



**The Abdus Salam
International Centre for Theoretical Physics**



2063-20

ICTP/FANAS Conference on trends in Nanotribology

19 - 24 October 2009

**Atomic friction: ways to determine the elastic and viscous properties of
nano-contacts**

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Atomic Friction: Ways to determine elastic and viscous properties of nano-contacts

Ernst Meyer

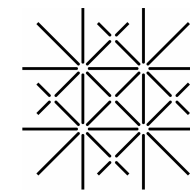
Institute of Physics

University of Basel, Switzerland

- Atomic-scale stick slip
 - loading dependence
 - multiple slips and estimation of damping
- Simultaneous measurement of normal and lateral contact stiffness
- Control of friction
 - actuation of nano-contacts



Acknowledgement



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Anisoara Socoliuc
(Nanonis)



Oliver Pfeiffer
(Individual Computing)



Sabine Maier
(LBL)



Jonas Gessler
(Antarctic)

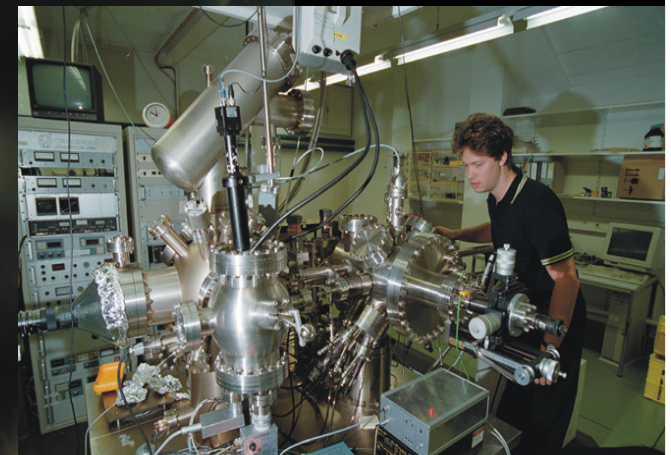
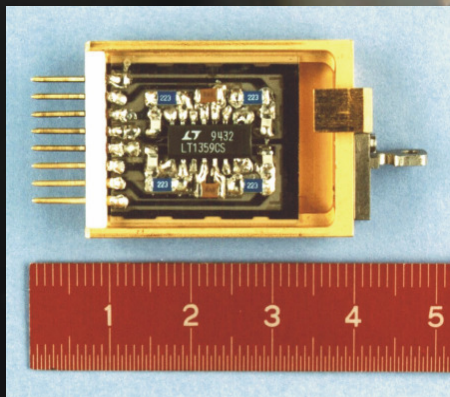
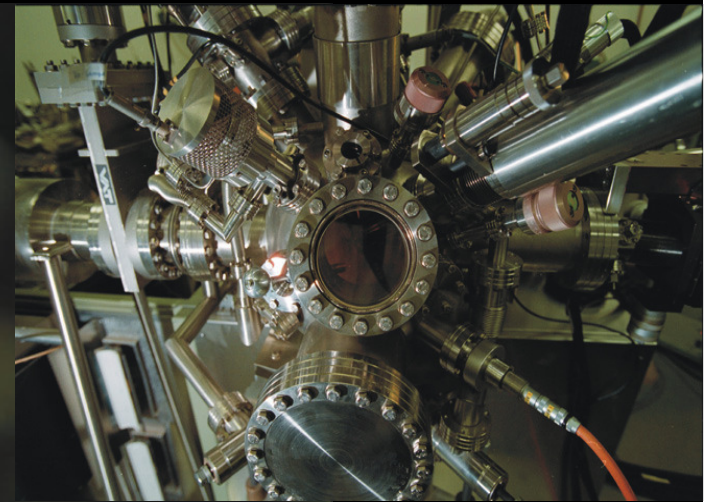
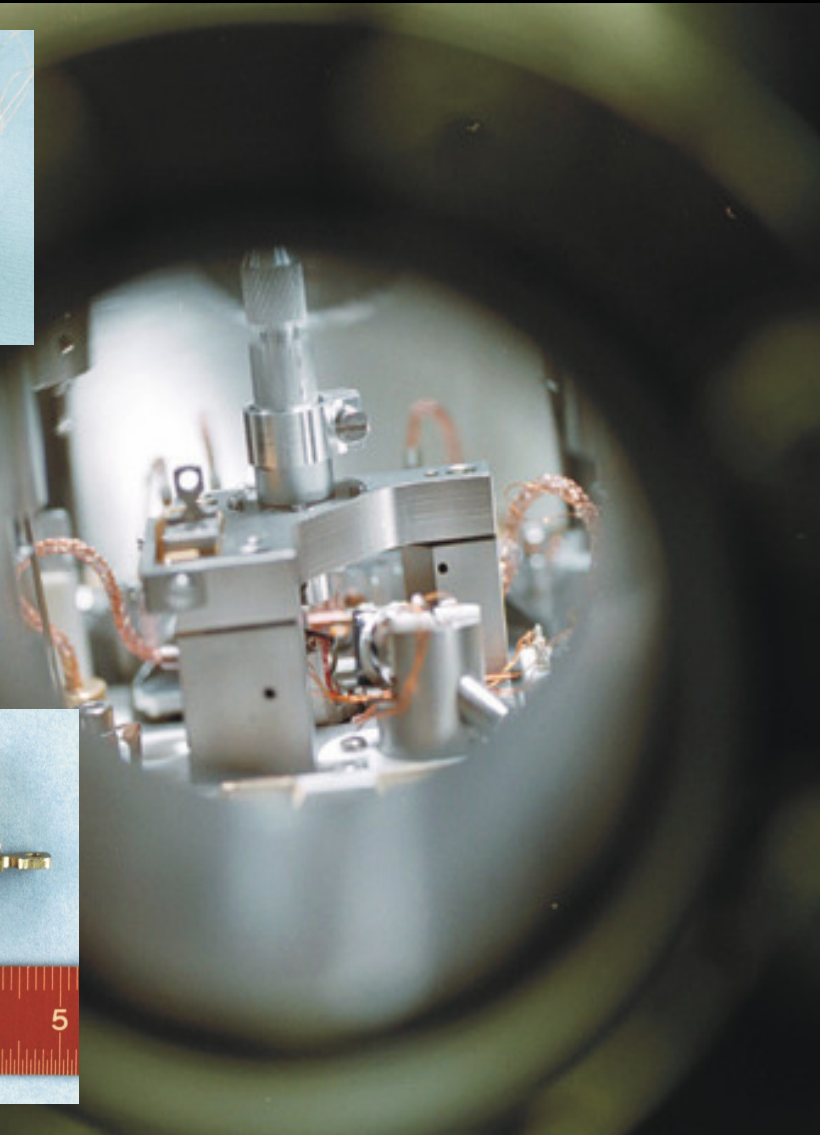
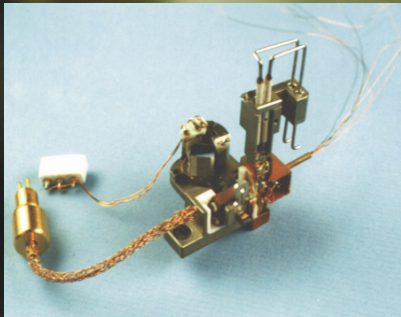


Roland Bennewitz
(Saarbrücken)



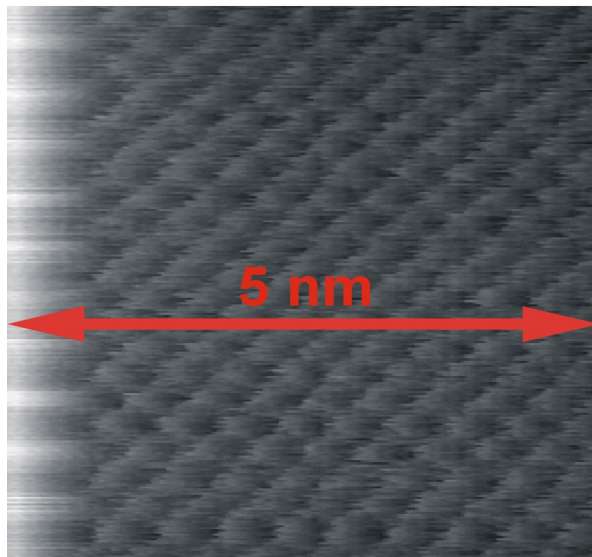
Lars Zimmerli
(Glas Trosch)

UHV-Force microscope with in-situ preamplifier



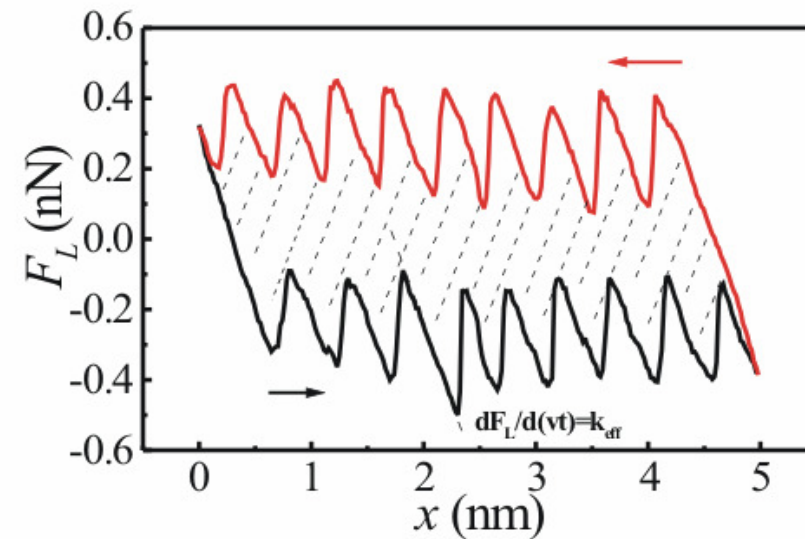
Friction on the Nanometer-scale: Atomic-Stick Slip

Atomic stick-slip



KBr(001)-crystal

Friction loop

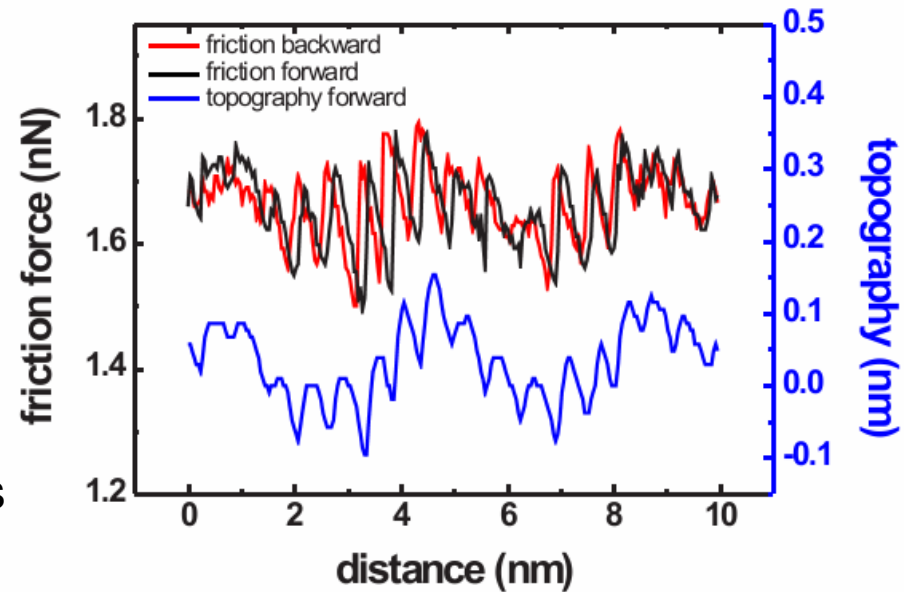
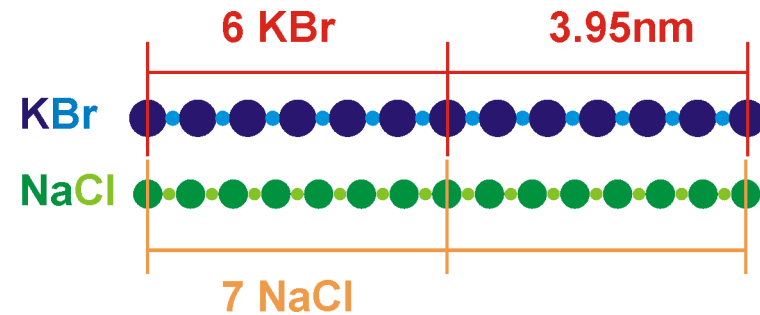
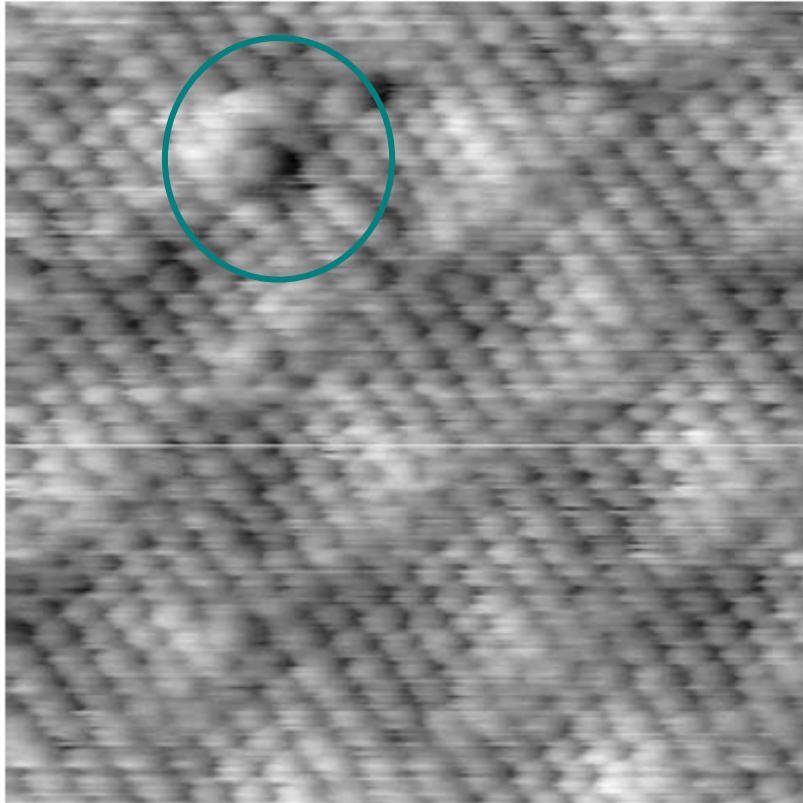


$$F_N = 0.44 \text{ nN}$$

$$E_{diss} = 1.4 \text{ eV}$$

(per slip)

