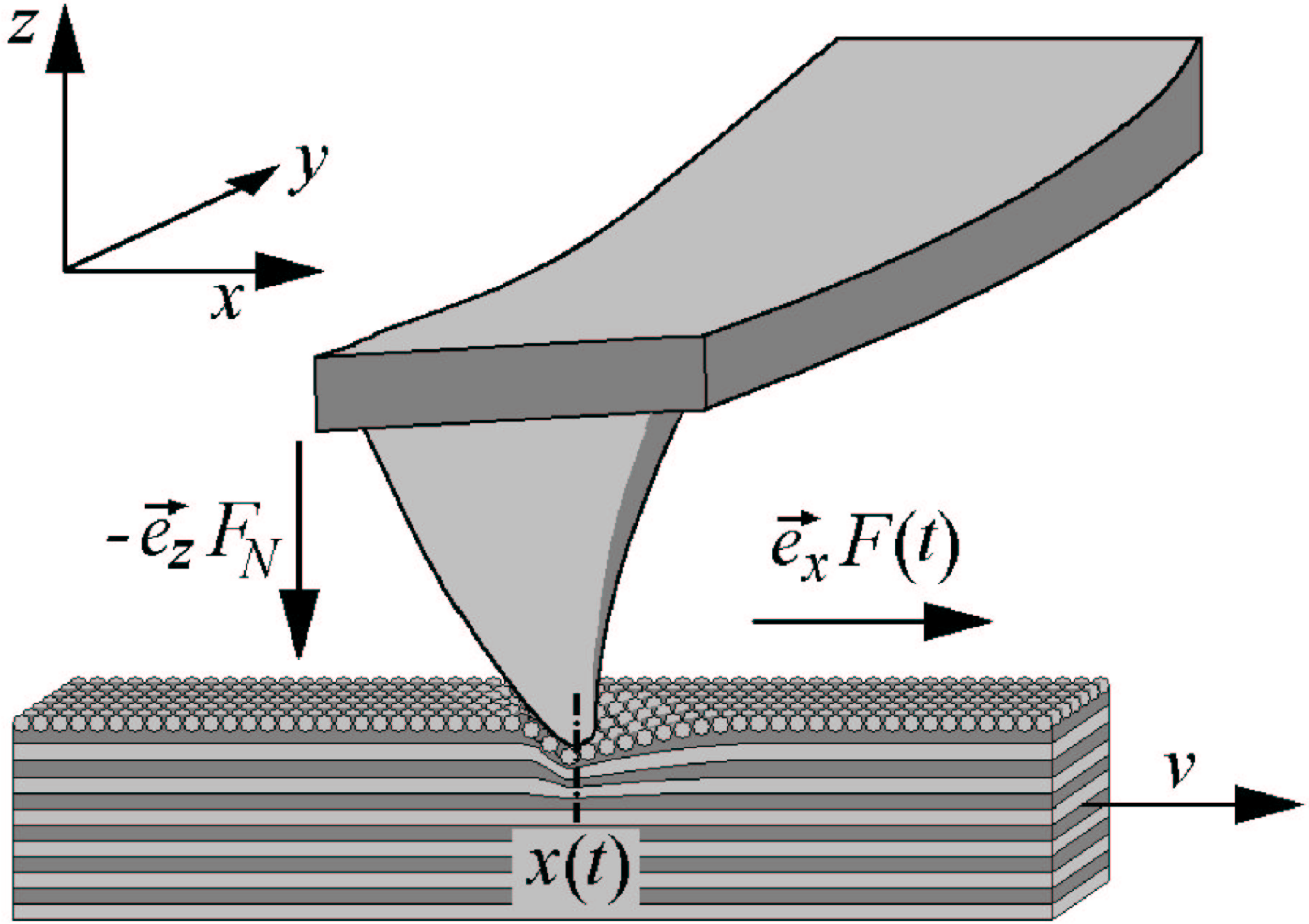
Velocity Dependence of Atomic Friction Beyond the Thermally Activated Hopping Regime

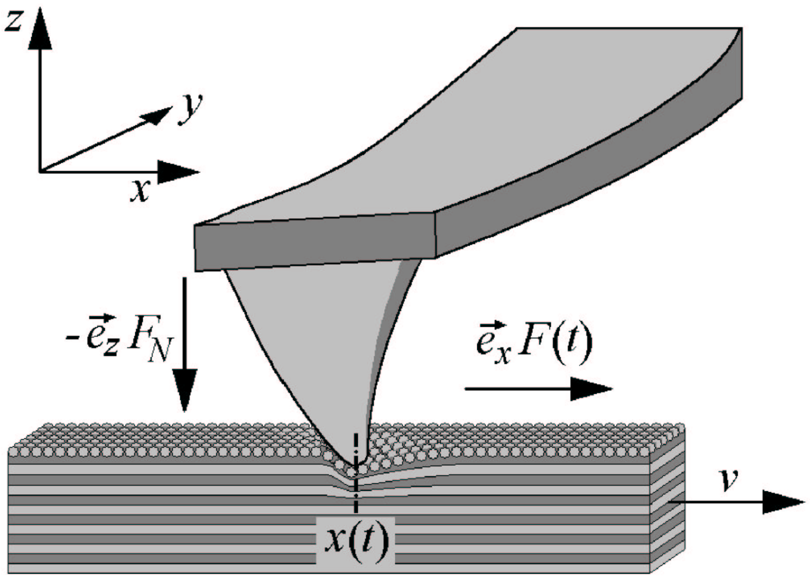
Peter Reimann, Mykhaylo Evstigneev (Theory)
André Schirmeisen, Lars Jansen, Harald Fuchs (Experiment)

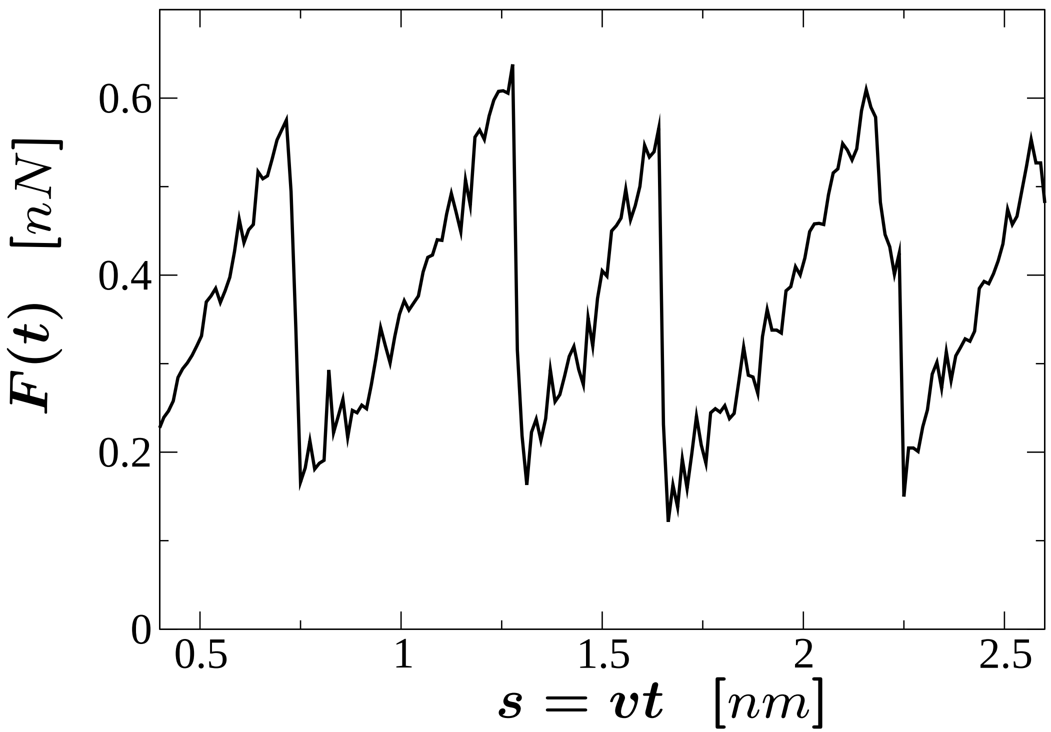
- **Experimental set-up and observations**
- **Simplified theoretical model**
- **Non-monotonic velocity dependence of atomic friction**
- **Slip statistics and rate theory**



- cantilever dimensions $\approx 200\ \mu m \times 50\ \mu m \times 1\ \mu m$
- tip height and basis radius $\approx 5\ \mu m \times 1\ \mu m$
- tip apex radius ≈ 10 nm
- lattice constant $L \approx 0.5$ nm

Friction Force Microscopy





- stick-slip motion
- "atomic resolution" ($L \approx 0.5$ nm)
- thermal noise effects

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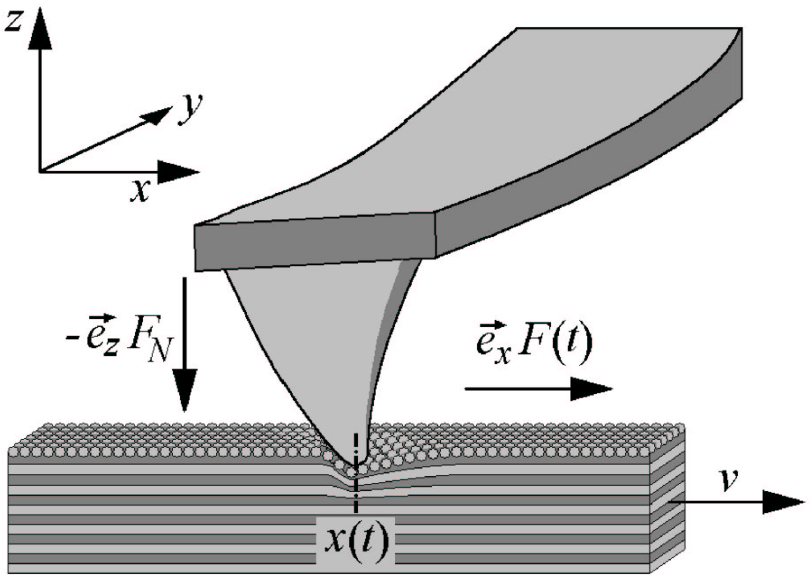

