Lecture 18b
Analytical Approaches – Peak Interaction Forces

Peak force during tapping – not directly observable

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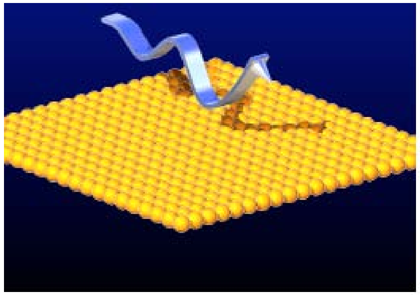
Observables/non-observables in dAFM



Observables- quantities directly measured in an AFM

- "Free" or initial amplitude A_0
- Setpoint amplitude A
- Phase lag ϕ
- Photodiode output $\theta(t)$, bending angle
- Energy dissipation
- Cycle averaged tip-sample interaction force $\langle F_{ts} \rangle$

"Known" parameters

- Cantilever equivalent stiffness k
- Natural and drive frequency ω_0, ω
- Q factor

Non- Observables- quantities that cannot be directly measured in dynamic AFM

- Tip-sample interaction force history $F_{ts}(t)$
- Peak interaction force F_{ts}^{peak}
- Adhesion, sample elasticity

This is a major point of departure from contact mode imaging where the applied force is known!

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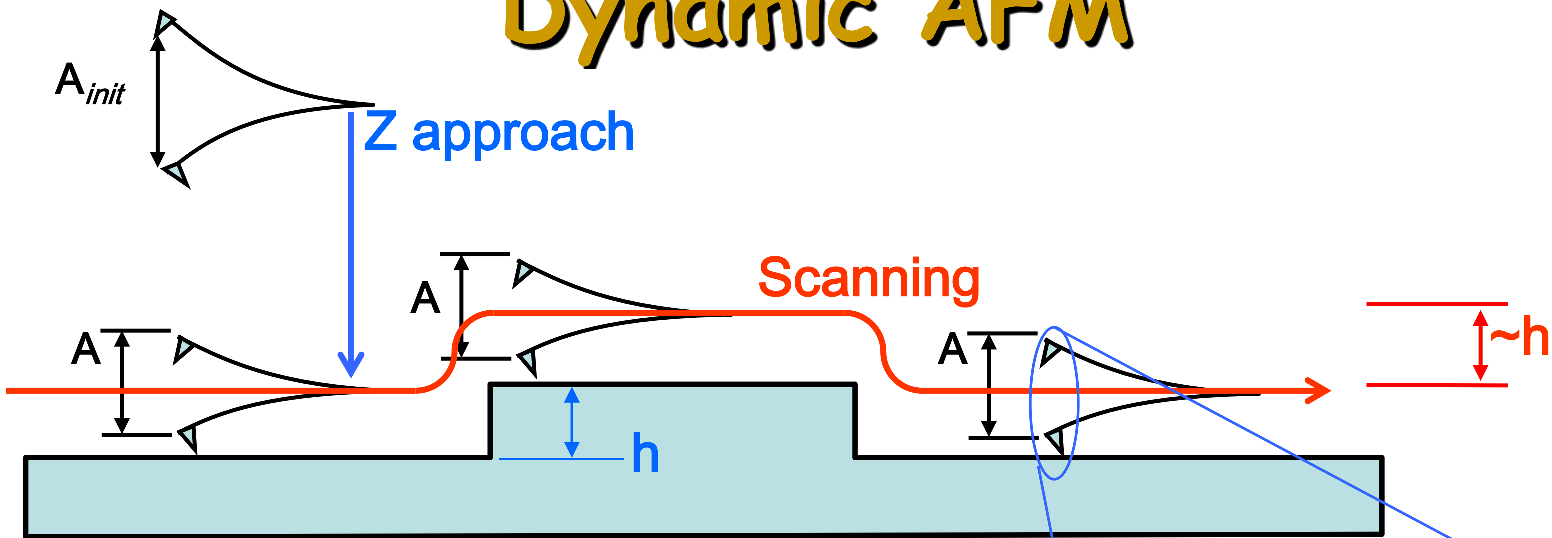
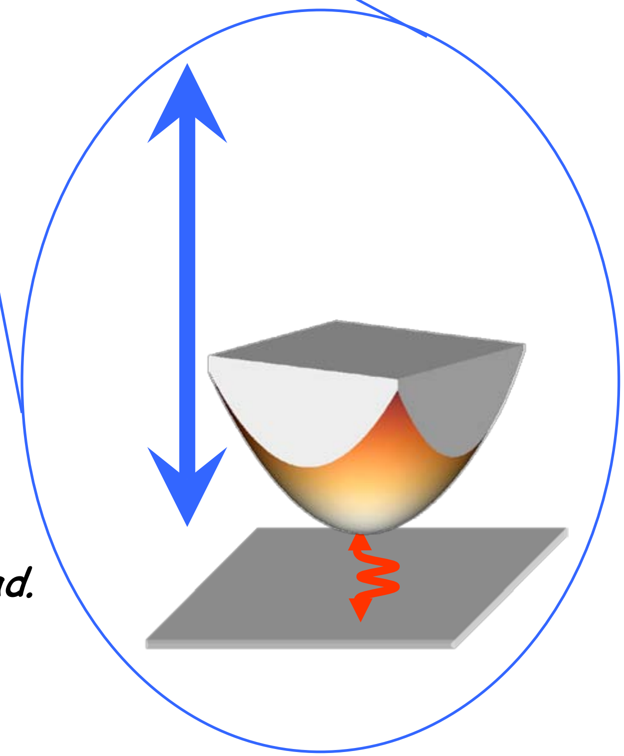
Dynamic AFM