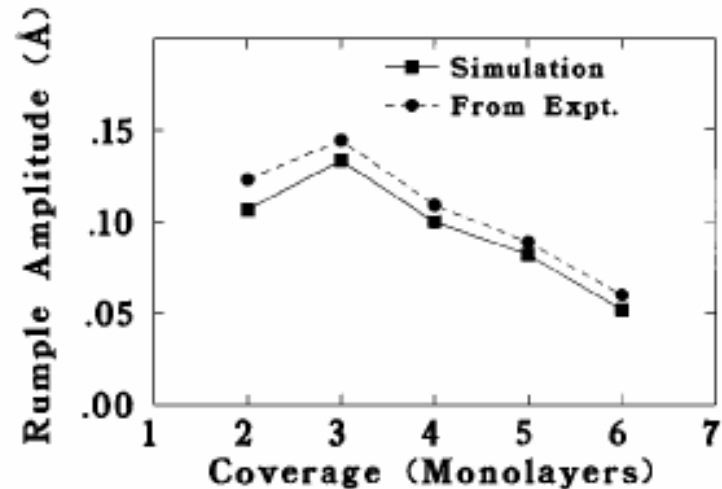
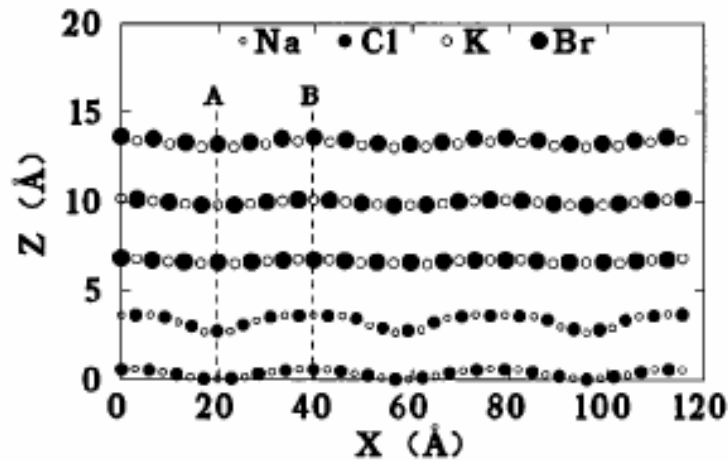
Observation of defects and superstructure of KBr on NaCl(001)



Contact size is smaller than 10 atoms
Contact stiffness is about 1N/m
 $F_{\max} \approx 0.1 \text{ nN}$

Monte Carlo Simulations of KBr/NaCl(001)

J. Baker and P.A. Lindgard, *Phys. Rev. B* **54**, R 11137 (1996)

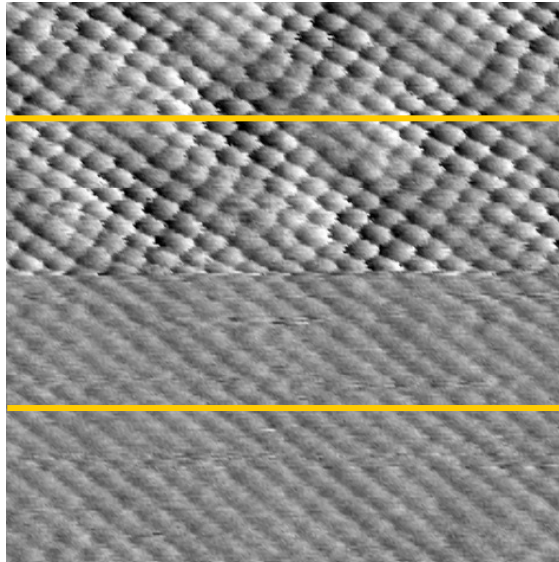


17% misfit leads to superstructure
6 KBr-units fit on 7 NaCl-units

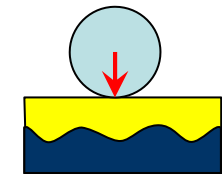
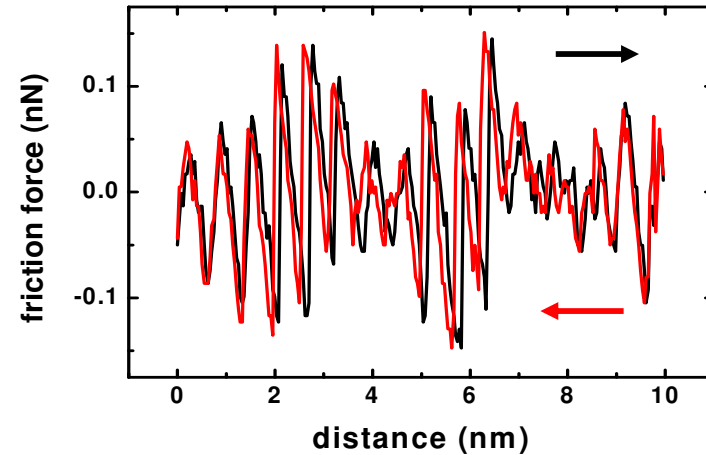
Rumpling of NaCl-interface is observed on the KBr-surface (0.01 nm for 2ML)

Agreement with Helium scattering data; Duan et al. *Surf. Sci.* **272**, 220 (1992)

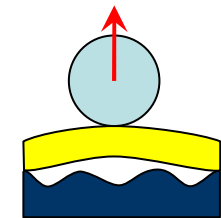
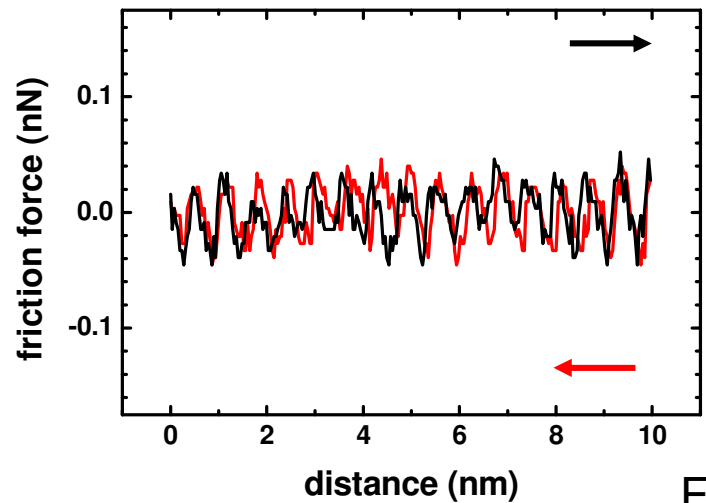
Loading dependence of atomic friction: KBr/NaCl(001) superstructure



10x10nm²:
Friction force map at 2 loads



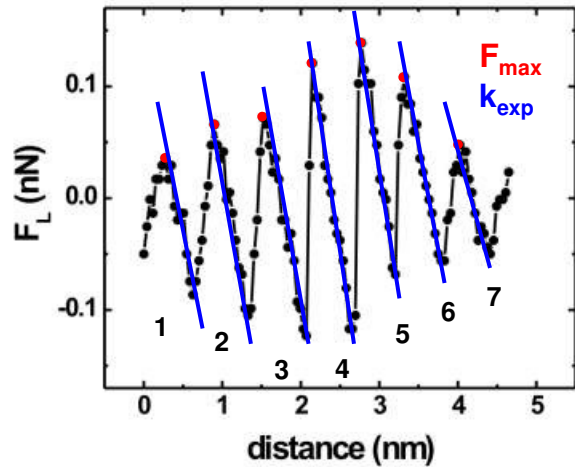
$F_N = 0.01$ nN



$F_N = -0.31$ nN
Close to jump-off

Superstructure is less pronounced at lower loads
Influence of the buried interface?

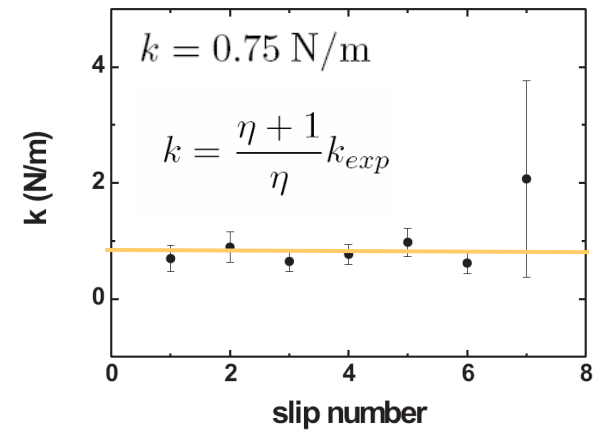
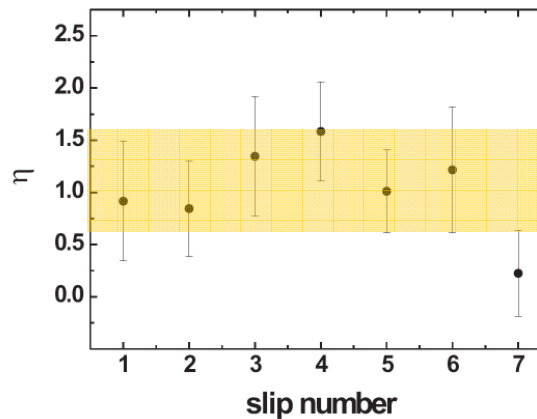
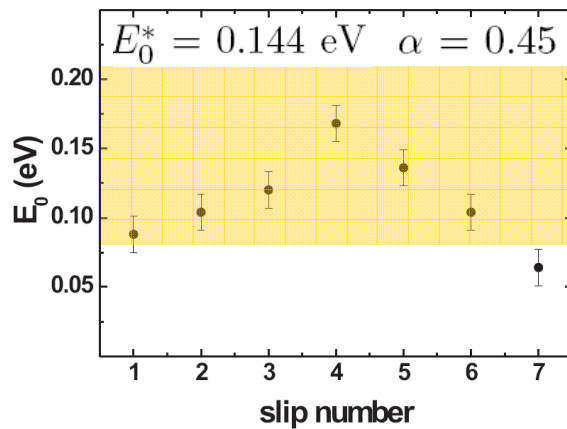
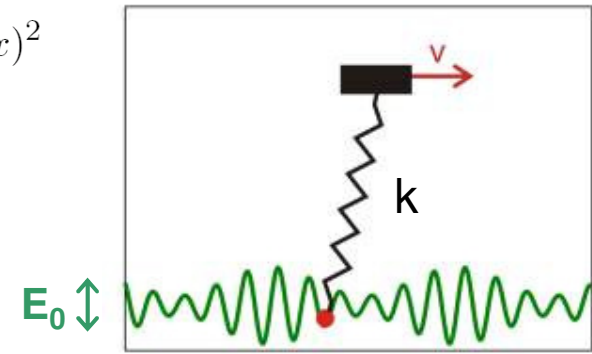
Modification of the Tomlinson Model



$$V = -\frac{E_0}{2} \cos\left(2\pi \frac{x_{tip}}{a}\right) + \frac{1}{2}k(x_{tip} - x)^2$$

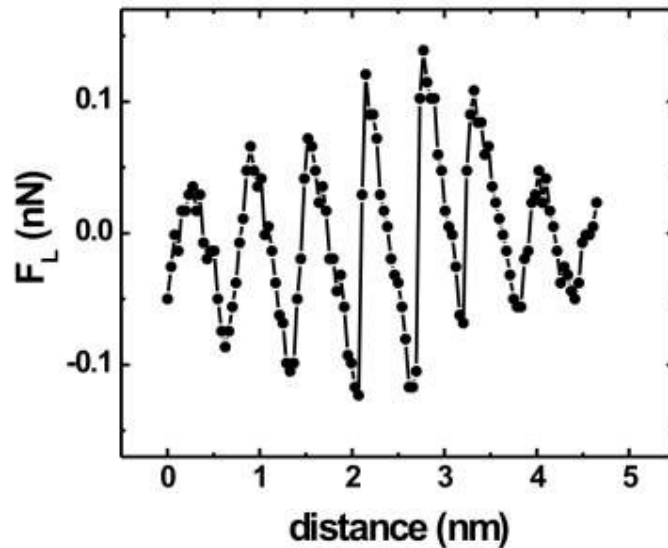
$$E_0 = E_0^* \left(\alpha \cos\left(\frac{2\pi x_{tip}}{b}\right) + 1 \right)$$