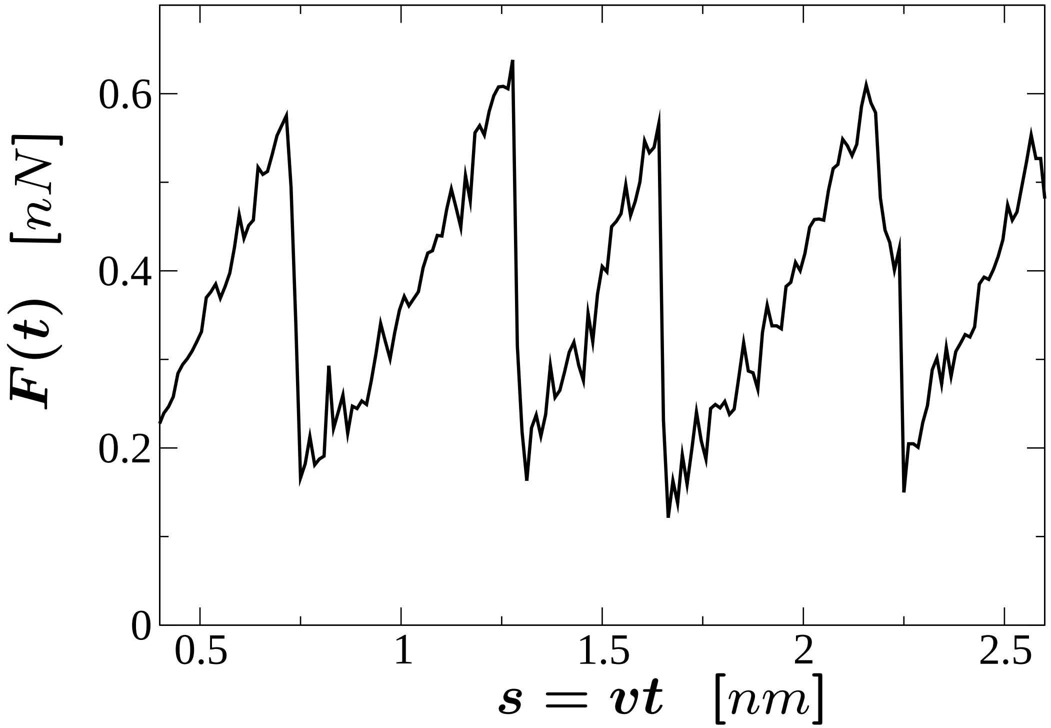

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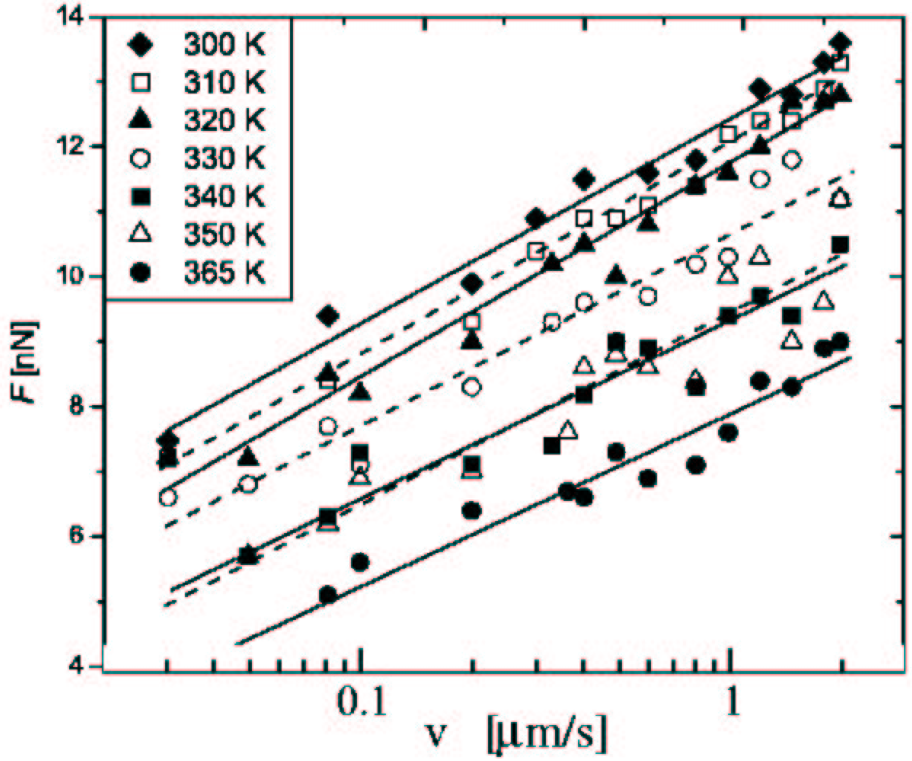
Quantity of main interest: $\bar{F} := \lim_{t\to\infty} \frac{1}{t} \int_0^t dt' \, F(t')$

$\bar{F}$ versus v



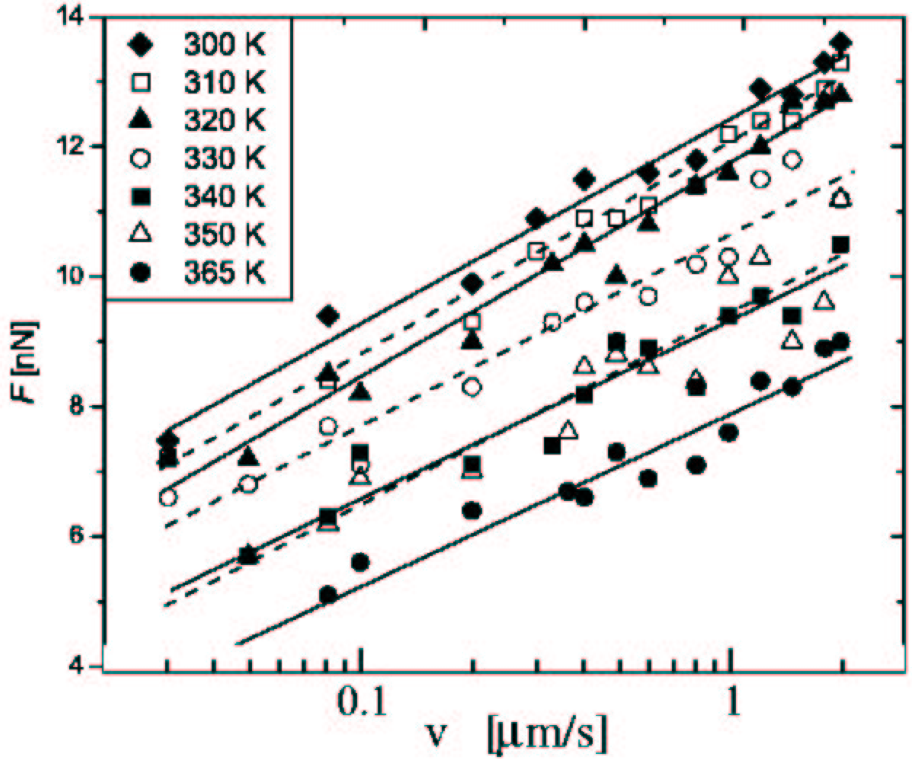
Sills and Overney, PRL 91, 095501 (2003)

glassy polysterene surface

$F_N = 15$ nN

- thermal noise matters

$\bar{F}$ versus v



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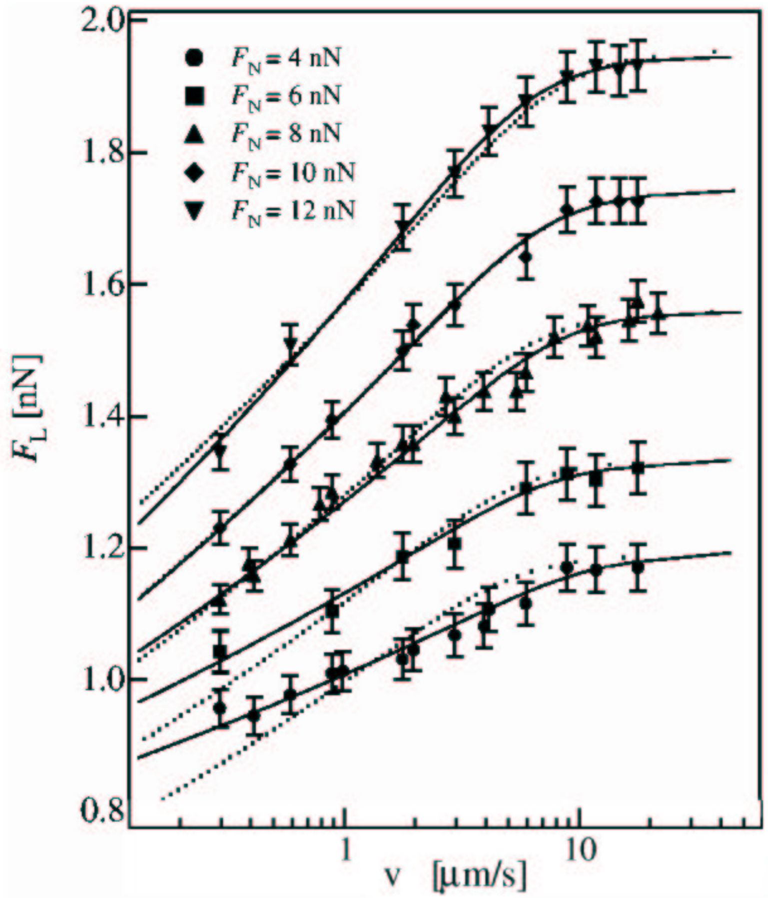