Challenges

- What is the peak interaction force?
  - Experimental methods[1,2]
  - Numerical simulations[3,4]
- What does it depend on?
- How does it scale?



[1] M. Stark, R. W. Stark, W. Heckl, R. Guckenberger, *Proc. Natl. Acad. Sci.*, 99, 8473, 2002

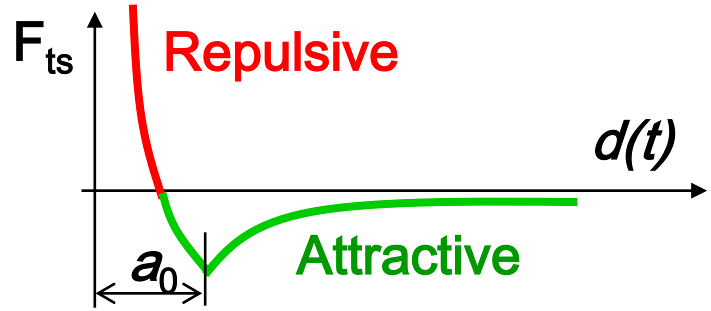
[2] J. Legleiter, M. Park, B. Cusick, T. Kowalewski, *Proc. Natl. Acad. Sci.*, 103, 4813, 2006, Xu et al., *Biophysical Journal*, 2007

[3] VEDA

Tip-sample interaction model

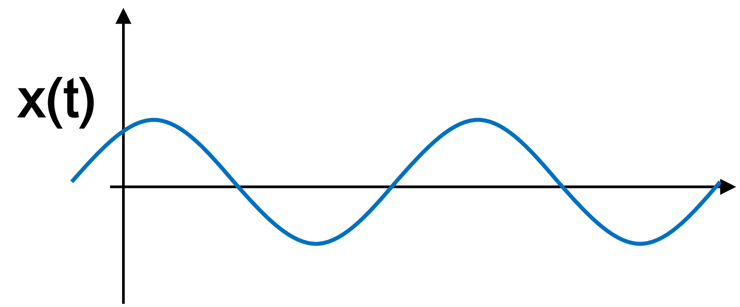
- Derjaguin-Toporov-Mueller contact mechanics

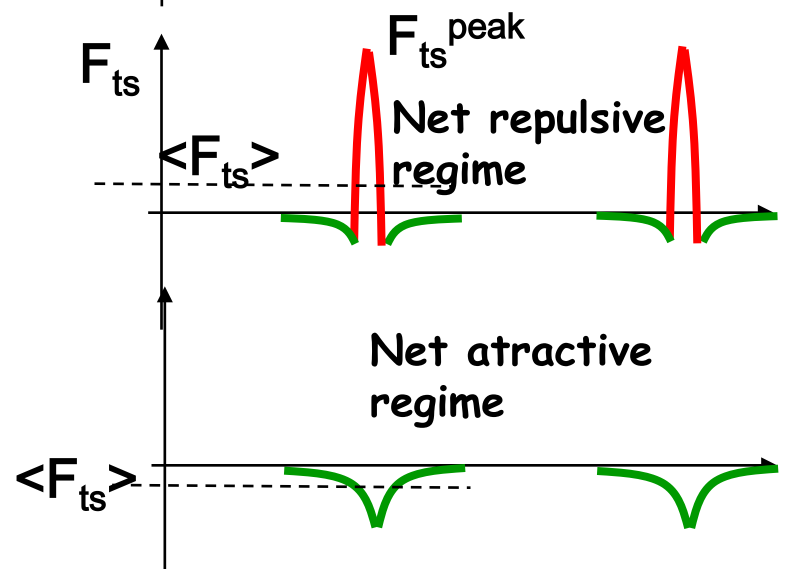
$$F_{ts}(d)=\begin{cases} F_{VdW}=-\dfrac{HR}{6d^2}, & for\ d > a_0 \\ F_{contact}=-\dfrac{HR}{6a_0^2}+\beta(a_0-d)^\alpha, & for\ d < a_0 \end{cases}$$