⇒ Modulation of the stiffness k or energy corrugation E_0

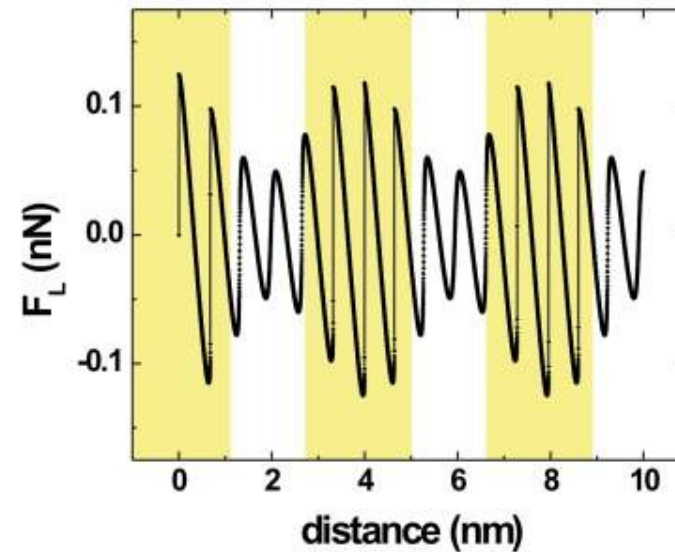


Modified 1D Tomlinson Model Comparison with Experimental Results

Experiment



Tomlinson Model

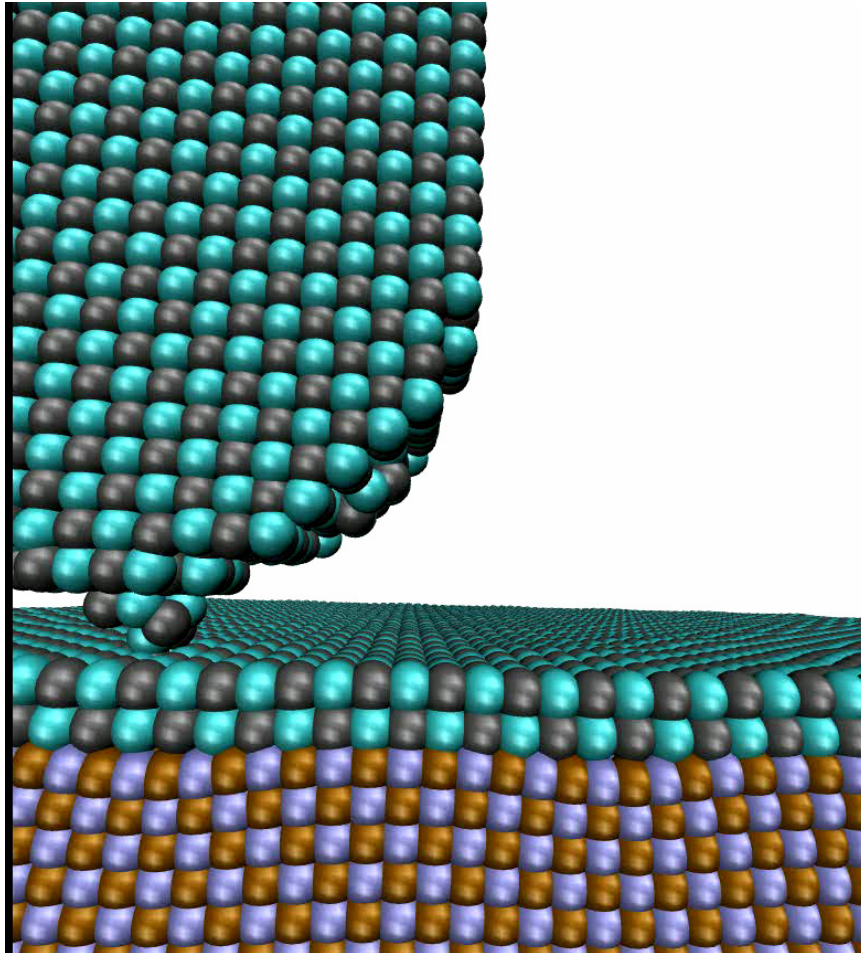


Parameters: $E_0^*=0.144$ eV, $\alpha=0.45$, $k=0.75$ N/m, $v=10$ nm/s, $a=0.66$ nm

⇒ It is possible to observe areas in the superlubricity regime ($\eta < 1$) and areas with stick slip ($\eta > 1$) due to the large variations of energy barriers

Atomistic Simulations: KBr/NaCl(001)

A. Ghasemi, S. Goedekker, Uni Basel



-Superstructure
observed

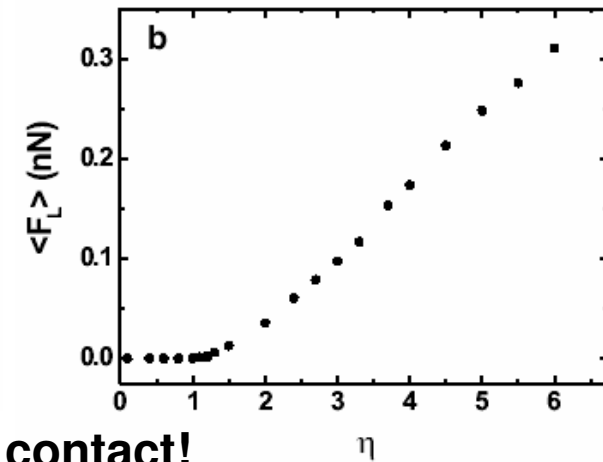
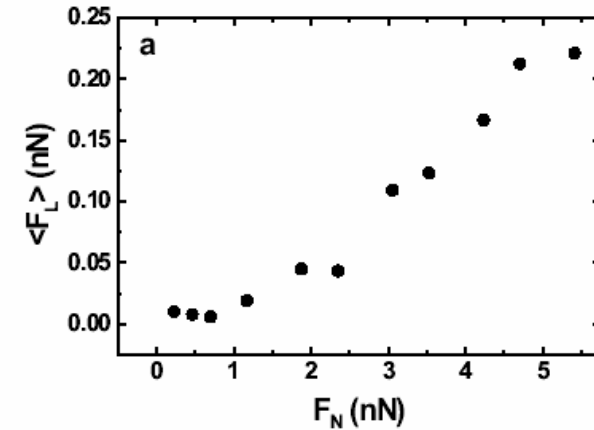
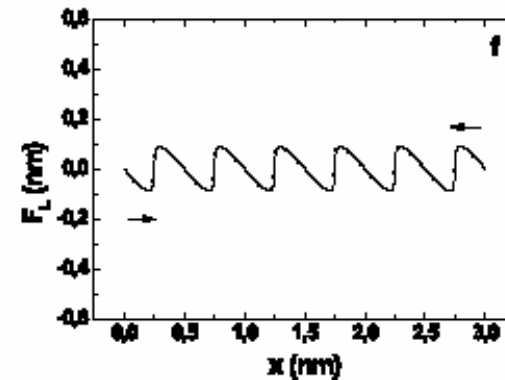
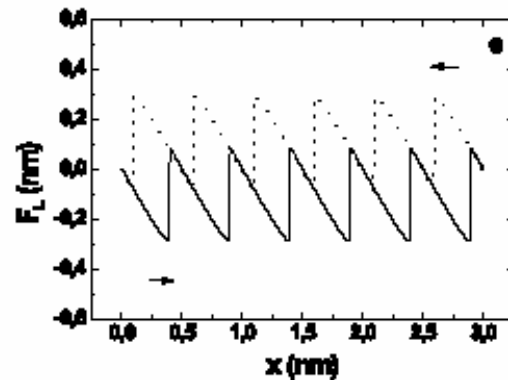
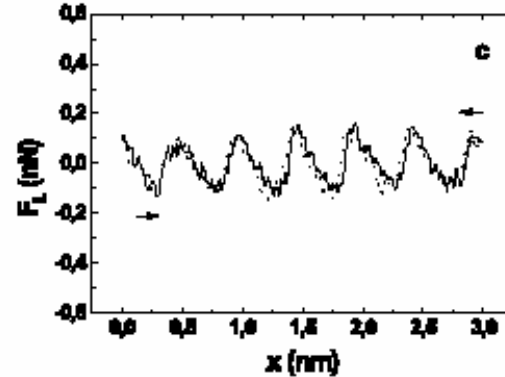
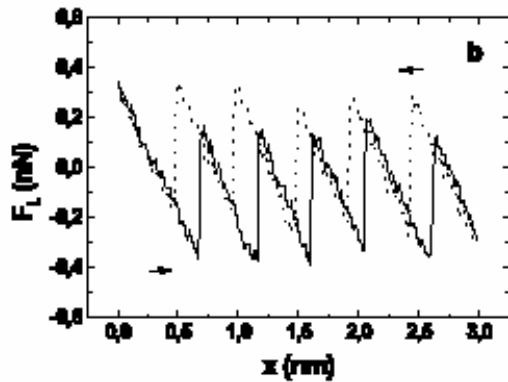
-small topographic changes

-Interface leads to strong
variations of atomic
friction

Tip (9000 atoms)
KBr/NaCl (70'000 atoms)

Loading dependence of Friction on NaCl(001) UHV FFM with sharp tip vs. Prandtl-Tomlinson model

$k_x = 29 \text{ N/m}$, $k_z = 0.05 \text{ N/m}$, $v_x = 3 \text{ nm/s}$, const. z
Scans along [100] showing maximum variation



Stick-slip

$$\eta > 1$$

Continuous sliding in contact!

$$\eta < 1$$

$$\text{mean load } F_N = F_z + 0.7 \text{ nN}$$

A. Socoliuc et al., *Phys. Rev. Lett.* **92**, 134301 (2004)

1d-Prandtl-Tomlinson-Model

Potential energy:

$$U = -\frac{E_0}{2} \cos\left(2\pi \frac{x_t}{a}\right) + \frac{1}{2} k(x_t - x_s)^2$$

Stability criterion:

$$\frac{\partial U^2}{\partial x_t^2} = \frac{2\pi^2}{a^2} E_0 \cos\left(2\pi \frac{x_t}{a}\right) + k > 0$$

$$\eta = \frac{2\pi^2 E_0}{ka^2} = \pi^2 \frac{E_0}{ka^2/2}$$

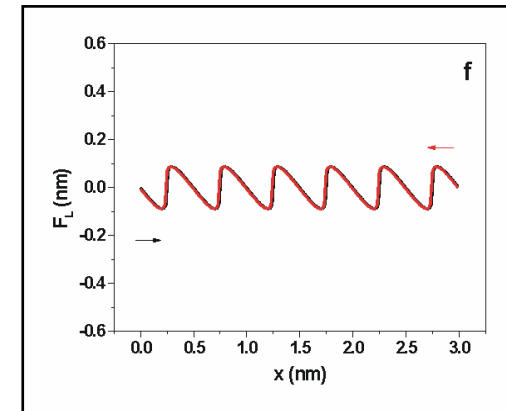
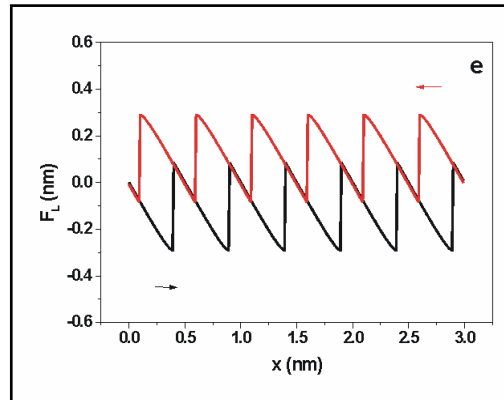
$\eta > 1$

$\eta < 1$

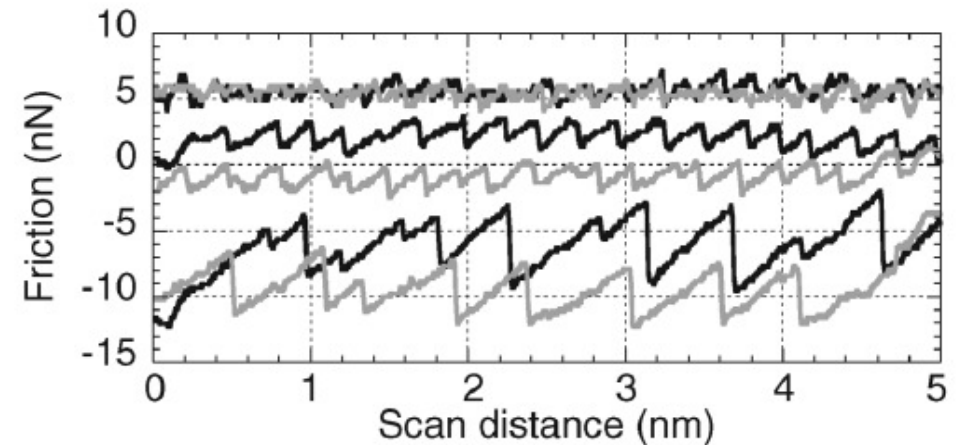
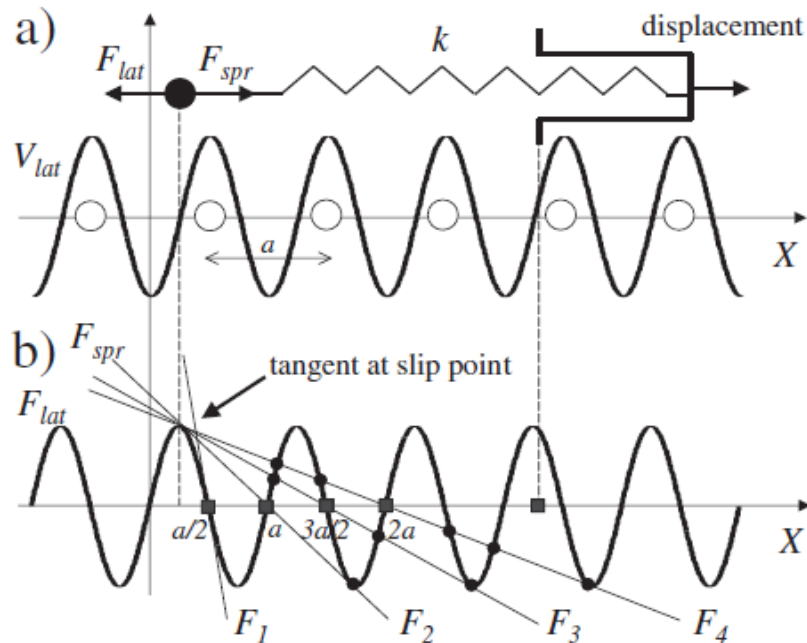
$\eta = 3$