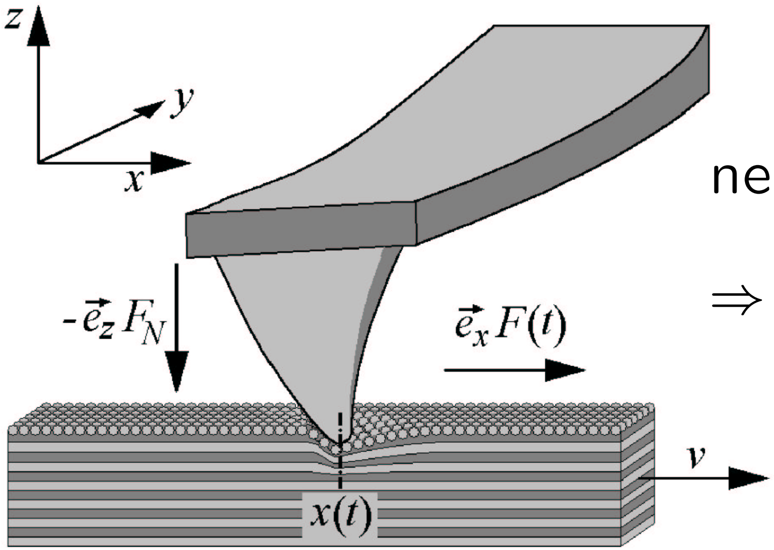
Riedo et al., PRL 91, 084502 (2003)

mica surface

$T = 293$ K

- "plateaux" at large v

Model



neglect "fast" thermal fluctuations of molecules

$\Rightarrow$ 2 "slow" state variables/collective coordinates:

x-coordinate of tip apex (rest position $x = 0$)

s : position of substrate along x-axis

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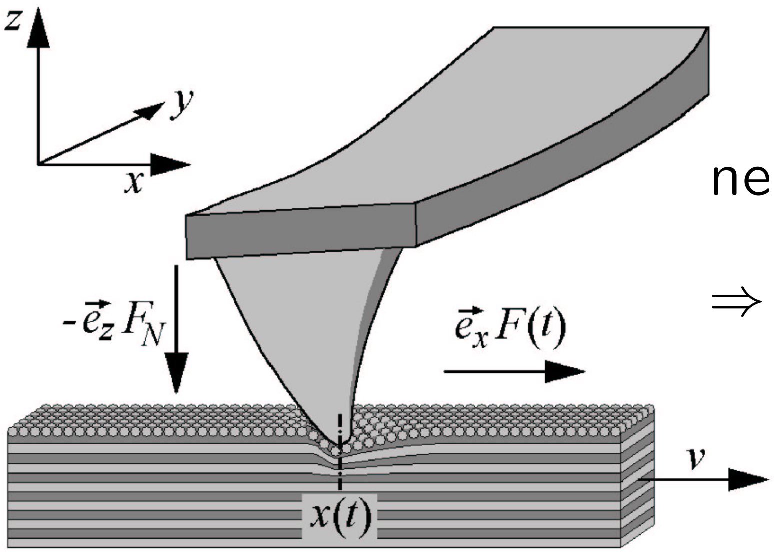

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- given x and s, the entire "global" configuration is uniqely fixed
- x, s "slow" $\Leftrightarrow$ "fast" molecular fluctuations always close to equilibrium
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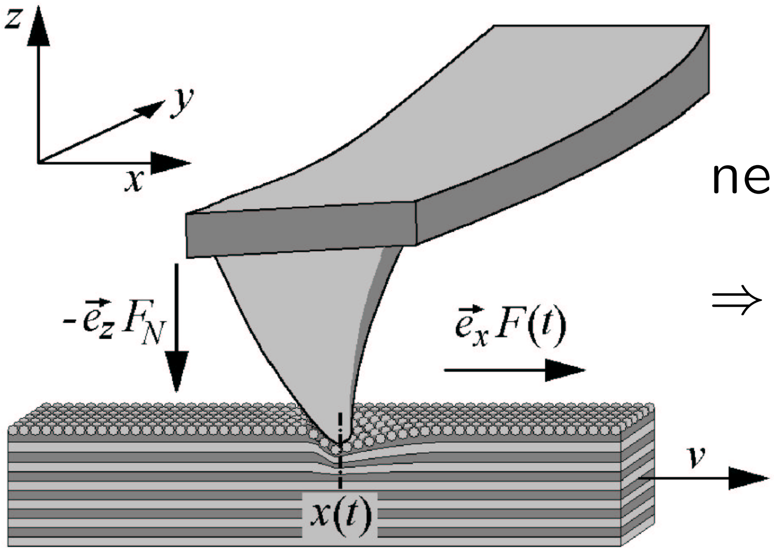

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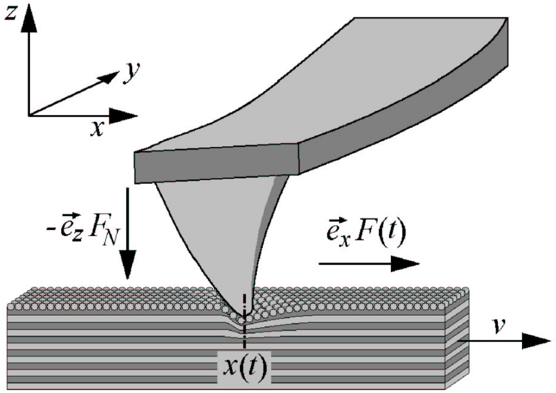
$\Rightarrow$ goal: equation of motion for $x(t)$



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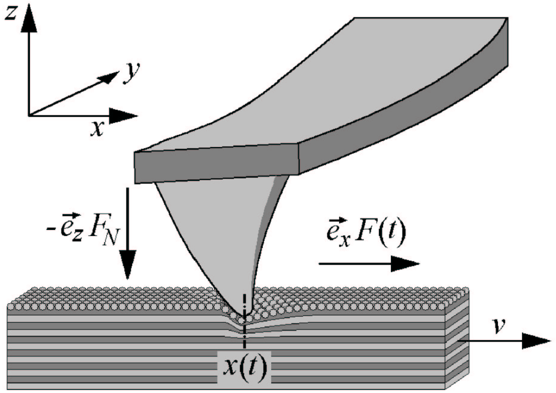
substrate potential $U(x-s)$ with $\boxed{U(x+L) = U(x)}$

elastic force $\boxed{-\kappa\, x(t) = -F(t)}$ [$\kappa \approx 1$ nN/nm]



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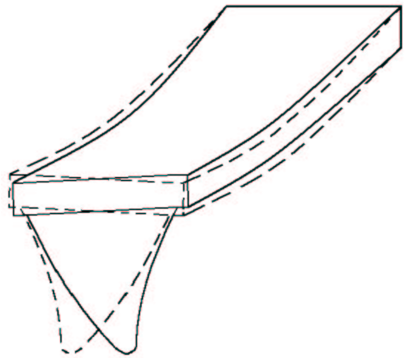

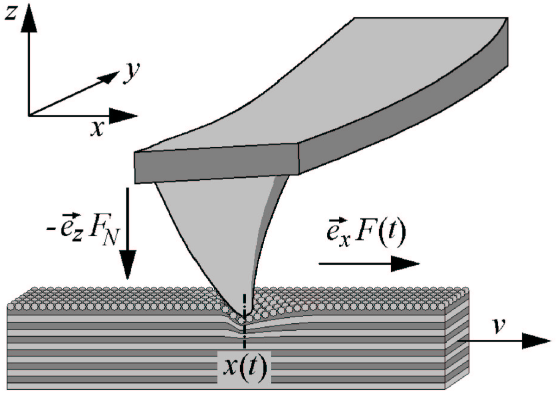

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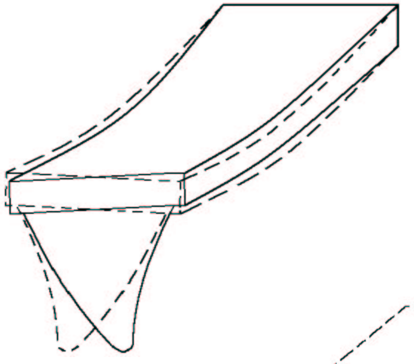

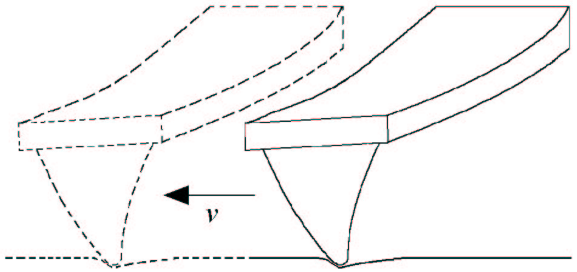

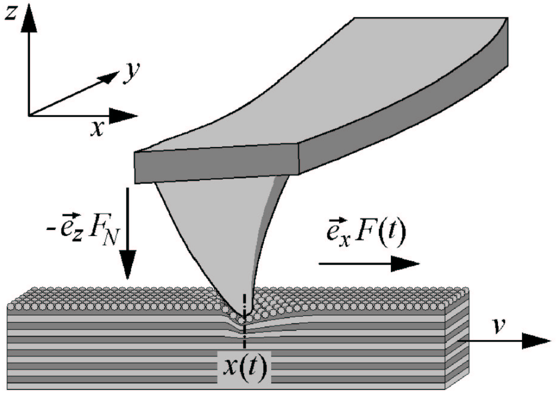

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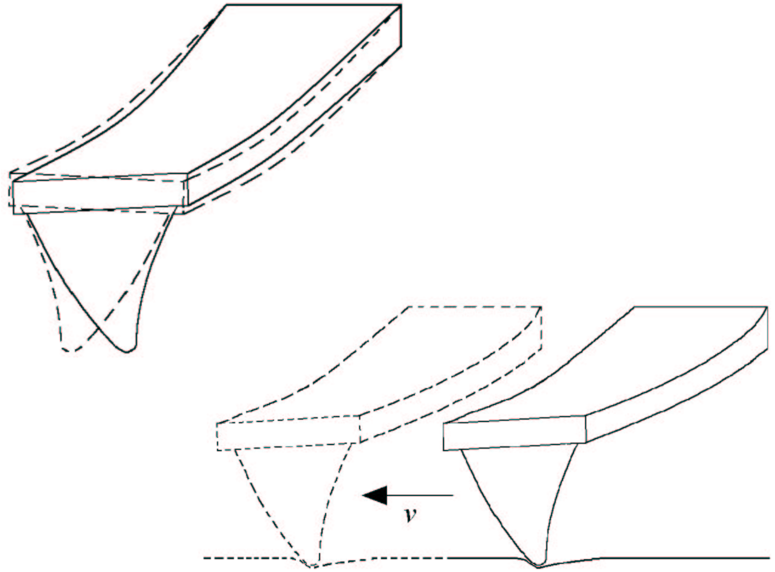
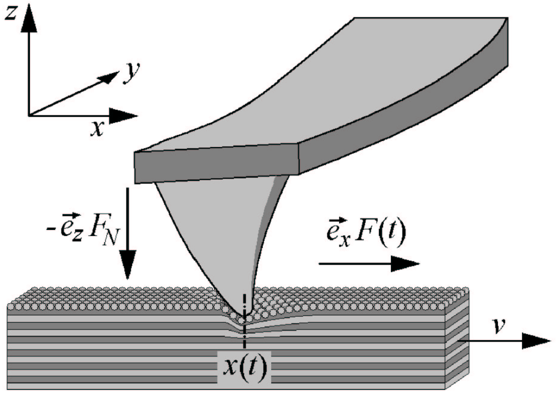


$$\boxed{m\ddot{x}(t) = -U'(x(t)-vt) - \kappa x(t) - \eta_c \dot{x}(t) + \sqrt{2\eta_c kT}\xi_c(t) - \eta_s(\dot{x}(t)-v) + \sqrt{2\eta_s kT}\xi_s(t)}$$