DMT contact mechanics: $\beta = \frac{4}{3}E^*\sqrt{R}$, $\alpha = \frac{3}{2}$

Linear sample stiffness model: $\beta = k_{ts}$, $\alpha = 1$





$d(t)$: Gap between sample and tip

R : Tip radius

H : Hamaker constant

E^* : Effective elastic modulus

k_{ts}: Sample contact stiffness

a_0 : Intermolecular distance

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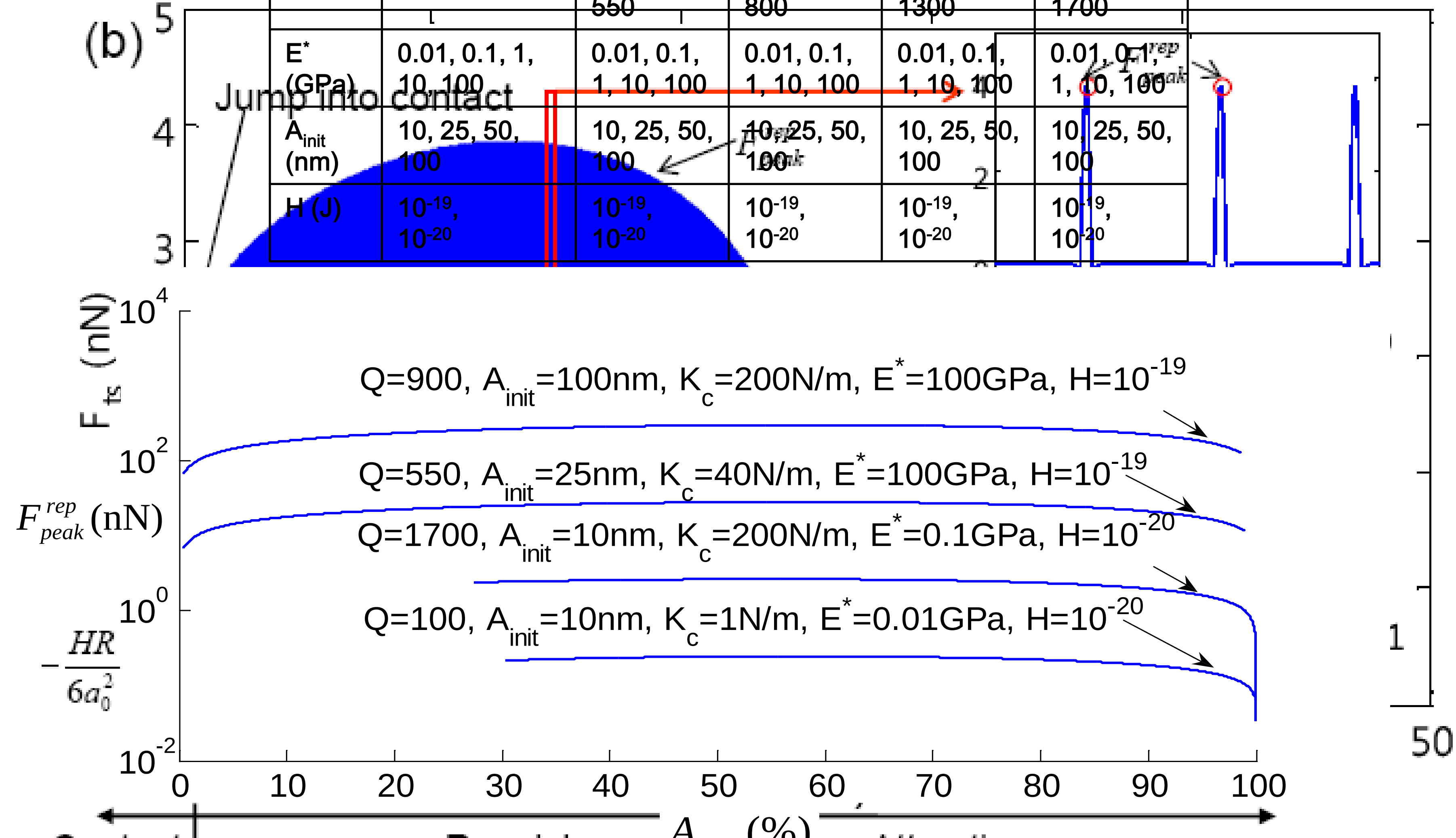
Peak forces from VEDA simulations