$\eta = 1$

$\eta < 1$: unique sliding solution
 $\eta > 1$: instabilities



Multiple Slips



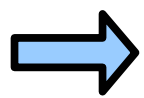
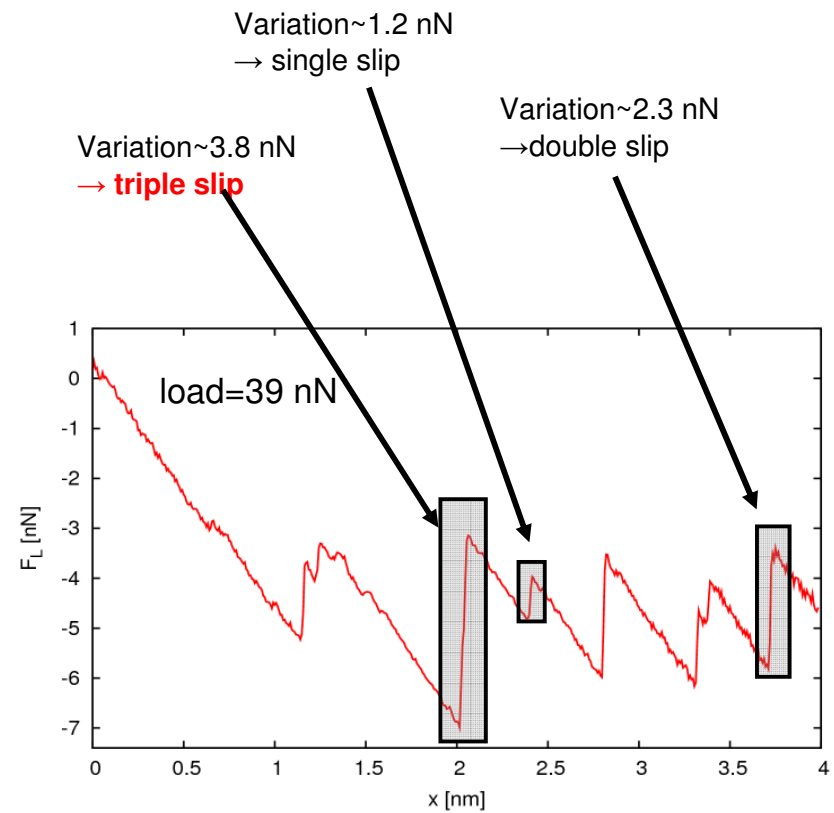
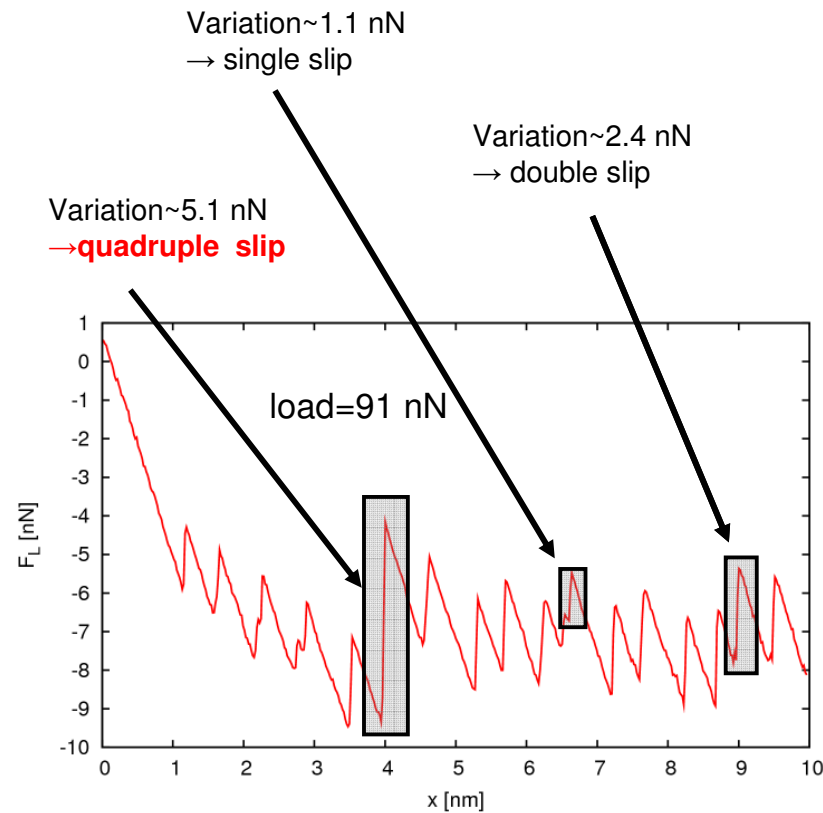
Silicon tip on graphite in air

Transitions for $\eta = 1$ / 4.604 / 7.788 /
10.95 / 12.66 ...

... but this is only valid for the quasi-static limit (and 1 dimensional).

S. Medyanik, W. Liu, I. Sung, R. Carpick, Phys. Rev. Lett. 97, 136106 (2006).

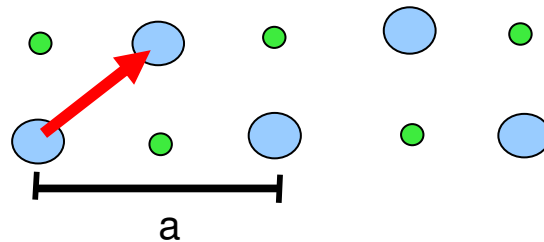
Experiments on NaCl(001) in UHV



Multiple slips do happen at relatively high loads, but they are quite rare (single events)

Classification of multiple slips on NaCl(001)

single slip



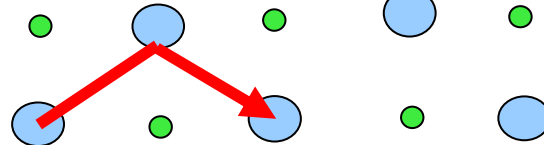
$$\text{Force-variation} = \frac{1}{2} a \times k_{\text{cont}} \sim 1.2 \text{ nN}$$

These jumps are
nothing special,
they also occur at
low loads



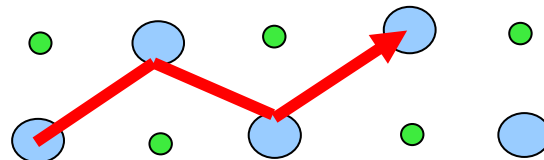
depends on
load
~4.6-5.4
N/m

double slip



$$\text{Force-variation} = 1 a \times k_{\text{cont}} \sim 2.4 \text{ nN}$$

triple slip

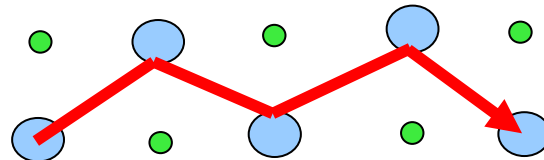


$$\text{Force-variation} = \frac{3}{2} a \times k_{\text{cont}} \sim 3.6 \text{ nN}$$

We are looking for these jumps!



quadruple slip

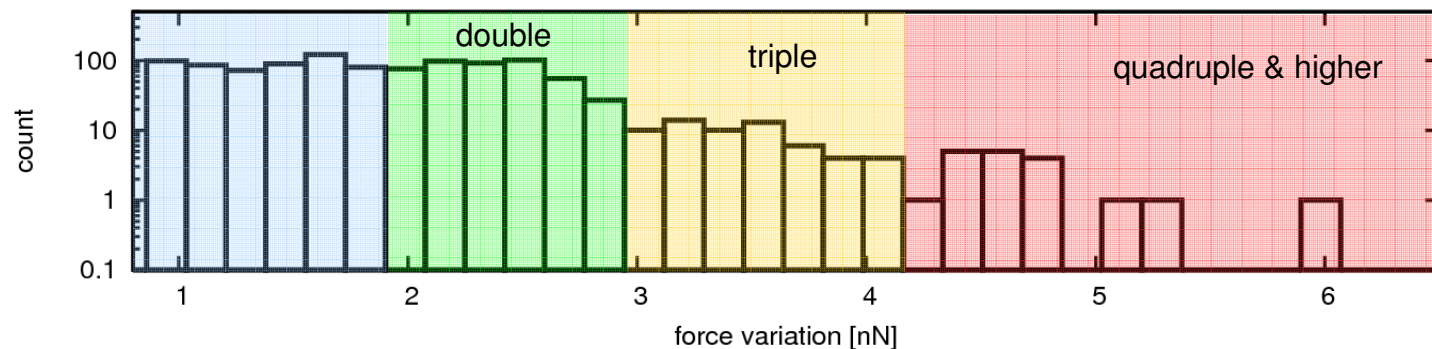
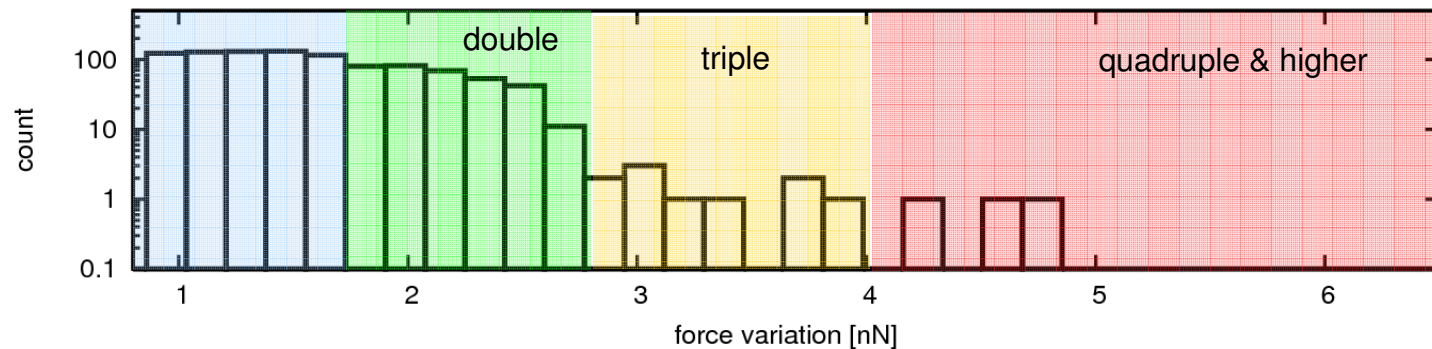
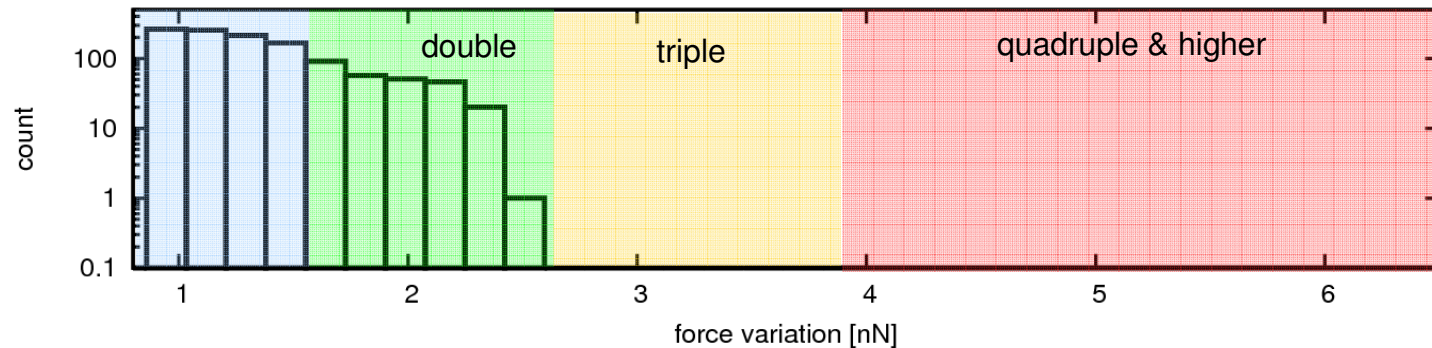


$$\text{Force-variation} = 2 a \times k_{\text{cont}} \sim 4.8 \text{ nN}$$

etc...

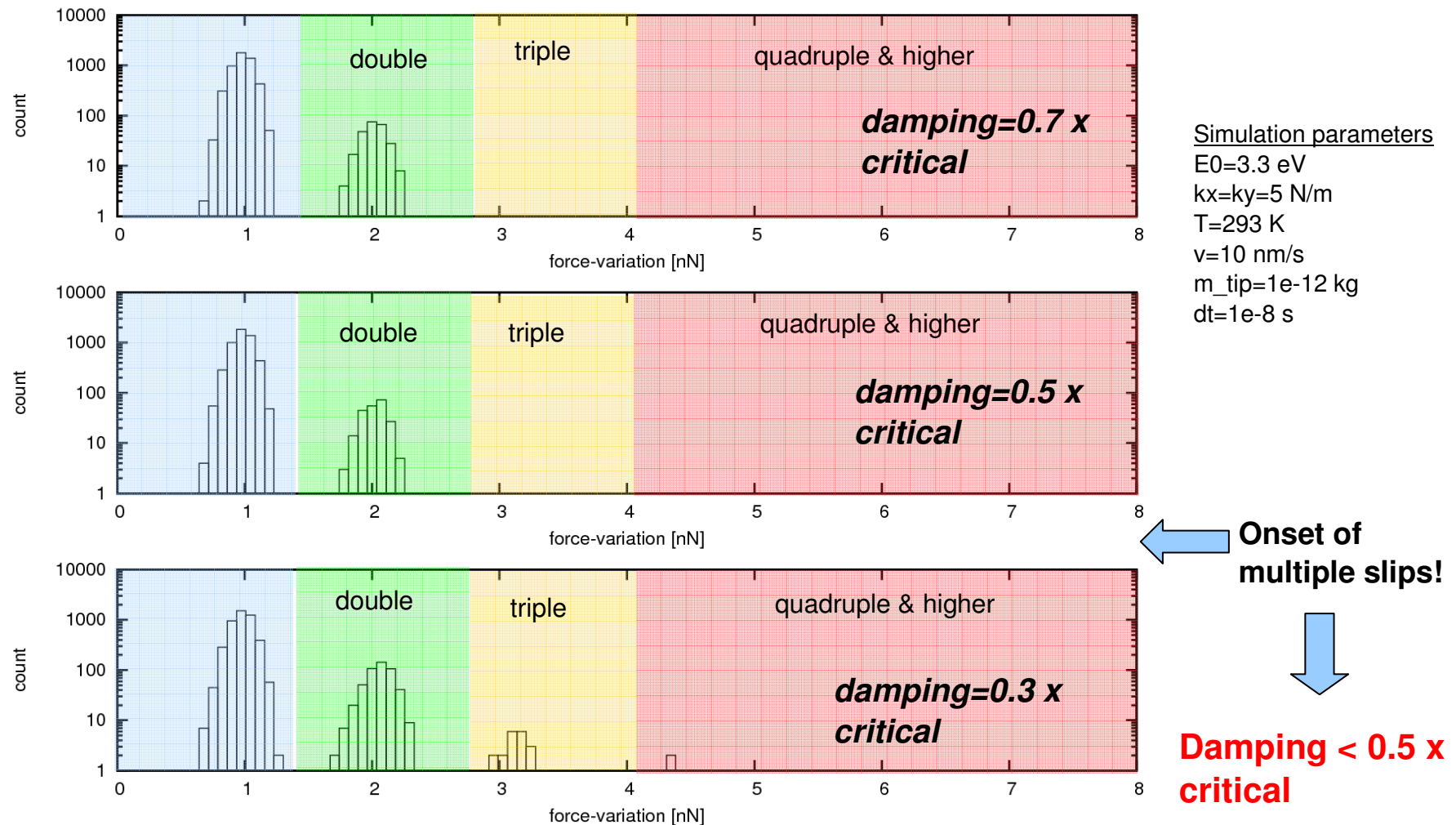
PS: Force variations are upper limits, since jump distance is actually smaller than multiples of $a/2$