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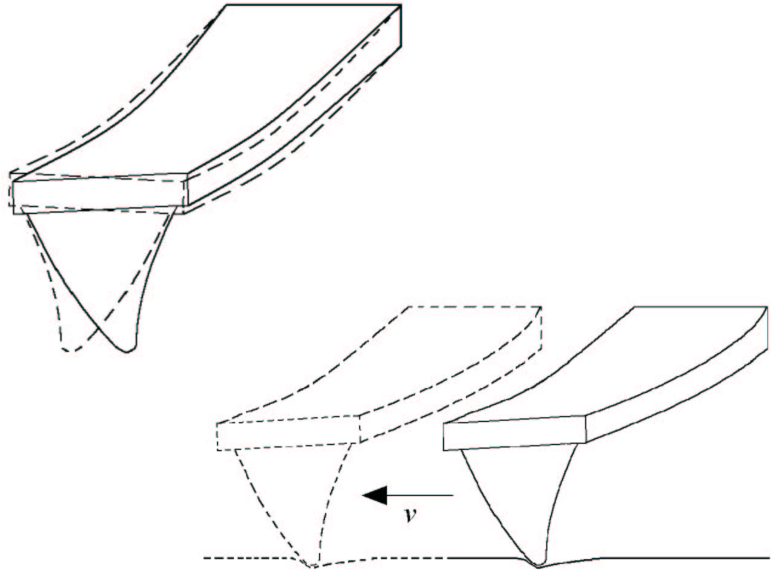

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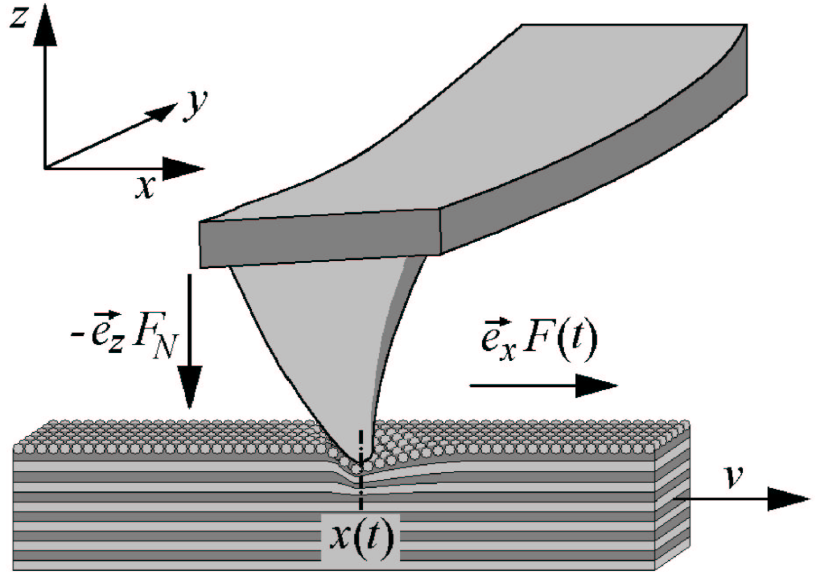
$$\boxed{\eta := \eta_c + \eta_s\ ,\quad \vartheta := \eta_c/\eta\ ,\quad X(t) := x(t) - v\,t\ ,\quad F(t) = \kappa\, x(t) = \kappa\,(X(t) + vt)}$$

$$\boxed{m\,\ddot{X}(t) = -U'(X(t)) - F(t) - \vartheta\eta v - \eta\dot{X}(t) + \sqrt{2\eta kT}\,\xi(t)}$$

Previous theories: bath effects of cantilever & tip ignored $\Leftrightarrow\ \vartheta = 0$



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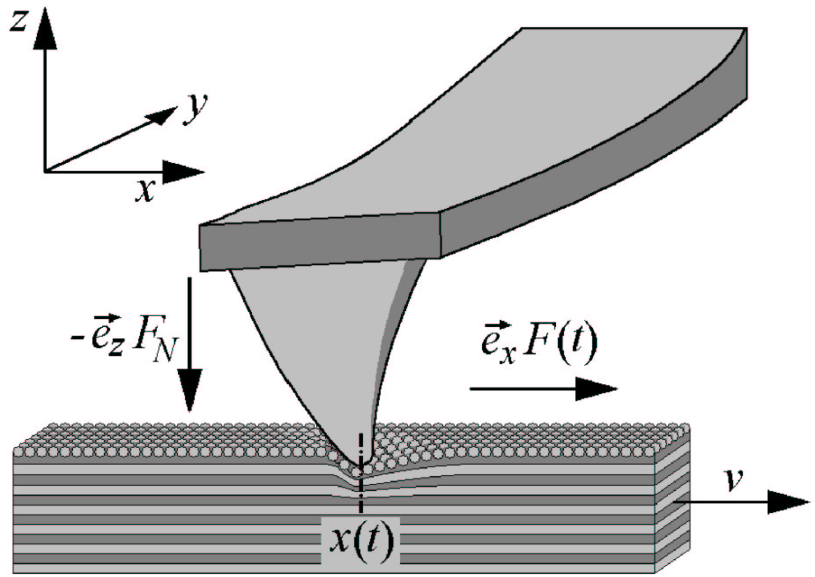
Elasticities: κ_c (cantilever), κ_t (tip-apex), κ_s (substrate)

κ (total): 3 springs in series: $\frac{1}{\kappa} = \frac{1}{\kappa_c} + \frac{1}{\kappa_t} + \frac{1}{\kappa_s}$

Typical values $\kappa_c \approx 75$ nN/nm, $\kappa \approx 1.2$ nN/nm

$\Rightarrow$ deformations mainly within small tip-substrate contact region



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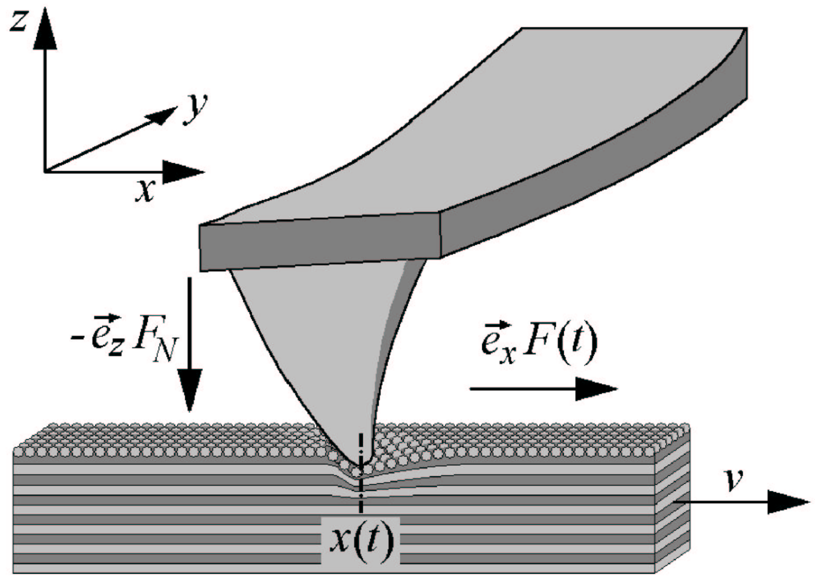

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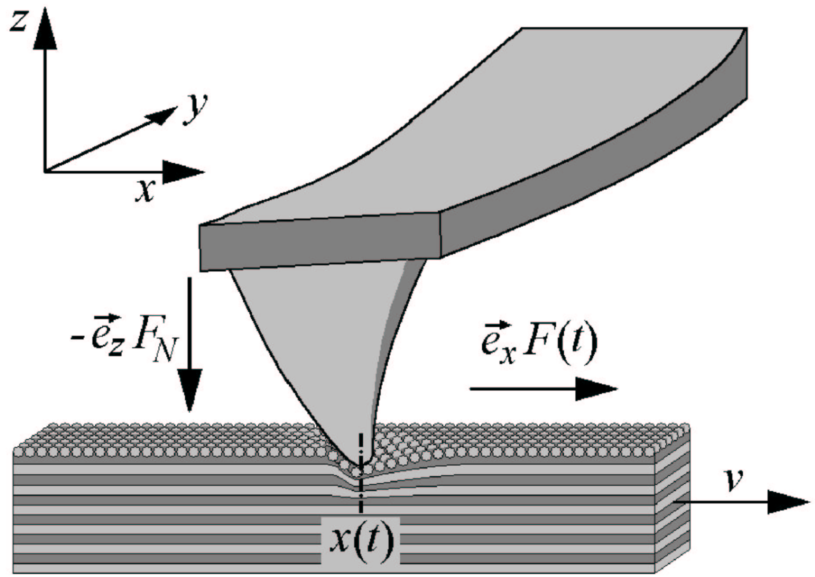
$\Rightarrow$ eff. mass $m \ll$ cantilever mass

$\Rightarrow$ dynamics overdamped ($m\ddot{X}(t) \simeq 0$)

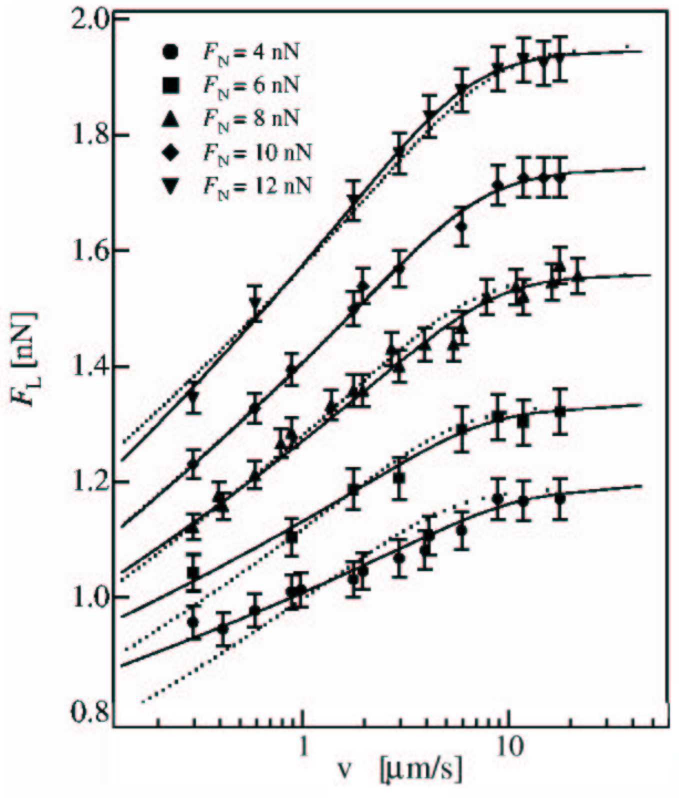


Previous theories: $m \approx$ cantilever mass $\Rightarrow$ dynamics underdamped