$\omega=\omega_0$, A_0= 25 nm, k_c=1 N/m, Q=50, E^*=1GPa (Si tip- polymer sample),
H=10^{-19} J, R=10nm, a_0=0.5 nm

K_c (N/m)	1	10	40	140	200
Q	50, 75, 100	250, 400, 550	300, 550, 800	700, 1000, 1300	900, 1300, 1700
E^* (GPa)	0.01, 0.1, 1, 10, 100	0.01, 0.1, 1, 10, 100	0.01, 0.1, 1, 10, 100	0.01, 0.1, 1, 10, 100	0.01, 0.1, 1, 10, 100
A_{init} (nm)	10, 25, 50, 100	10, 25, 50, 100	10, 25, 50, 100	10, 25, 50, 100	10, 25, 50, 100
H (J)	10^{-19}, 10^{-20}	10^{-19}, 10^{-20}	10^{-19}, 10^{-20}	10^{-19}, 10^{-20}	10^{-19}, 10^{-20}

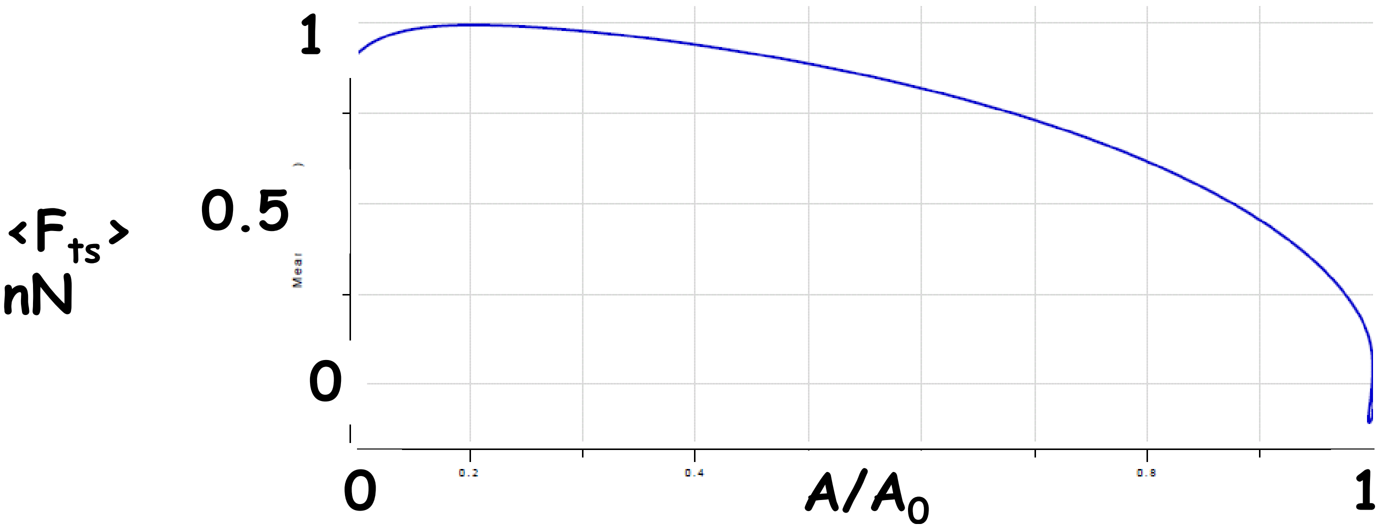


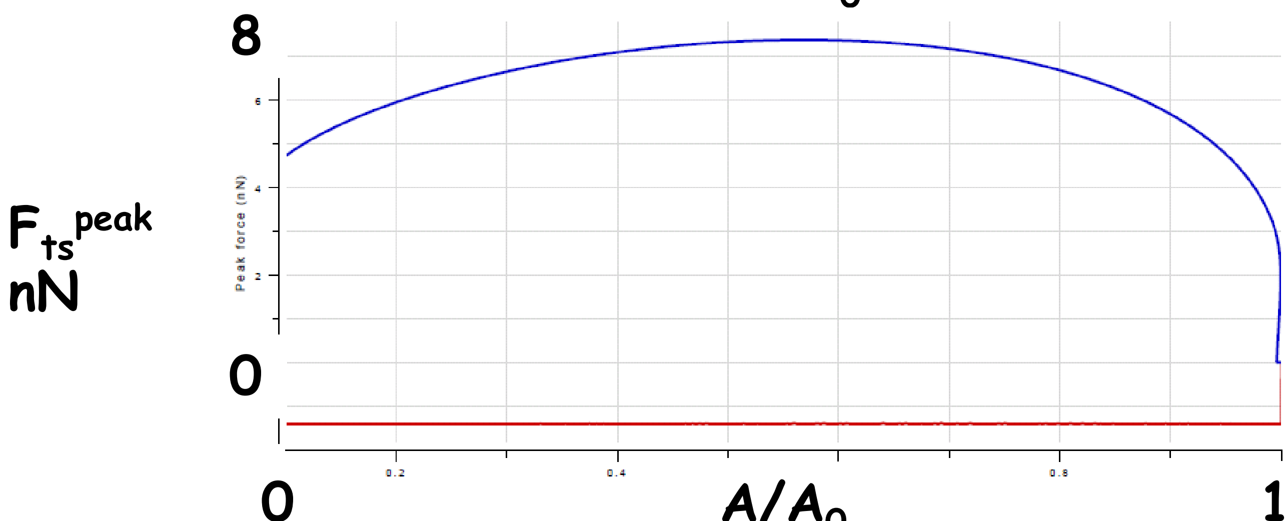
- Peak repulsive forces span 4 orders of magnitude

Average vs. peak forces

$\omega=\omega_0=100kHz$, $A_0=20nm$, $k=20N/m$, $Q=100$ $E_s=1$ GPa, $F_{ad}=1.4$ nN DMT

Hint: Under "Simulation parameters" tab in VEDA choose X axis as amplitude ratio





- Peak force >> average force
- Very different dependence on amplitude setpoint

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Peak forces - analytical expressions

- Using perturbation methods, it is possible to estimate the peak interaction forces for specific tip-sample interaction models[1,2]
- DMT model in net repulsive regime

$$F_{peak}^{rep} = 1.995\left(E^{*}\sqrt{R}\right)^{1/4}\left(k_c / Q\right)^{3/4} A_0^{9/8}\left(A_{ratio} - A_{ratio}^{3}\right)^{\frac{3}{8}}$$

Or

$$\bar{F}_{peak}^{rep} = \left(E^{*}\sqrt{R}\right)^{-1/4}\left(Q / k_c\right)^{3/4} A_0^{-9/8}\,F_{peak}^{rep} = 1.995\left(A_{ratio} - A_{ratio}^{3}\right)^{\frac{3}{8}}$$

[1] S. Hu, A. Raman, *App. Phys. Lett.*, 91, 123106, 2007
[2] X. Xu, C. Carrasco,P. J. de Pablo, J. Gomez-Herrero, A. Raman, *Biophysical Journal*, 95(5), 2520, 2007