Statistics of multiple slips on NaCl(001)



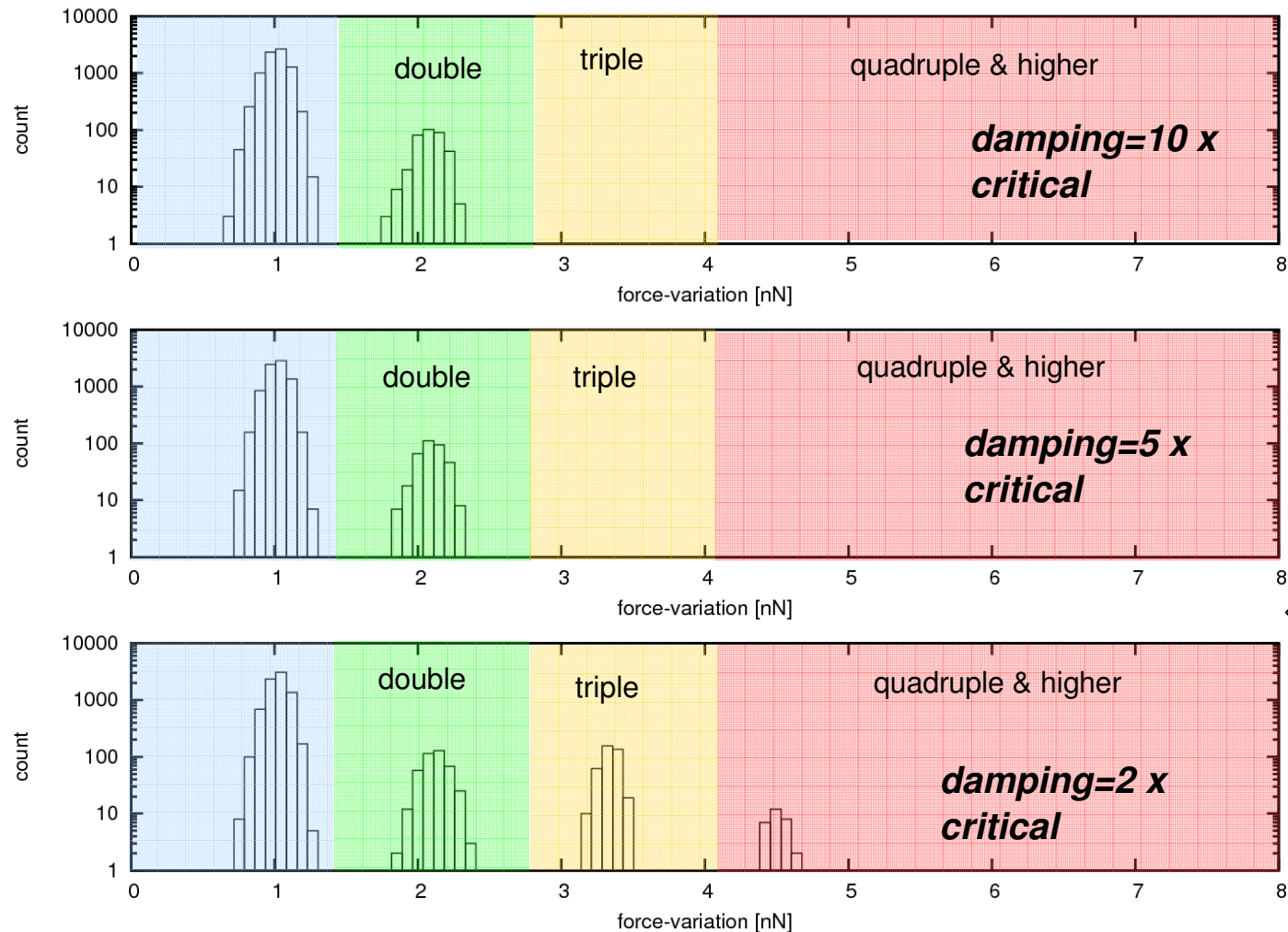
Comparison with simulations ($\eta=8.2$)

Same slip-recognition program run with output of 2D thermal Tomlinson simulation program:



Comparison with simulations ($\eta=12.5$)

Same slip-recognition program run with output of 2D thermal Tomlinson simulation program:



Simulation parameters
E0=5 eV
kx=ky=5 N/m
T=293 K
v=10 nm/s
m_tip=1e-12 kg
dt=1e-8 s

← Onset of multiple slips!

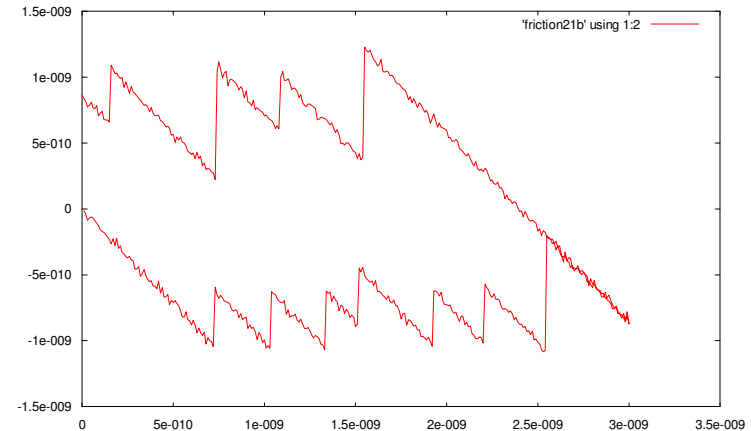
↓
Damping < 5 x critical

Multiple slips: An indicator for damping

$$d^2x_{\text{tip}}/dt^2 + \Gamma_{\text{tip}} dx_{\text{tip}}/dt + \omega_{\text{tip}}^2 (x_{\text{tip}} - x_s) = - (\pi E_0/a) \sin (2\pi x_{\text{tip}}/a)$$

$$\omega_{\text{tip}} = \sqrt{\frac{k}{m}} \quad \Gamma_{\text{tip}} = \frac{\gamma}{m}$$

$$\text{Critical damping: } \Gamma_{\text{crit}} = 2\sqrt{\frac{k}{m}}$$



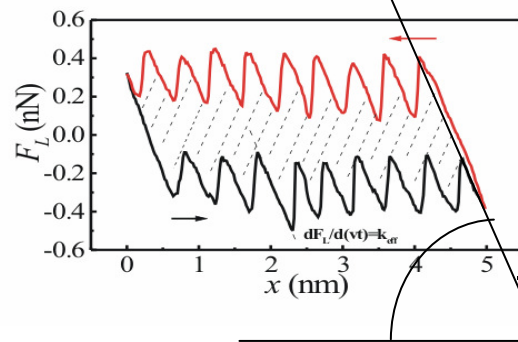
Observation of multiple slips indicate that the slightly underdamped case is present for intermediate loadings (39nN):

$$\gamma < 0.5\gamma_{\text{crit}}$$

At high loads (78nN), there seems to occur a transition to the overdamped case.

$$\gamma < 5\gamma_{\text{crit}}$$

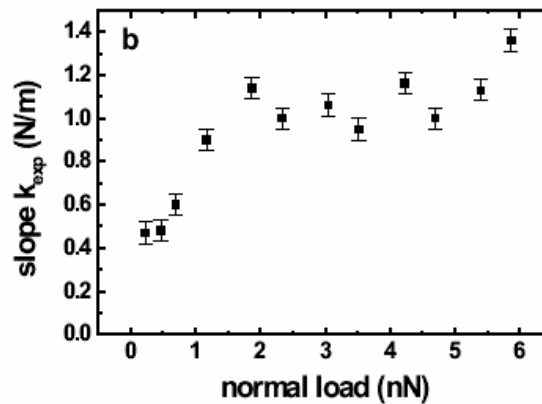
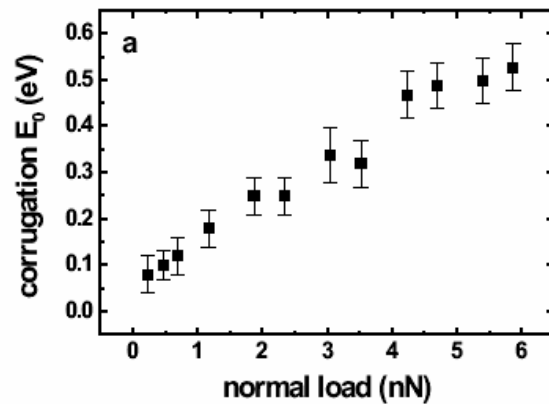
Dependence of Tomlinson Parameters



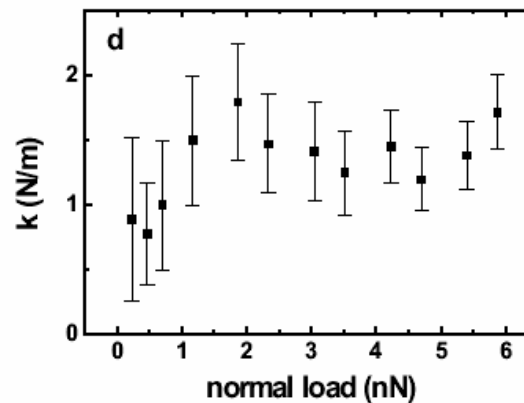
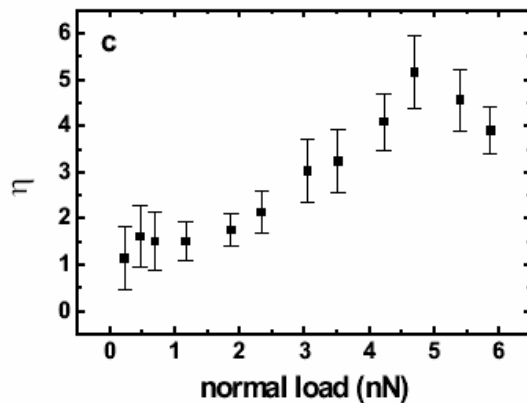
$$F_L^{\max} \longrightarrow E_0 = \frac{a F_L^{\max}}{\pi}$$

$$k_{\text{exp}} \longrightarrow \eta = \frac{2\pi F_L^{\max}}{k_{\text{exp}} a} - 1$$

$$k = \frac{\eta + 1}{\eta} k_{\text{exp}}$$

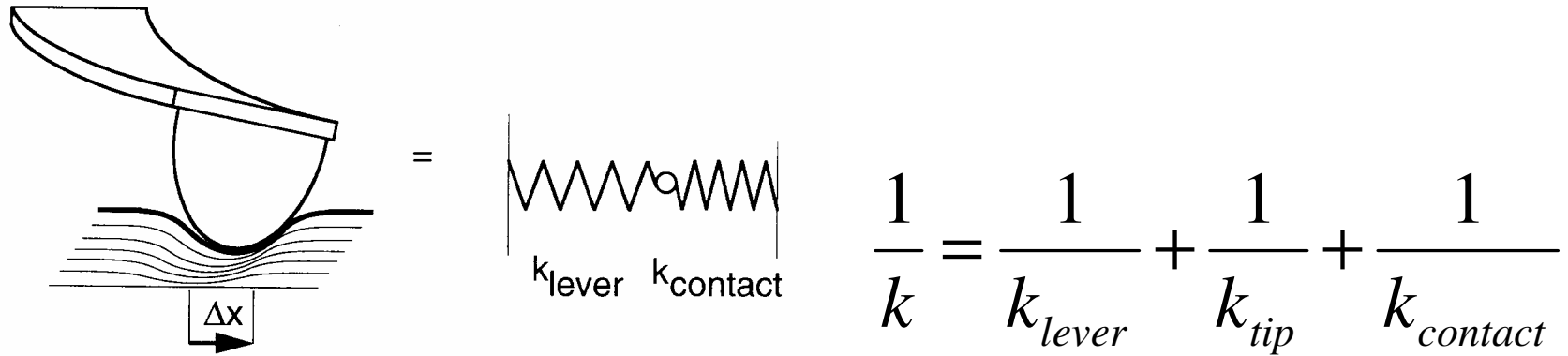


E_0 : linear increase with normal forces



k : rather independent (contact area const.?)