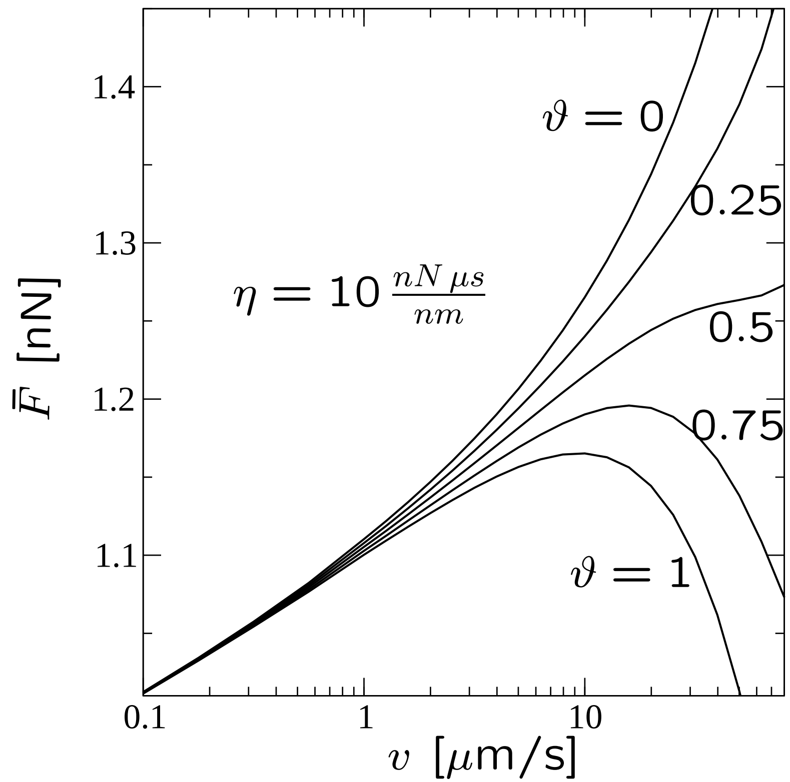
$$\eta \dot{X}(t) = -U'(X(t)) - F(t) - \vartheta \eta v + \sqrt{2\eta kT}\,\xi(t)$$

$$F(t) = \kappa\,[X(t) + v\,t]\ , \quad \bar{F} := \lim_{t\to\infty} \tfrac{1}{t}\int_0^t dt'\,F(t')$$

- $\eta \mapsto \alpha\eta \Leftrightarrow$ shifting $\bar{F}(v)$ curve along log(v)-axis by -log(α)
- $\bar{F}(v,\vartheta) = \bar{F}(v,\vartheta=0) - \vartheta\eta v$



mica surface, Riedo et al., PRL 91, 084502 (2003)



Numerics for $U(x) = A\sin(2\pi x/L)$, $A = 0.5$ nN nm

common parameters: $L = 0.52$ nm, $\kappa = 1.2$ nN/nm, $T = 293$ K

- Experiment implies $\vartheta > 0.5$

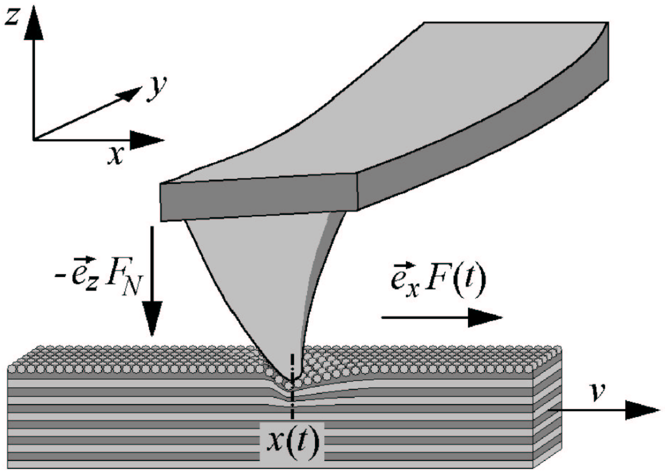
$\Leftrightarrow$ friction and noise due to tip apex exceed those due to substrate

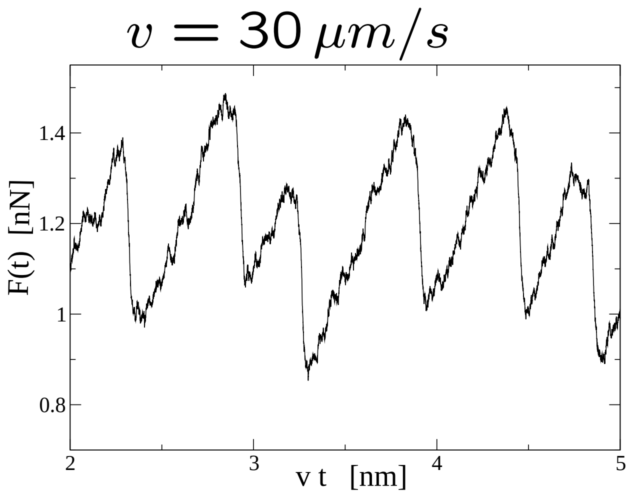
- first theoretical explanation of “plateaux” in $\bar{F}(v)$

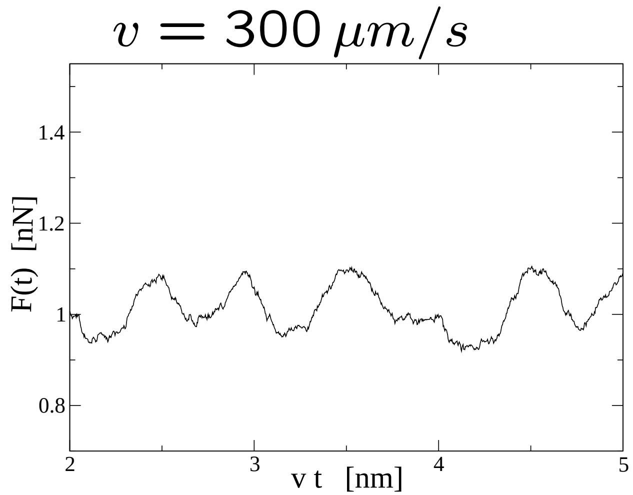
- Prediction of decreasing $\bar{F}(v)$ upon further increasing v

- For perfect fit $U(x) = A\,\mathsf{sin}(2\pi x/L)$ too simple

Physical Mechanism







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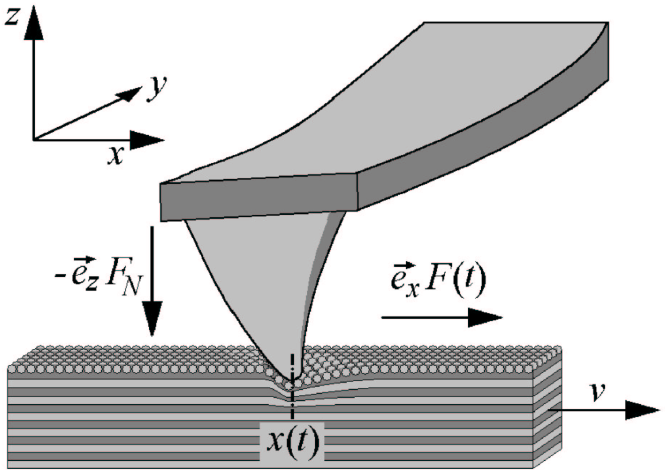
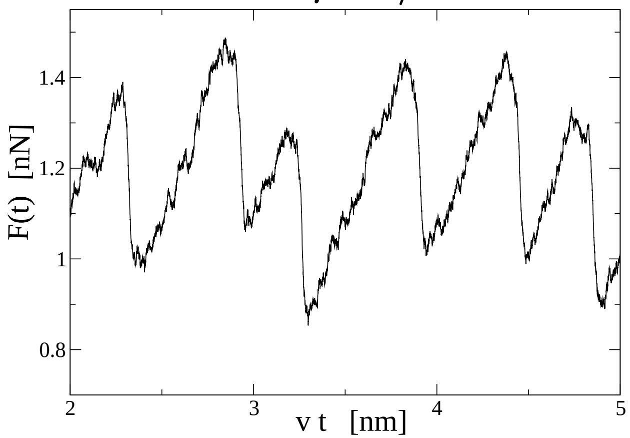


$v = 30\,\mu m/s$



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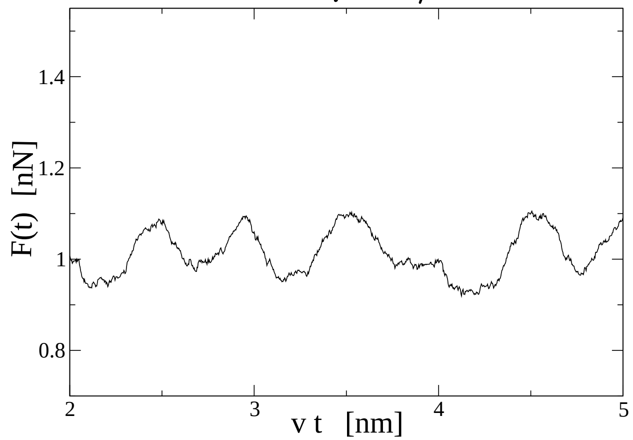

- stick-slip amplitude $\hat{=}$ dissipation
  $\Rightarrow \bar{F}(v)$ decreasing