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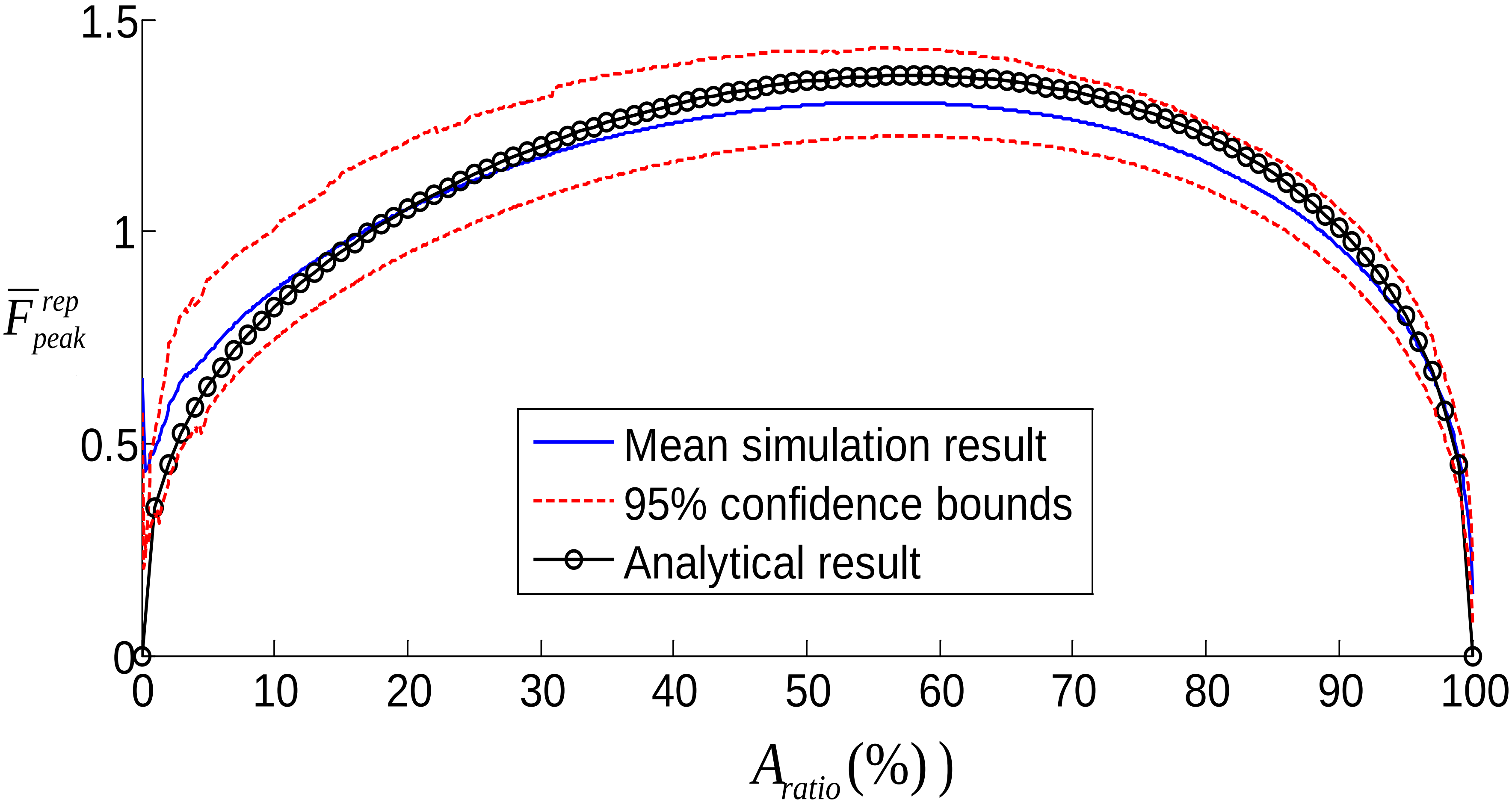
Approximate scaling law for peak forces



- Max forces at setpoint between 50-60% !!!! Very important result
- Sample viscosity has little effect on the result
- Results are excellent for stiff lever, UHV simulations
- Similitude implies commonality of interaction physics

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Other peak force expressions

- DMT in net attractive force regime

$$F_{peak}^{att} = -2 \times 3^{1/3} \left(HR\right)^{-1/3} \left(k_c / Q\right)^{4/3} A_0^{\ 2} \left(A_{ratio} - A_{ratio}^3\right)^{\frac{2}{3}}$$

- Linear contact spring k_{ts}

$$F_{peak}^{rep} = 2^{-5/3} 3^{2/3} \pi^{2/3} k_{ts}^{1/3} (k_{eff} / Q)^{2/3} A_0 (A_{ratio} - A_{ratio}^3)^{1/3}$$