Lateral contact stiffness



R. Carpick et al, Appl. Phys. Lett. 70, 1548-1550 (1997)

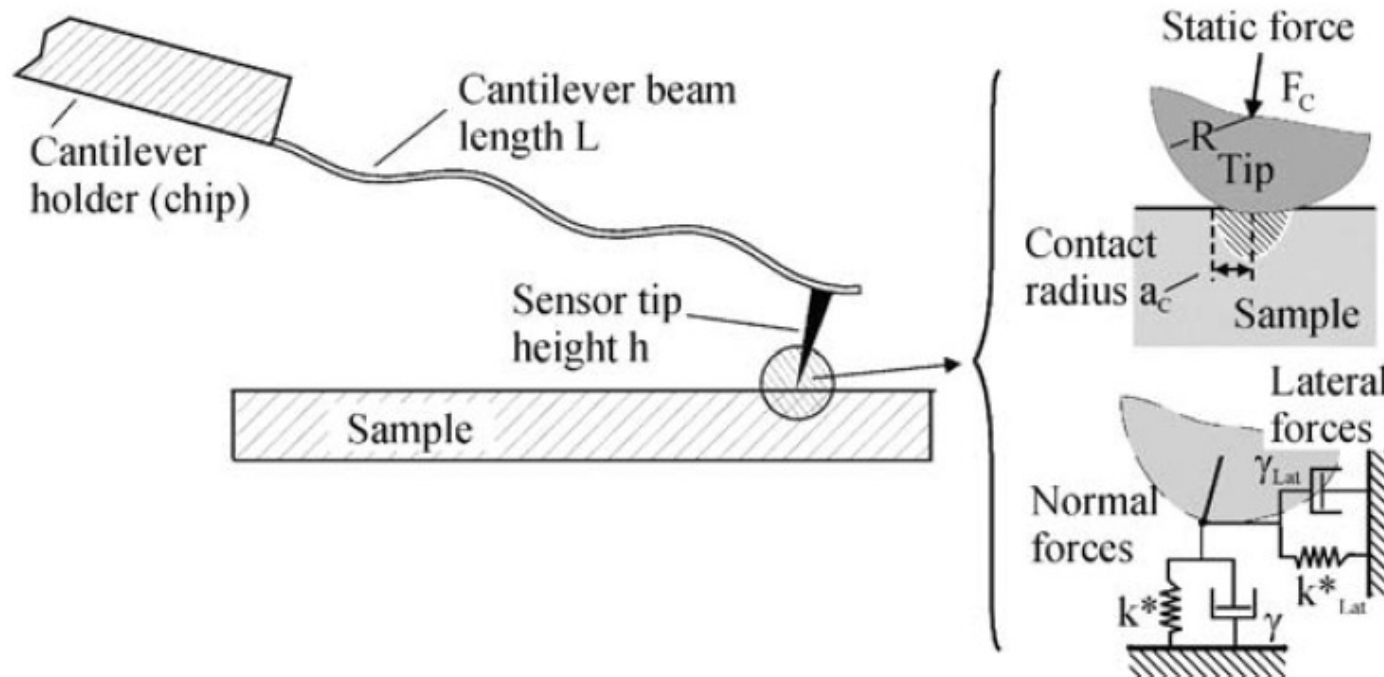
Here: $k_{\text{lever}} = 29 \text{ N/m} \gg k \Rightarrow k_{\text{contact}} \approx 1\text{-}2 \text{ N/m}$

Continuum model :

$k_{\text{contact}} = 8 \text{ a G} \Rightarrow a < 1 \text{ \AA} ?$

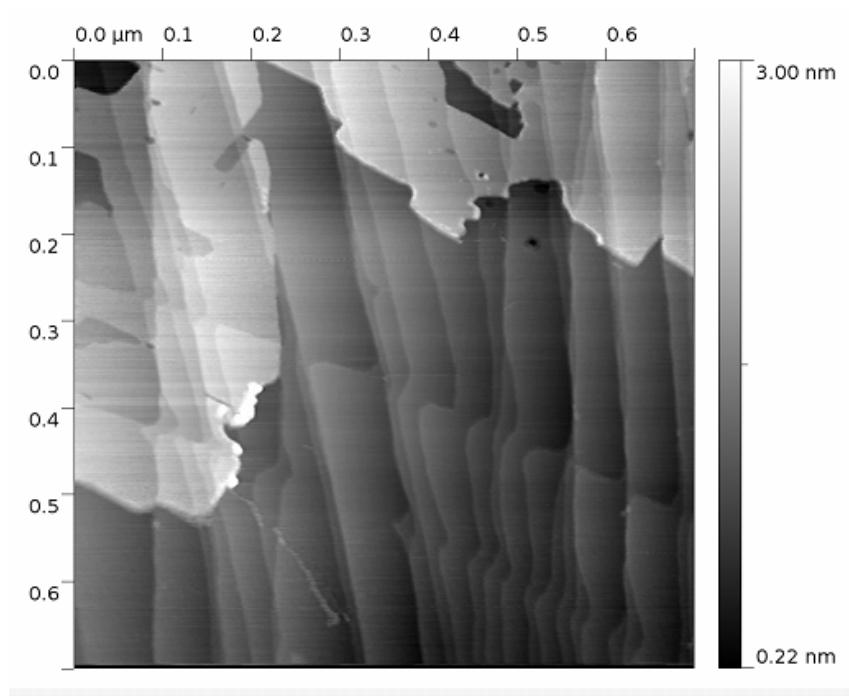
\Rightarrow Atomistic model needed

Contact resonance frequencies and normal stiffness k^*

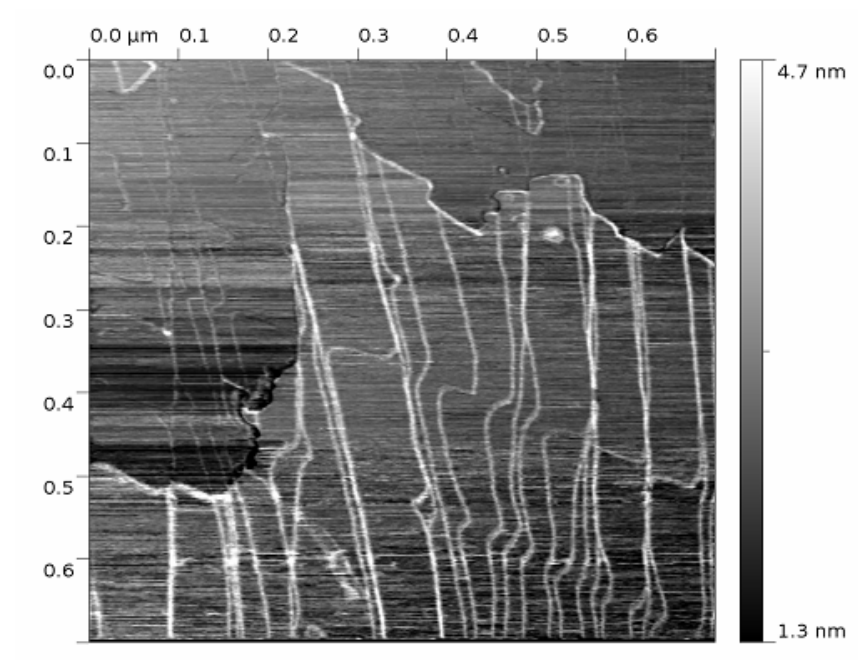


U. Rabe in Applied Scanning Probe Methods II, p. 39ff
Eds. H. Fuchs, B. Bhushan, Springer-Verlag, Berlin

Contact mode imaging with excitation of NaCl(001) on Cu(111) and amplitude measurement at contact resonance



Topography



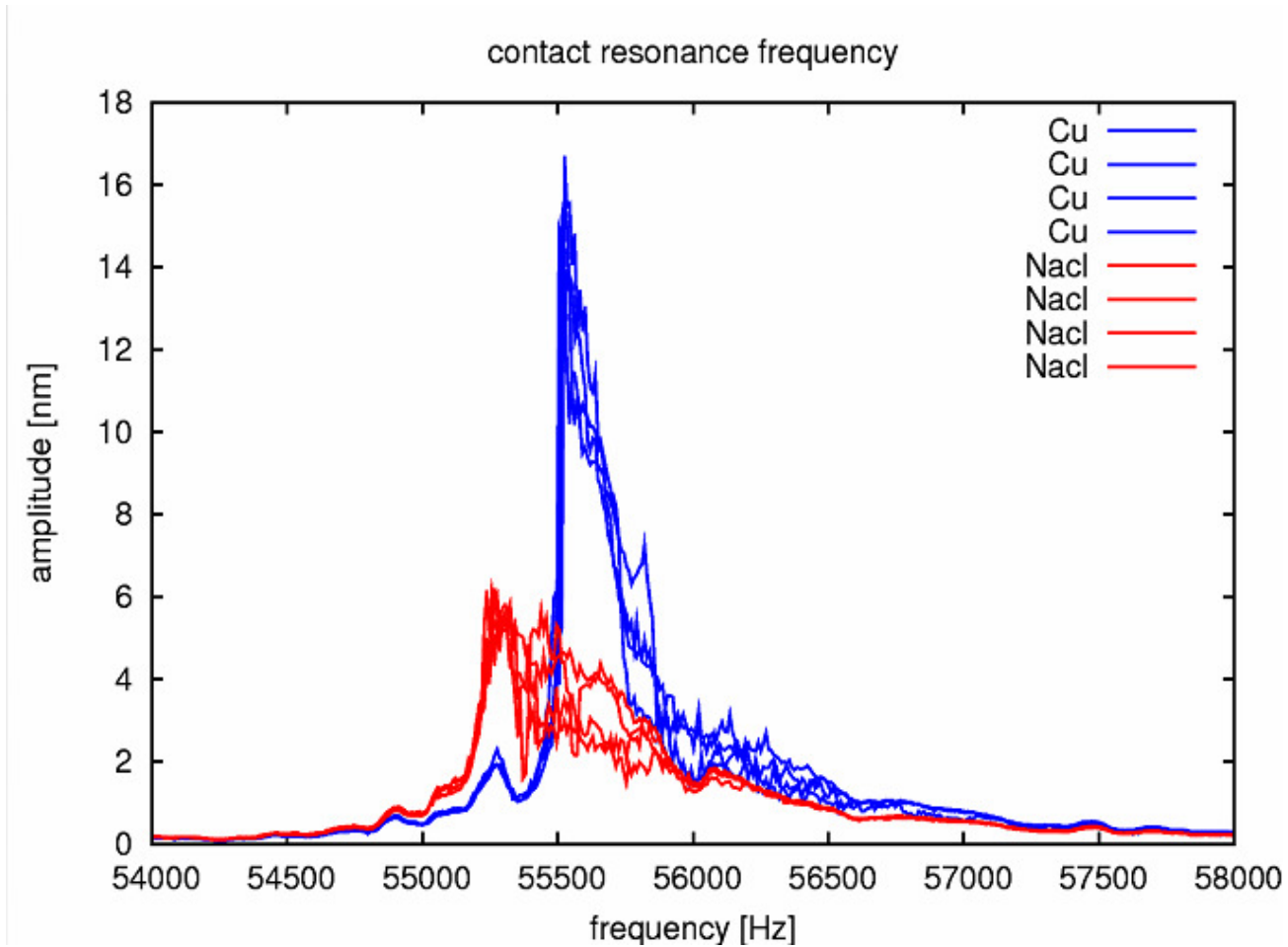
Lock-in amplitude at 56.2kHz

Fixed frequency: 56.2kHz

Lock-In measurement of amplitude

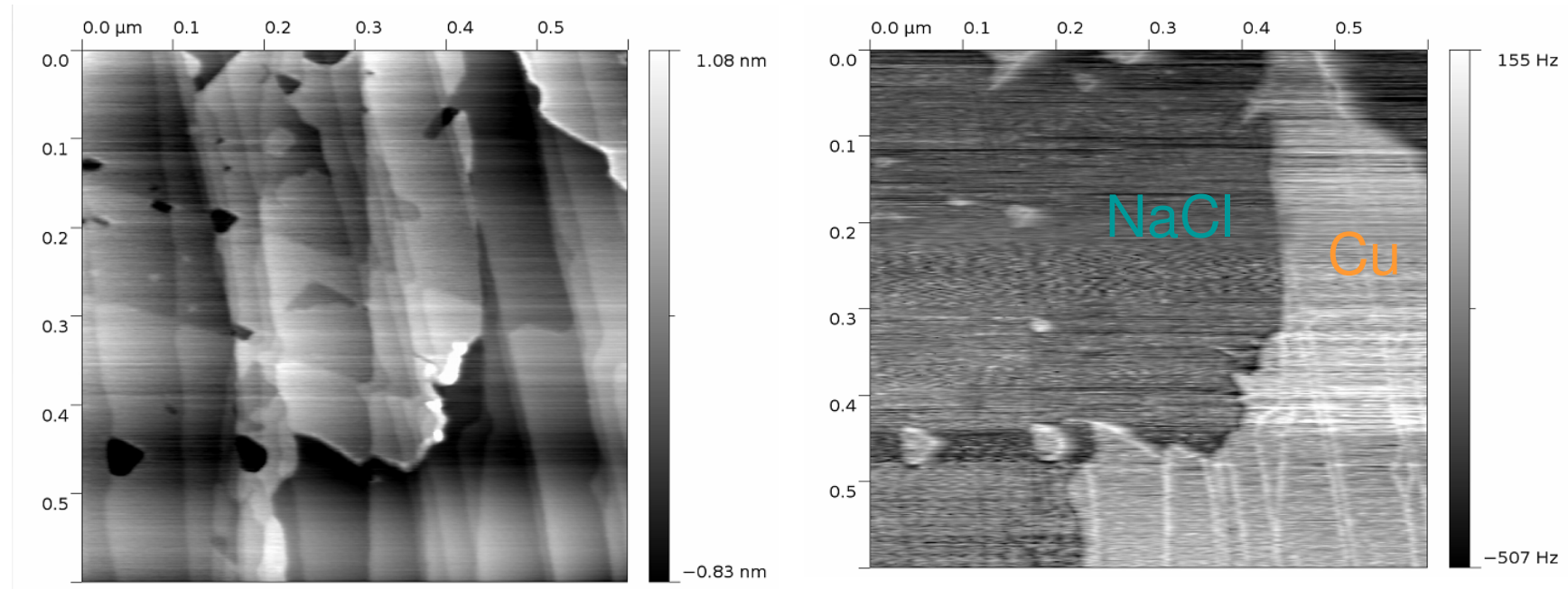
⇒ Local variations of normal contact stiffness

Contact Resonances



Free cantilever: 11325Hz; In Contact: 55.3kHz and 55.5kHz

Imaging of contact resonance by PLL NaCl(001) on Cu(111)