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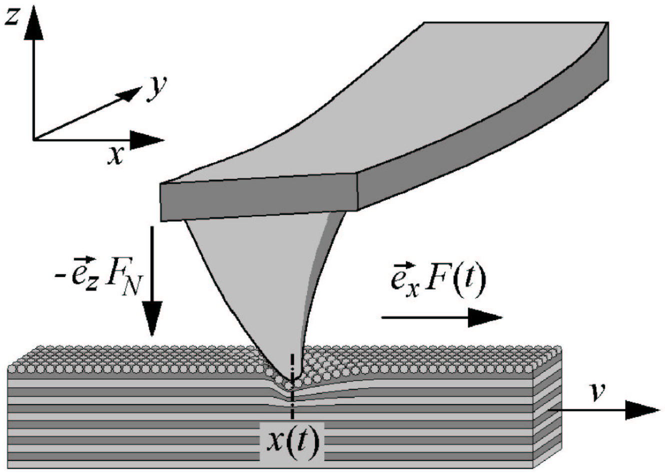

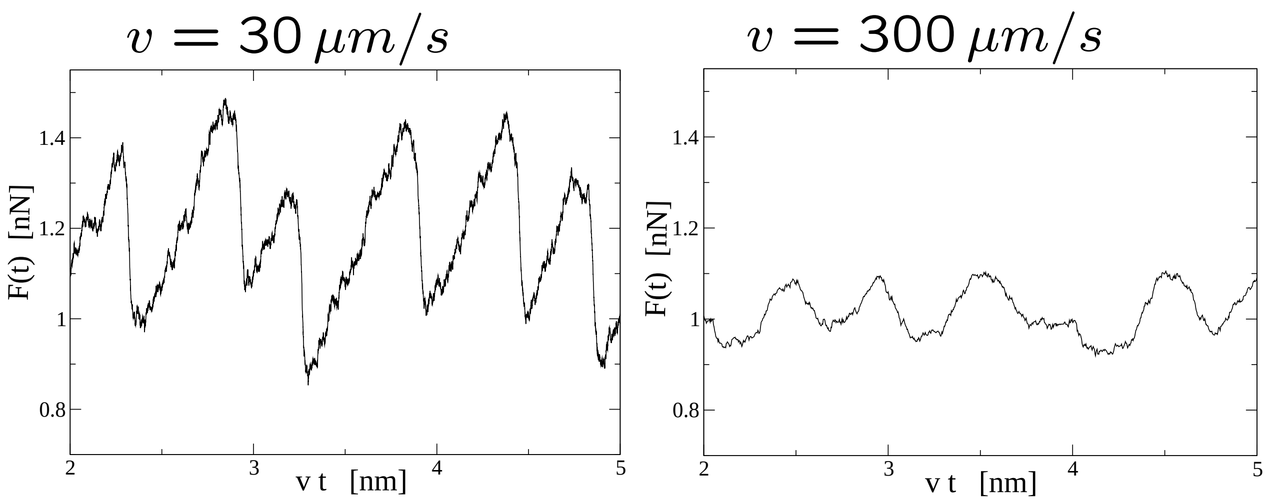

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- slips: thermally activated transitions

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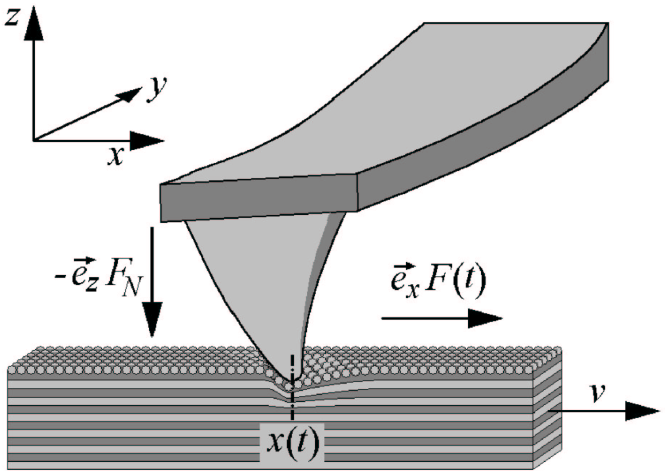

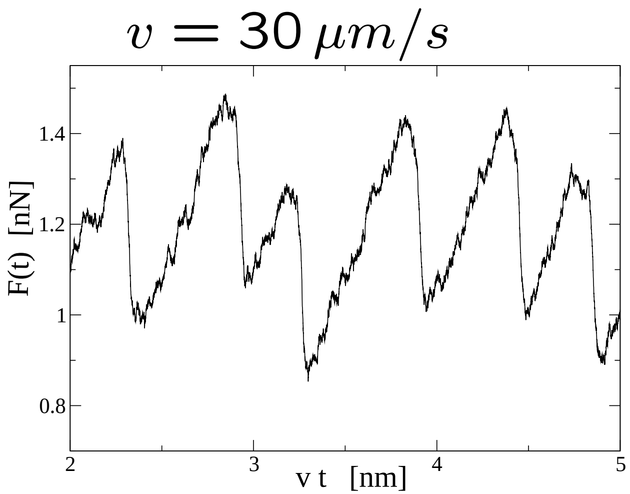

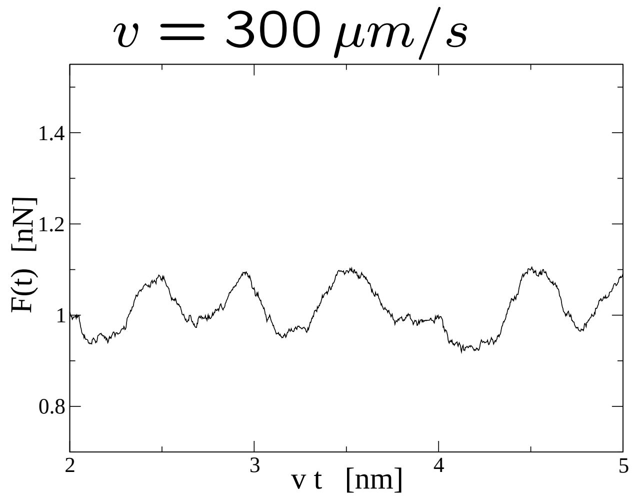

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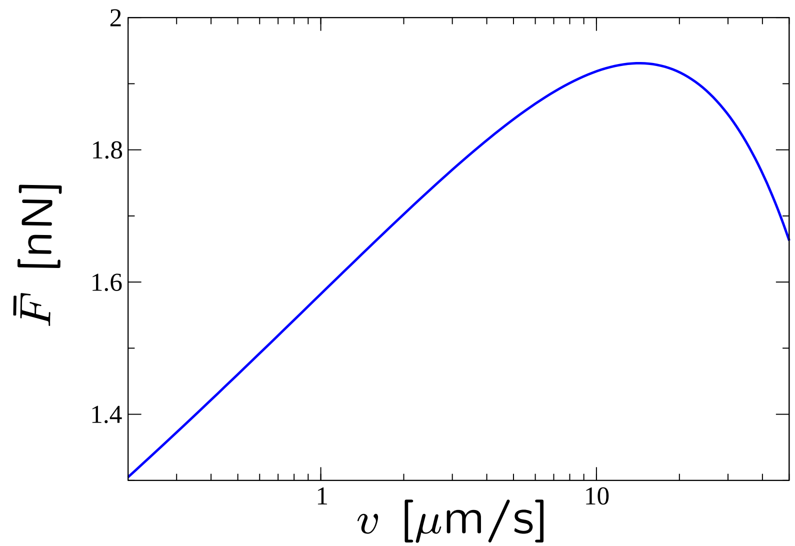
together **$\bar{F}(v)$ non-monotonic**



[Reimann & Evstigneev, New J. Phys. **7**, 25 (2005)]

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Approximation $F(t) \approx \bar{F}$ (exact for $\kappa \to 0$ or $v \to \infty$)

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Stratonovich 1957: General parametric solution (parameter f; $\langle \dot{X} \rangle = -v$):

$$v(f) \simeq \frac{L\, k\, T\, [1 - e^{-Lf/kT}]}{\eta \int_0^L dx \int_x^{x+L} dy \;\; e^{[U(x)-U(y)+(x-y)f]/kT}} \quad , \qquad \bar{F}(f) \simeq f - \eta v(f)$$

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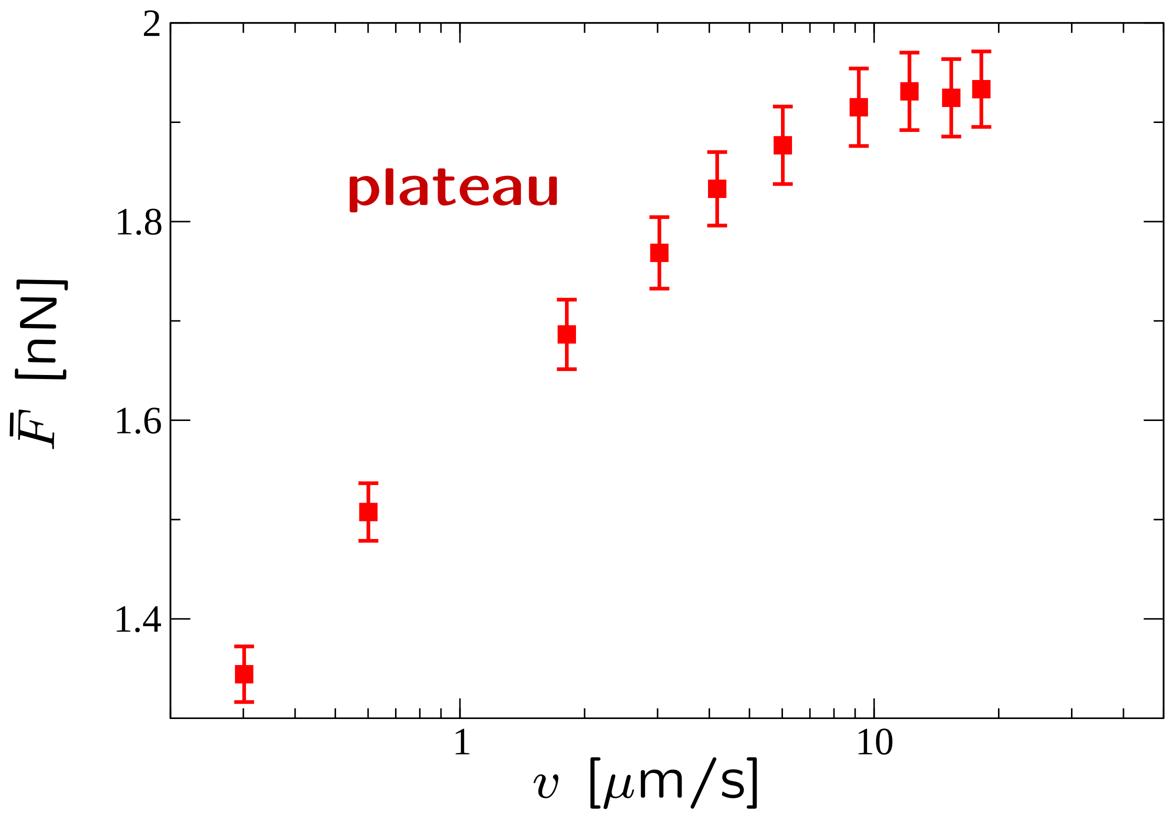

