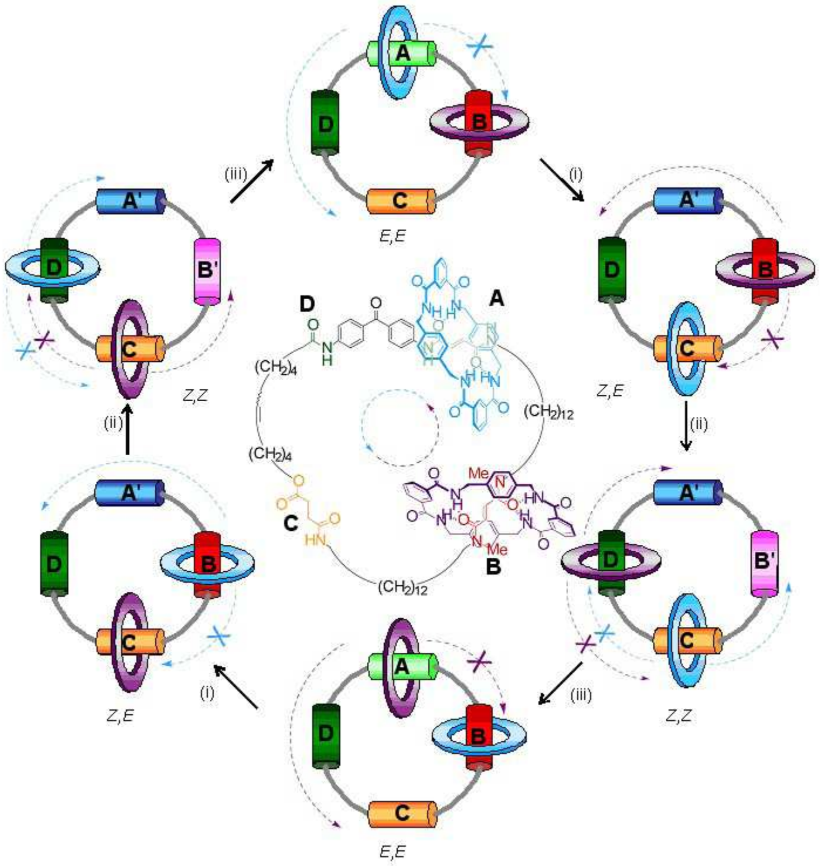


Why interesting?

Molecular nanomotor (chemical reactions)

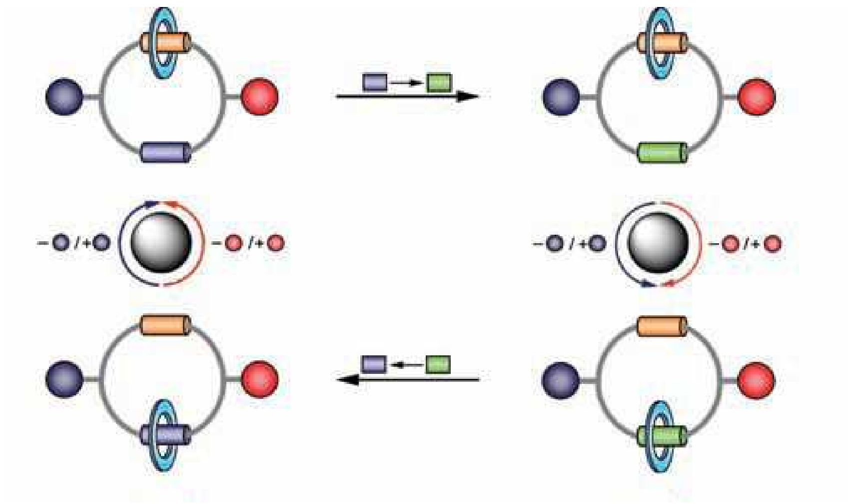
Leigh et al., Nature 424:174, 2003

Long- and short-wavelength breaks different bonds → unidirectional rotation



Leigh et al., Science 306:1532, 2004

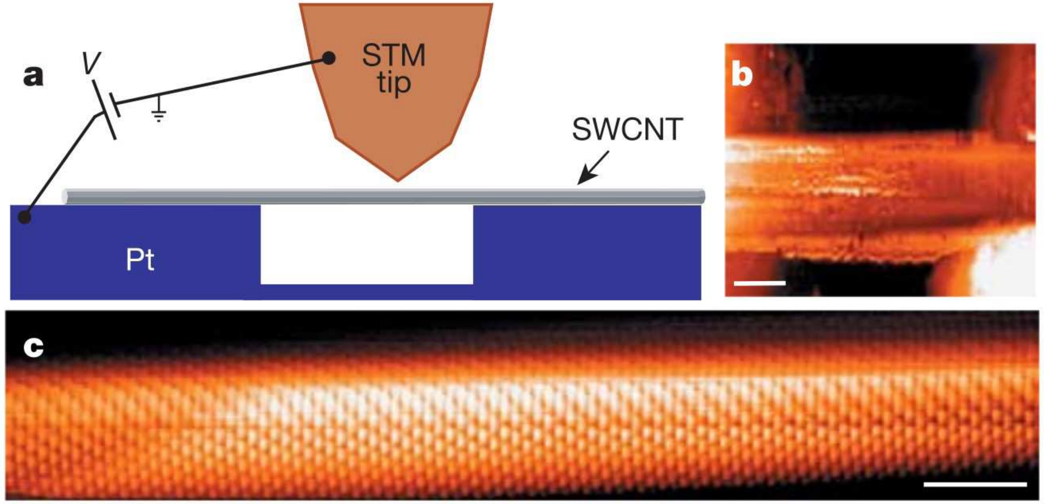
Brownian particle transport → unidirectional rotation



Why interesting?

Our dynamical chiral symmetry breaking, backed by continuum model analysis, represents a first idealized, pure physical nanomotor: **from nano-sliding to nano-rotation**

Electron-phonon coupling: low frequency breathing mode can be excited by STM tip (LeRoy et al. Nature 432:371, 2004)



Conclusion

Giant nano-friction is due to phonon **resonant excitations**

Energy nonlinearities → chiral symmetry breaking, thus sliding → rotation

New element in nanoscale: **Umklapp process**, crucial in tube sliding

Not only interesting, but also **phonon-electron** coupling

Zhang, Santoro, Tartaglino, Tosatti. Phys. Rev. Lett. **102**, 125502 (2009)

Thank you for your attention !