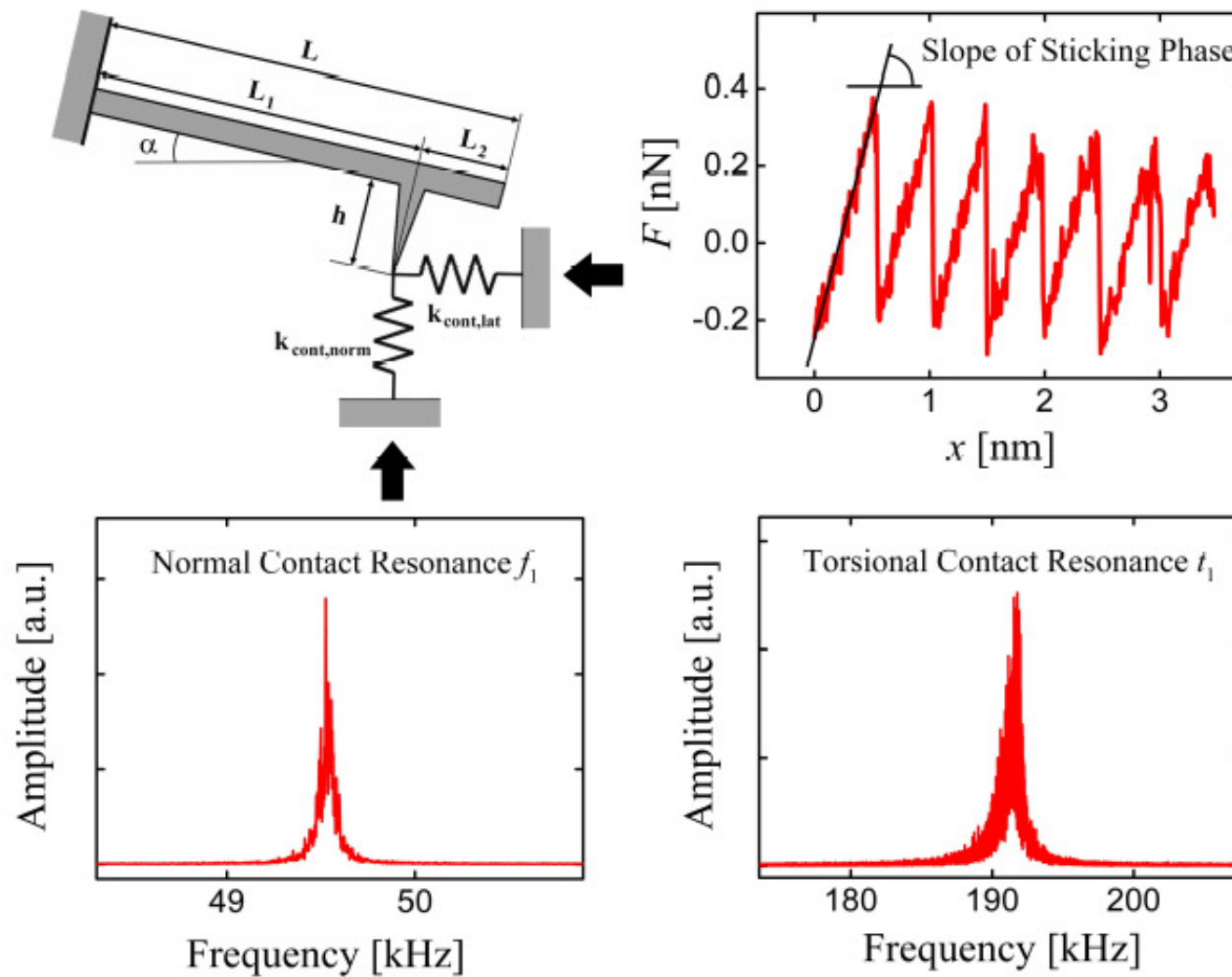
Topography

Frequency shift
measured by PLL
Amplitude=400pm

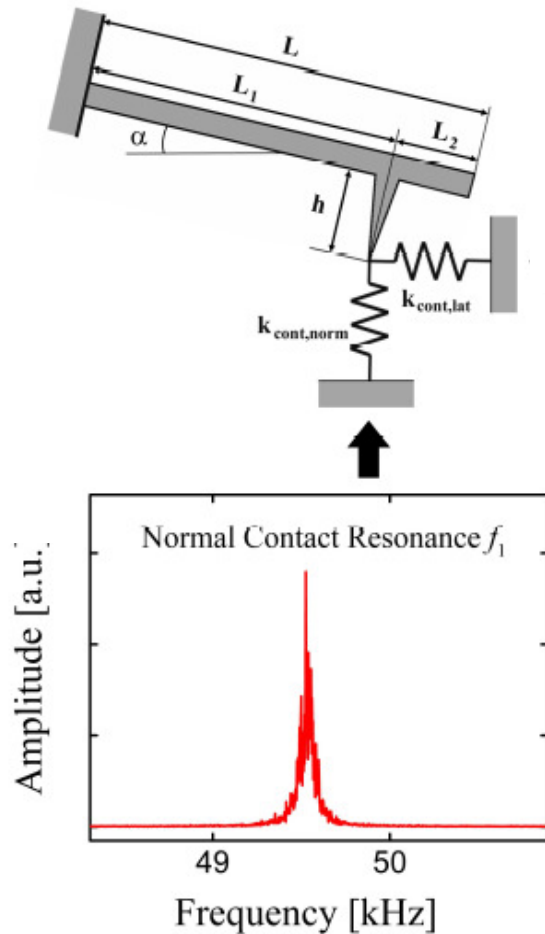
Contrast between copper and NaCl: 195Hz

Free cantilever: 11325Hz; In Contact: 55.3kHz and 55.5kHz

Simultaneous determination of lateral and normal contact stiffness

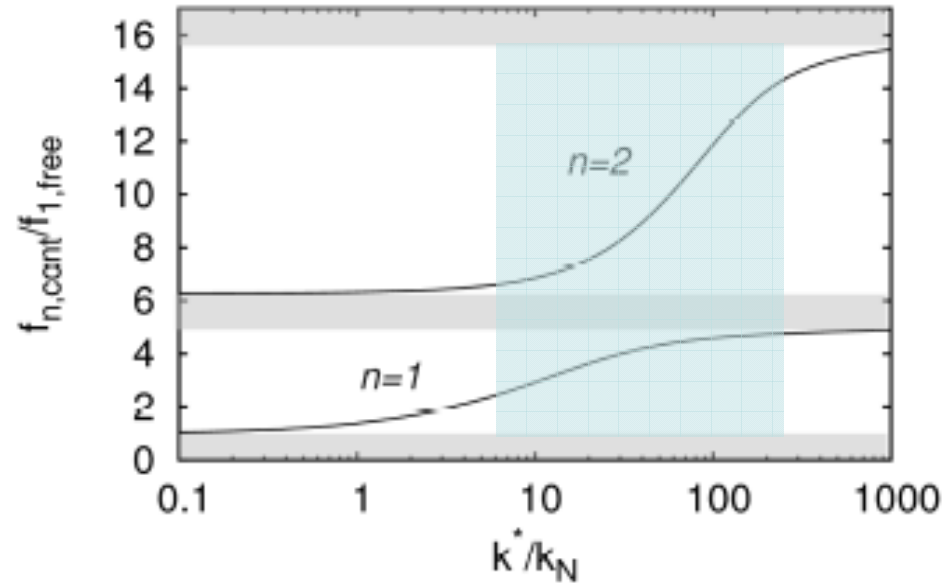


Determination of normal contact stiffness



$$k_N = 0.095 \text{ N/m}$$

$$f_1 = 49.5 \text{ kHz} \quad f_1^0 = 10.2 \text{ kHz}$$



$$\frac{k_{\text{cont,norm}}}{k_{\text{norm}}} = \frac{-B \pm \sqrt{B^2 - 4AC}}{6A}$$

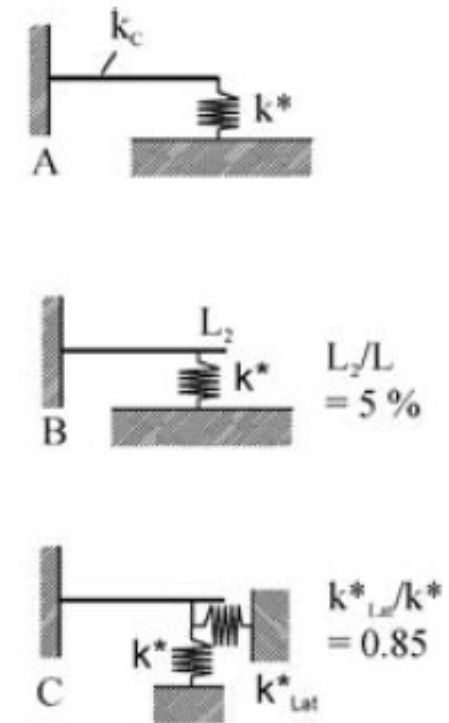
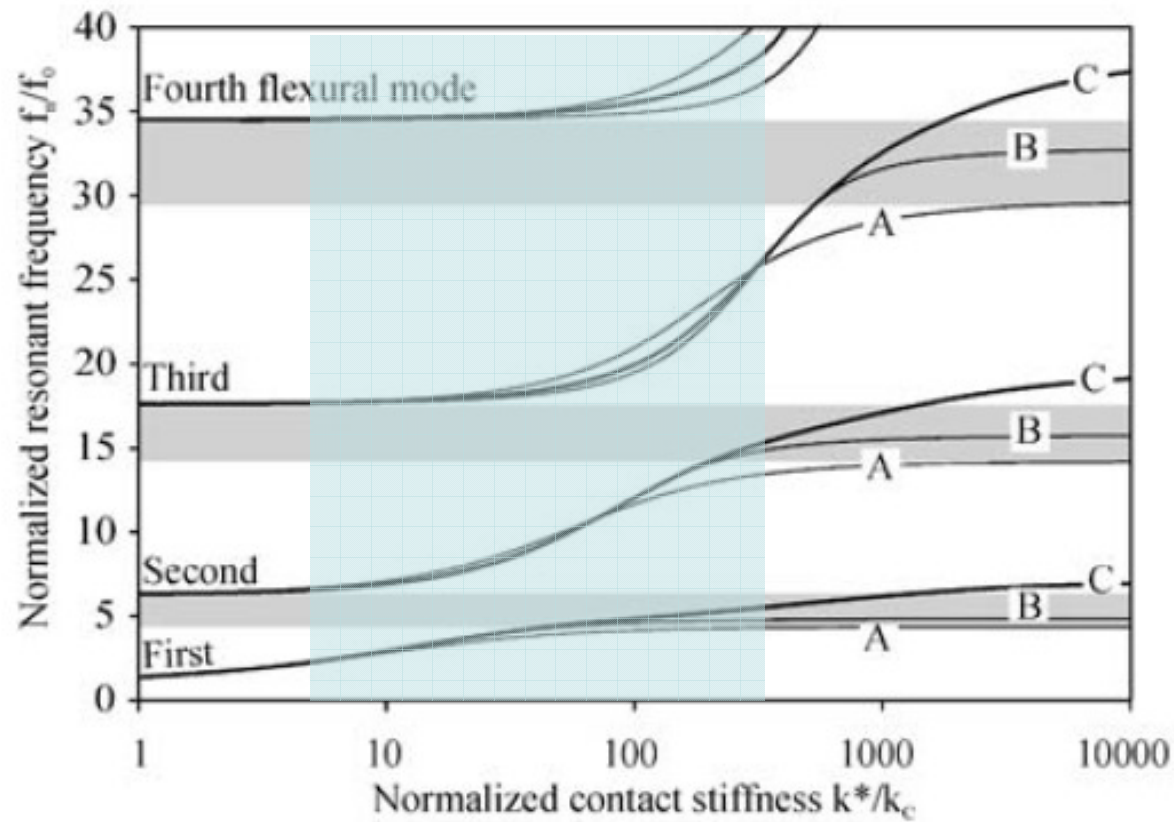
$$A = \left(\frac{k_{\text{cont,lat}}}{k_{\text{cont,norm}}} \right) \left(\frac{h}{L_1} \right)^2 (1 - \cos(x_n L_1) \cosh(x_n L_1)) \times (1 + \cos(x_n L_2) \cosh(x_n L_2)),$$

$$B = B_1 + B_2 + B_3,$$

$$C = 2(x_n L_1)^4 (1 + \cos(x_n L) \cosh(x_n L)),$$

$$x_1 L = x_1^0 L \sqrt{\frac{f_1}{f_1^0}},$$

Contact resonance frequencies as a function of normalized contact stiffness



U. Rabe in Applied Scanning Probe Methods II, p. 39ff
Eds. H. Fuchs, B. Bhushan, Springer-Verlag, Berlin

Comparison of lateral and normal contact stiffness

sample	k_N [N/m]	η	κ [N/m]	$k_{\text{cont lat}}$	$k_{\text{cont norm}}$	$\frac{k_{\text{cont norm}}}{k_{\text{cont lat}}}$	
				k_{eff} [N/m]	k^* [N/m]	$\frac{k^*}{\kappa}$	$\frac{k^*}{k_{eff}}$
NaCl(100)	3.1	5.7	1.72	2.07	13.1	7.6	6.33
NaCl(100)	0.095	4.9	1.24	1.49	21.1	17.1	14.16
NaCl(100)	0.082	4.0	1.43	1.83	19.0	13.0	10.38
KBr(100)	0.082	1.3	0.96	1.72	14.9	15.5	8.68
Cu(111)	0.091	5.7	2.72	3.20	40.4	14.9	12.63
NaCl(100) on Cu(111)	0.091	3.1	1.65	2.18	32.7	19.8	15.00

$$\eta = \frac{2\pi F_L^{\max}}{k_{exp} a} - 1. \quad k_{eff} = \frac{\eta + 1}{\eta} \cdot \kappa$$