Data for $F_N = 12\,$nN from Riedo et al., PRL 91, 084502 (2003)

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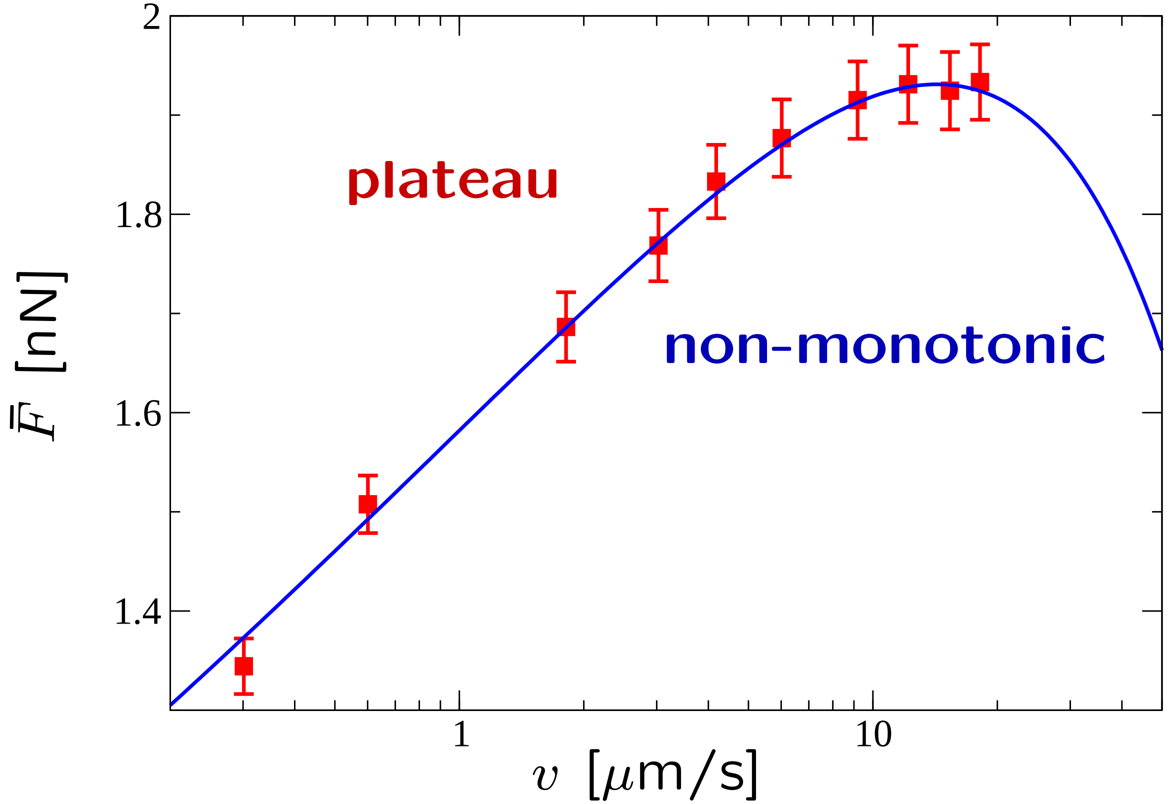
$$v(f) \simeq \frac{L\,k\,T\,[1-e^{-Lf/kT}]}{\eta \int_0^L dx \int_x^{x+L} dy\;\; e^{[U(x)-U(y)+(x-y)f]/kT}} \quad , \qquad \bar{F}(f) \simeq f - \eta v(f)$$



$\vartheta = 1$, $\eta = 20$ nN μs/nm, $L = 0.52$ nm, $\kappa = 1.2$ nN/nm, $T = 293$ K

$$\eta \dot{X}(t) = -U'(X(t)) - F(t) - \vartheta\eta v + \sqrt{2\eta kT}\,\xi(t)$$

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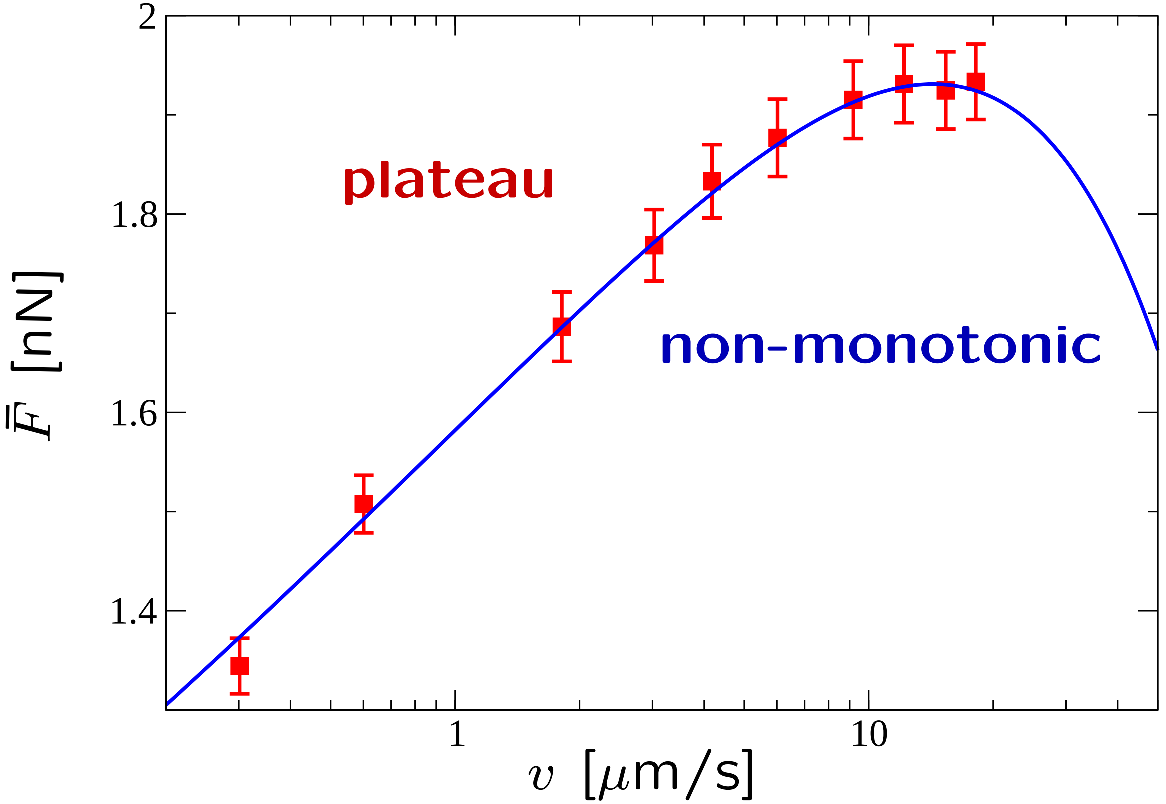