- These formulas suggest peak forces scale with A_0, A_{ratio} and k/Q mainly

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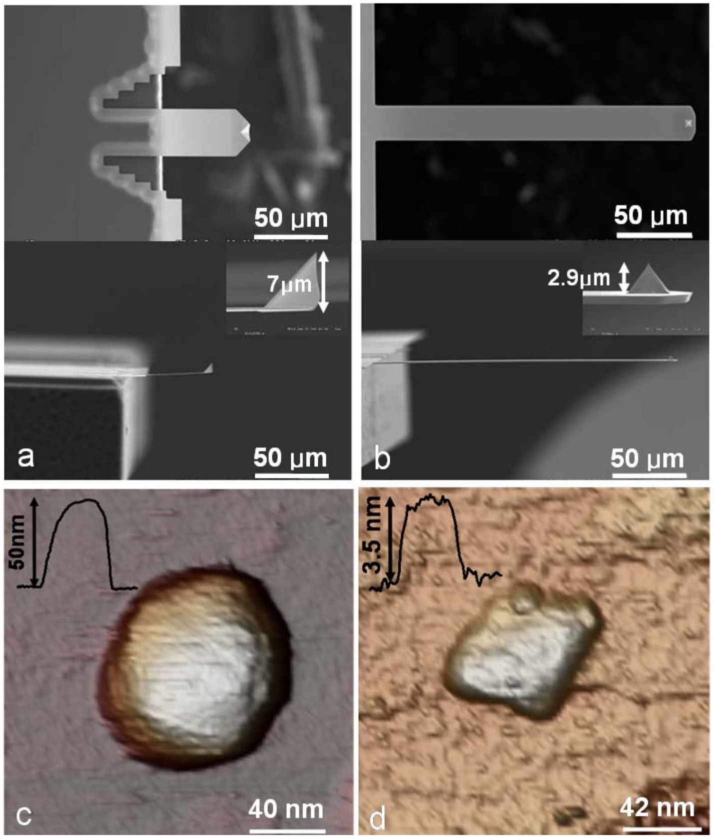
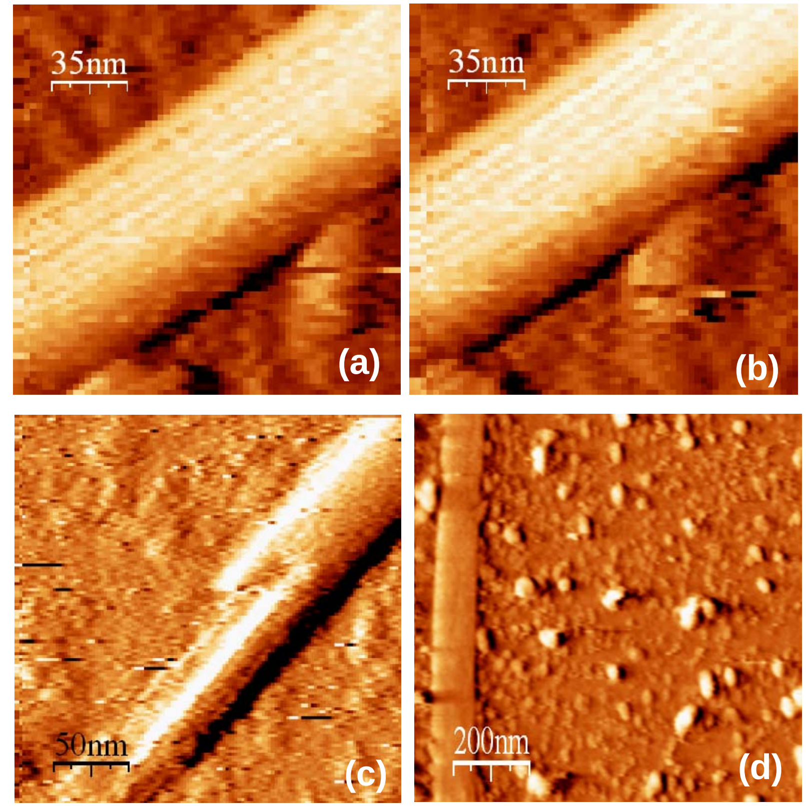
Case study



SEM of (a) the *small lever* (SL) and (b) *conventional lever* (CL) used for this study and phage Φ29 capsids imaged with the SL and the CL using acoustic dAFM under nominally similar operating conditions. (c) A tapping mode image of the viral capsid taken with the SL with the inset profile showing the correct height of the capsid. (d) A tapping mode image of the same kind of capsid scanned with the CL with the inset profile showing a collapsed virus capsid.



Microtubules scanned by SL for the 1st (a) and 80th (b) time, show that the same microtubule can stand the scanning forces for at least 80 times. Microtubules scanned by CLare either destroyed (c) or flattened (d)

Why?