Comparison of lateral and normal contact stiffness

Lateral contact stiffness under atomic stick slip condition

($F_N=0.1-1\text{ nN}$; $\eta=3-5$):

$$k_L=1-3\text{ N/m}$$

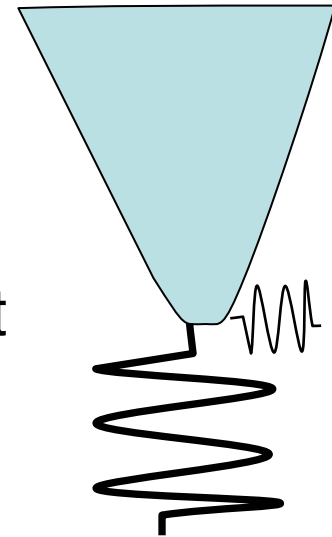
Normal contact stiffness determined from contact resonances:

$$k^*=13-40\text{ N/m}$$

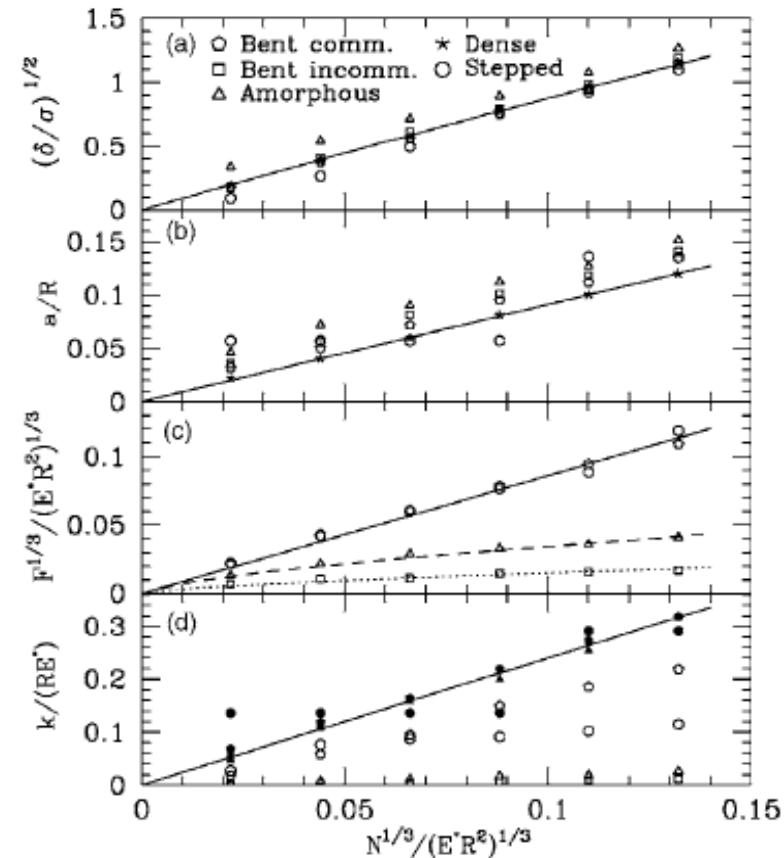
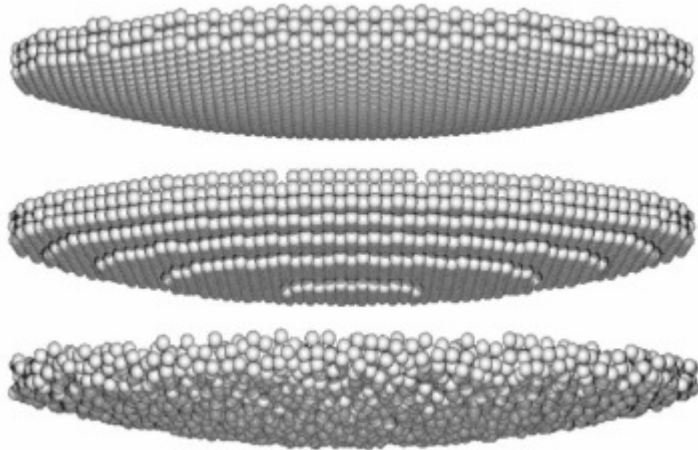
Ratio of normal to lateral contact stiffness:

$$k^*/k_L=6-15$$

Normal contact stiffness is larger than lateral contact stiffness
From continuum models a ratio of $E/G=2-4$ is expected!



Normal and lateral contact stiffness



- Normal contact stiffness in reasonable agreement with continuum models
- Lateral contact stiffness differs from the continuum model for small radii

B. Luan and M. Robbins, Phys. Rev. E 74, 026111 (2006).

Contact area from normal contact resonance frequencies measurements

$$k_{\text{cont, norm}} = 32 \text{ N/m on NaCl(001)/Cu(111)}$$

$$k_{\text{cont, norm}} = 40 \text{ N/m on Cu(111)}$$

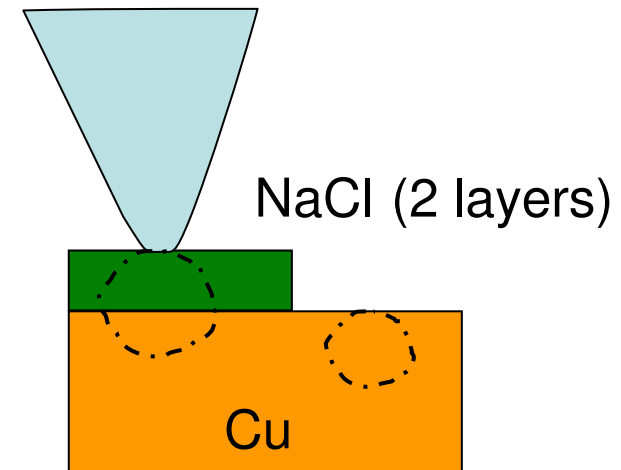
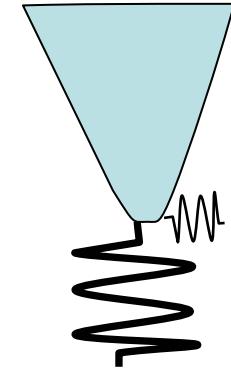
Application of Continuum model (flat punch):

$$2a = \frac{k_{\text{cont, norm}}}{E^*} = 0.9 \text{ nm} / 0.5 \text{ nm}$$

$$\frac{1}{E^*} = \left(\frac{1 - \nu_{\text{tip}}^2}{E_{\text{tip}}} \right) + \left(\frac{1 - \nu_{\text{sample}}^2}{E_{\text{sample}}} \right)$$

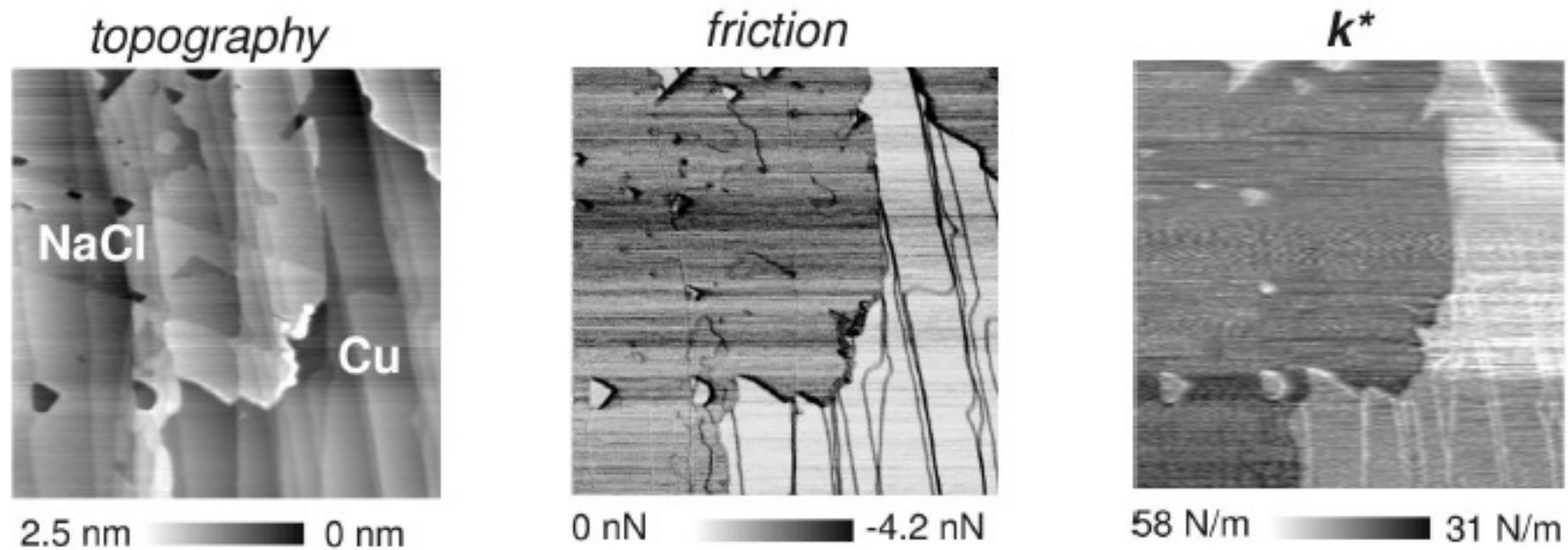
$$E_{\text{tip}} = 169 \text{ GPa} \quad \nu_{\text{tip}} = 0.33$$

$$E_{\text{sample}} = 40 \text{ GPa} / 120 \text{ GPa} \quad \nu_{\text{sample}} = 0.25 / 0.34$$



⇒ Area from normal contact stiffness seems in agreement with resolution

Simultaneous imaging of lateral forces and normal contact stiffness: NaCl(001) on Cu(111)



Lowest friction on Cu(111)

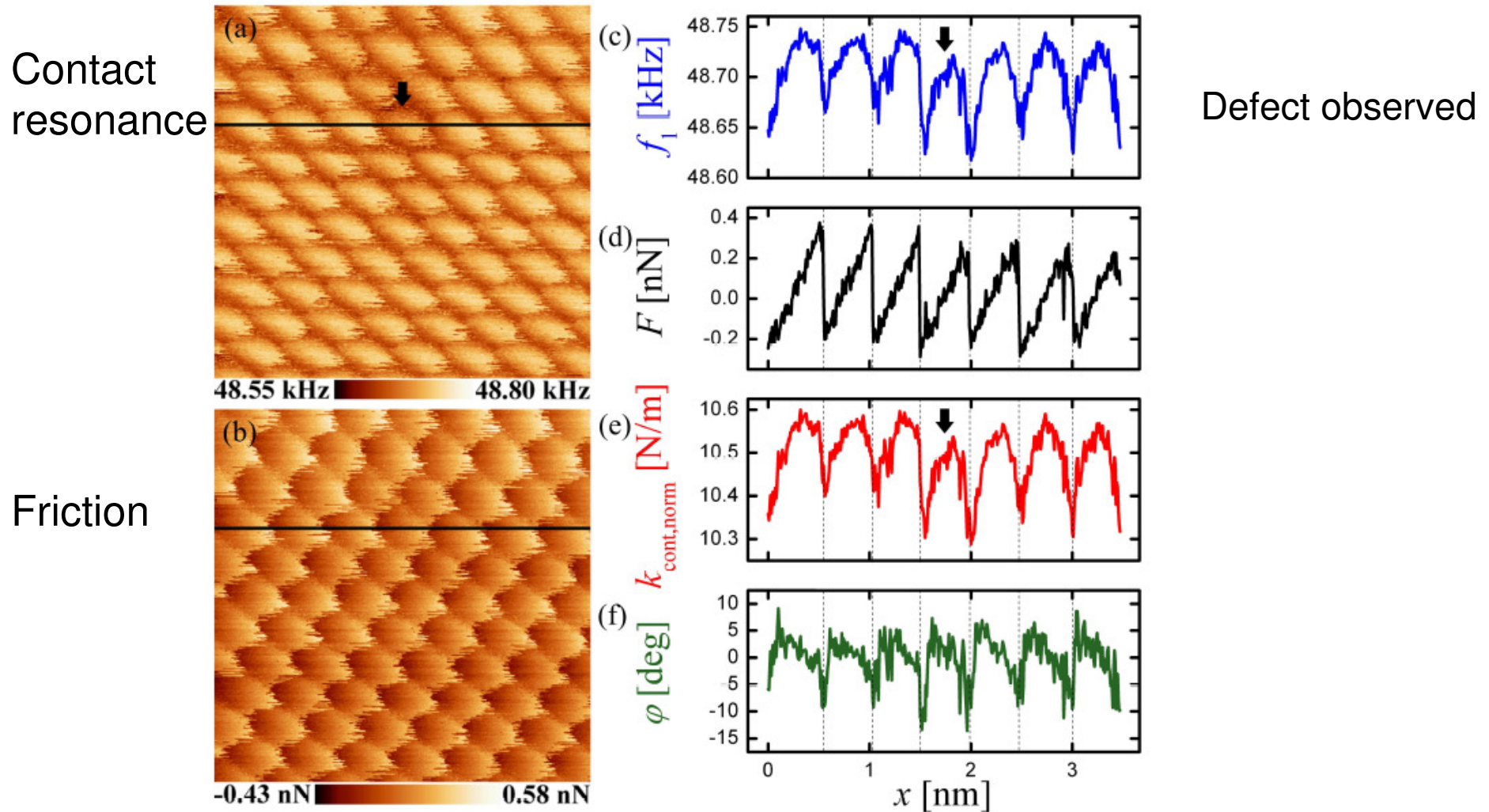
Contact stiffness on NaCl $k^*(\text{NaCl})=32\text{N/m}$

Contact stiffness on Cu(111) $k^*(\text{Cu})=40\text{N/m}$

Contact diameter: $2a=k^*/E^*=0.9\text{nm}$ (0.5nm)

Contact stiffness rather independent of number of layers

Simultaneous measurement of atomic stick slip and normal contact resonances on NaCl(001)



⇒ Maximum normal contact resonance is observed for $F_L=0$

Conclusions

- Observation of atomic-scale stick slip with single molecular and single atomic resolution
- Observation of multiple slips: A tool to estimate damping coefficients
- Simultaneous determination of normal and Lateral contact stiffness by contact resonance frequency measurements