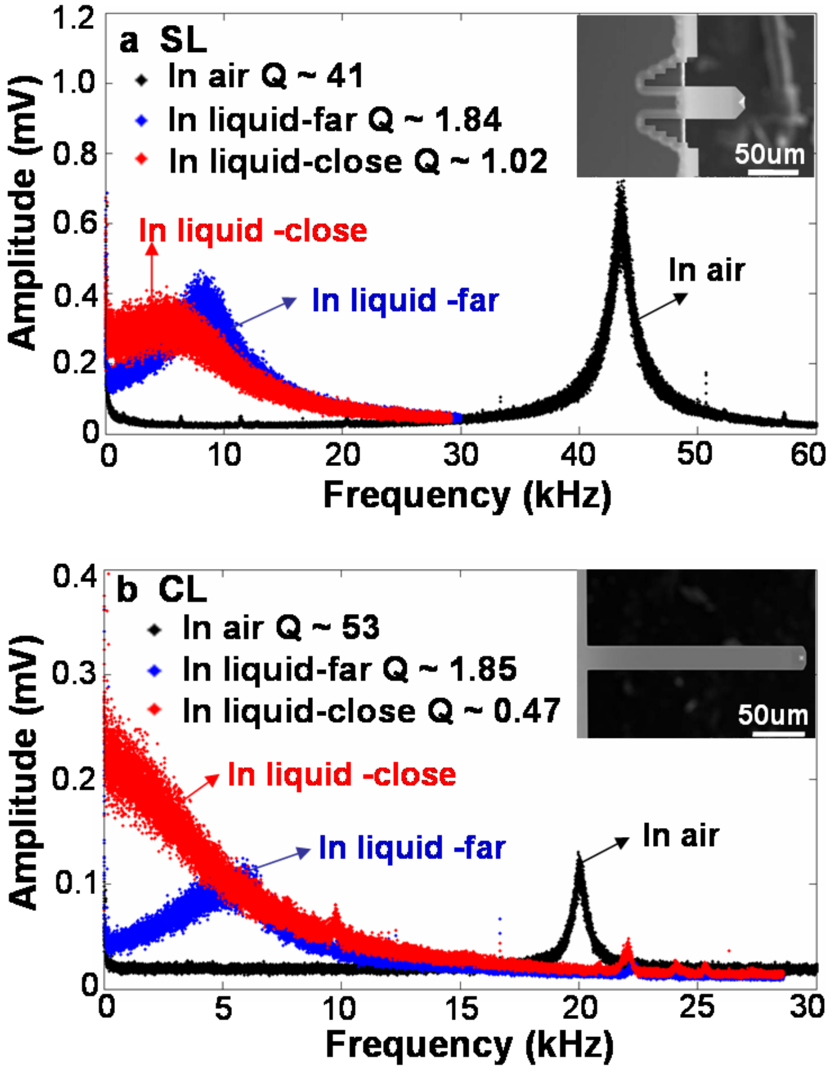
X. Xu, C. Carrasco, P. J. de Pablo, J. Gomez-Herrero, A. Raman, *Biophysical Journal*, 95(5), 2520, 2007

Evidence

	(SL) BioLever	(CL) OMCL-RC800
Resonance frequency in air (kHz)	43.6	20.1
Q-factor in air	41	53
Resonance frequency in liquid - far from surface (kHz)	9.3	6.0
Resonance frequency in liquid - close to surface (kHz)	8.3	5.4
Q-factor in liquid - far from surface	1.84	1.85
Q-factor in liquid - close to surface	1.02	0.47
Cantilever stiffness* (N/m)	0.063	0.072
Effective mass in liquid - close to surface (kg)	1.9×10^{-11}	5.2×10^{-11}
Effective mass in liquid - close to surface (kg)	2.4×10^{-11}	6.4×10^{-11}

One possible solution

$$F_{peak}^{rep} = 2^{-5/3} 3^{2/3} \pi^{2/3} k_{ts}^{1/3} (k_{eff} / Q)^{2/3} A_0 (A_{ratio} - A_{ratio}^3)^{1/3}$$



- Q of CL near surface is >2 times that of SL
- K of SL is slightly softer
- Thus force applied is also ~100% greater using CL
- Viral capsids and microtubules have critical loads where they rupture/buckle (typically ~ 1nN)

Next time

- Feedback controller for scanning