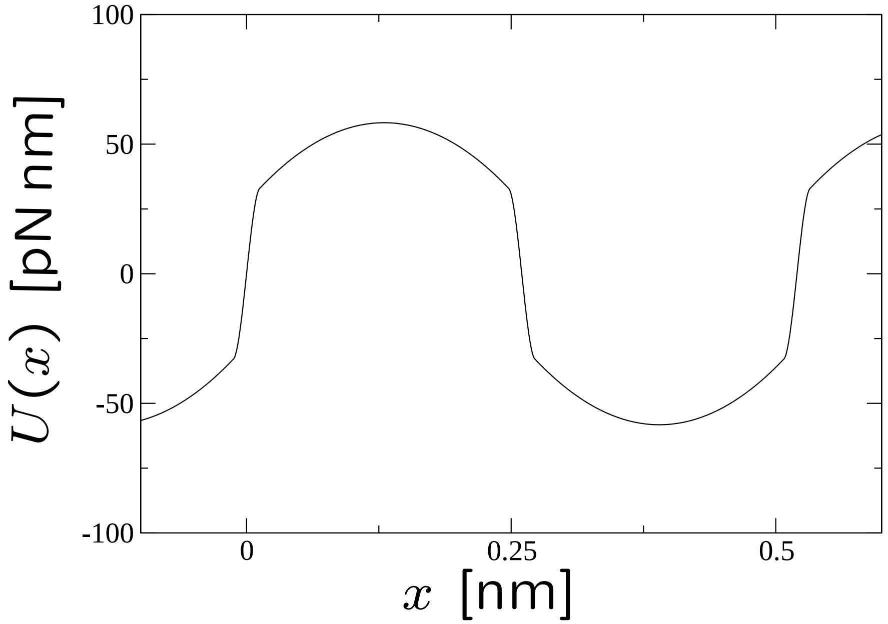

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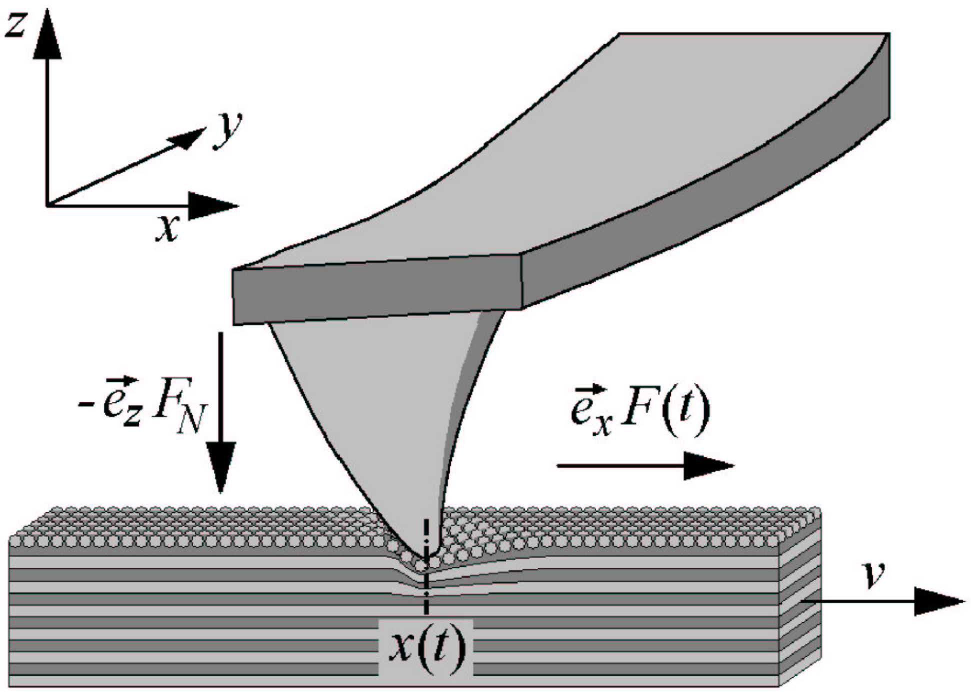
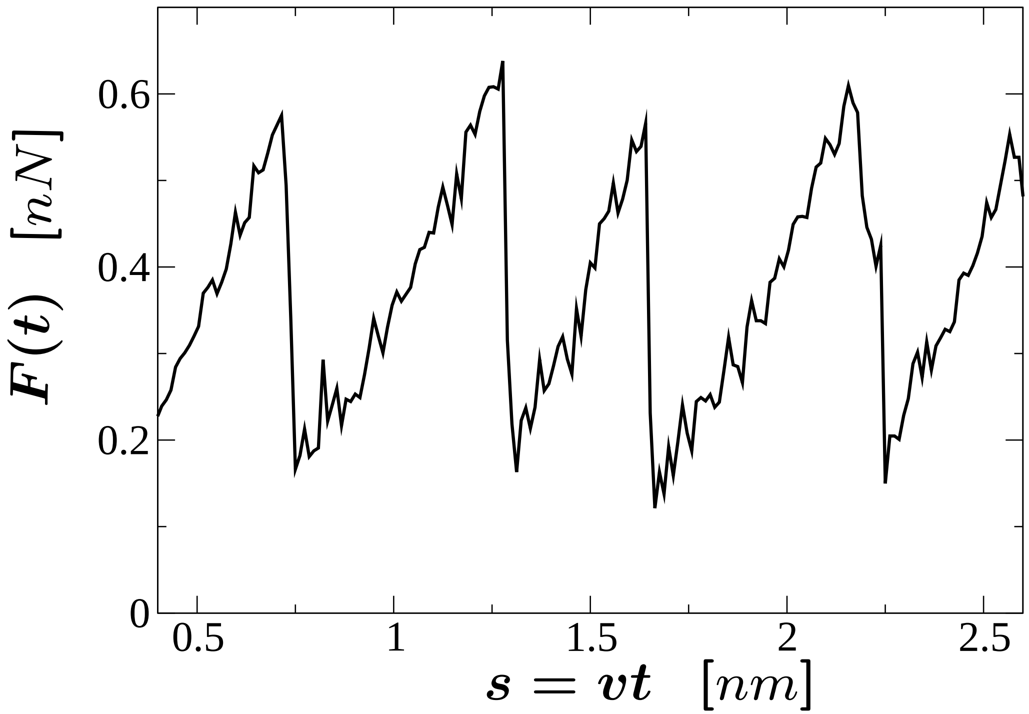
Slip-statistics and Rate Theory

[Evstigneev, Schirmeisen, Jansen, Fuchs, Reimann, PRL **97**, 240601 (2006)]





$$\dot{p}_v(F(t)) = -r(F(t))\, p_v(F(t))$$

$F(t)$ instantaneous force, $r(F)$ “slip-rate”, $p_v(F)$ “stick-probability”

Slip-statistics and Rate Theory

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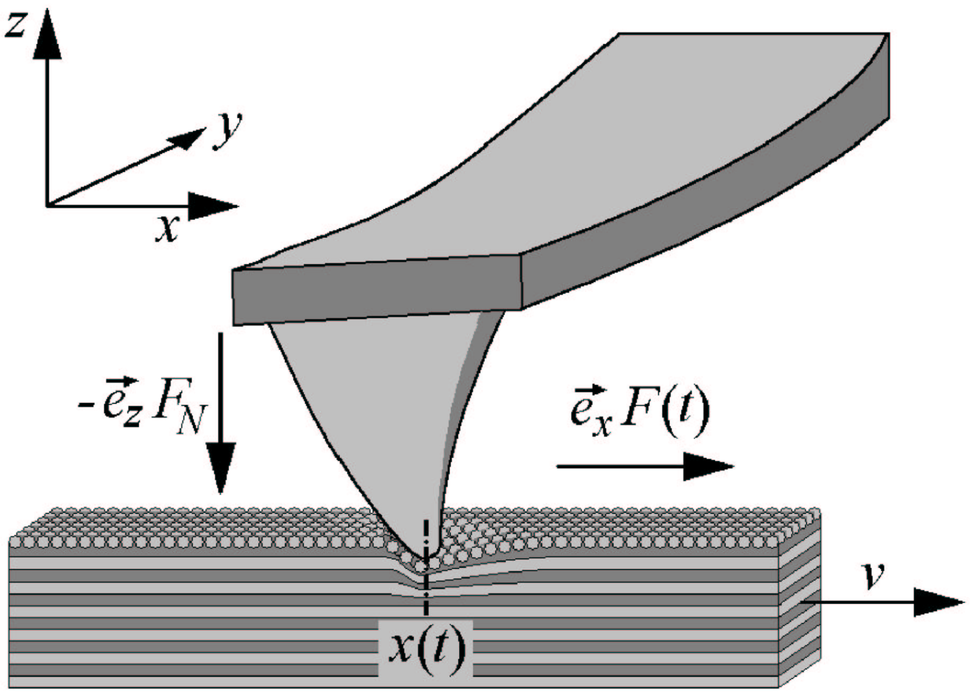

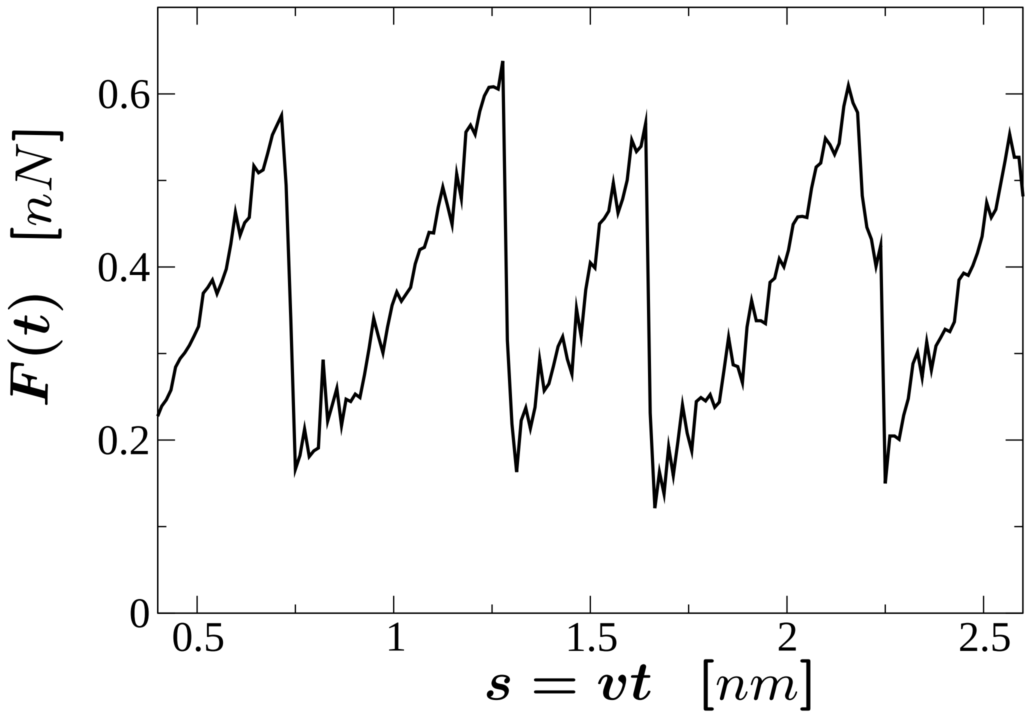

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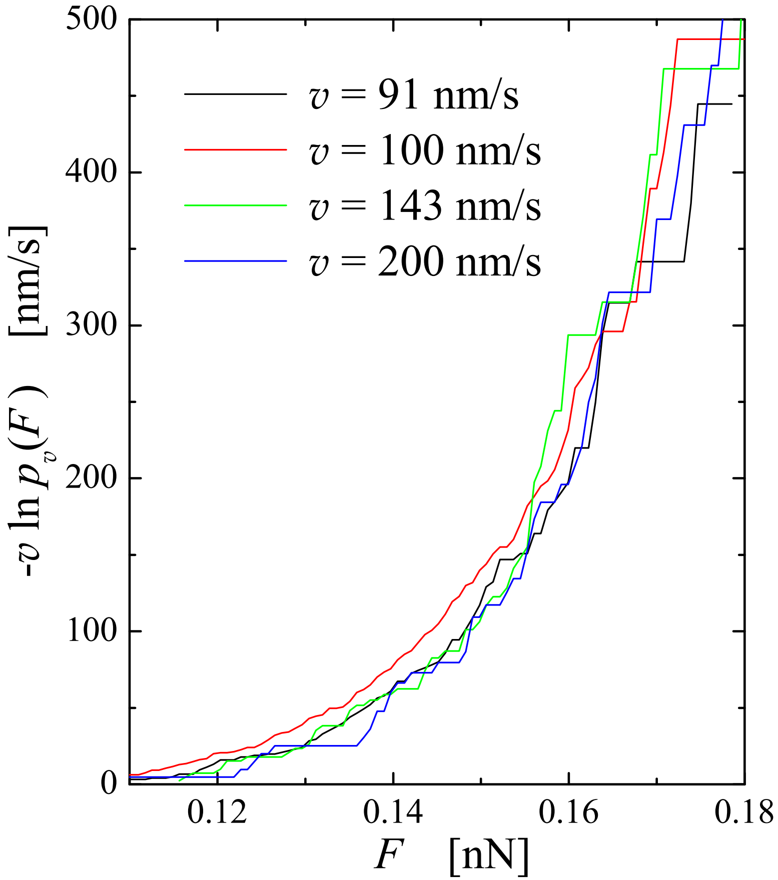

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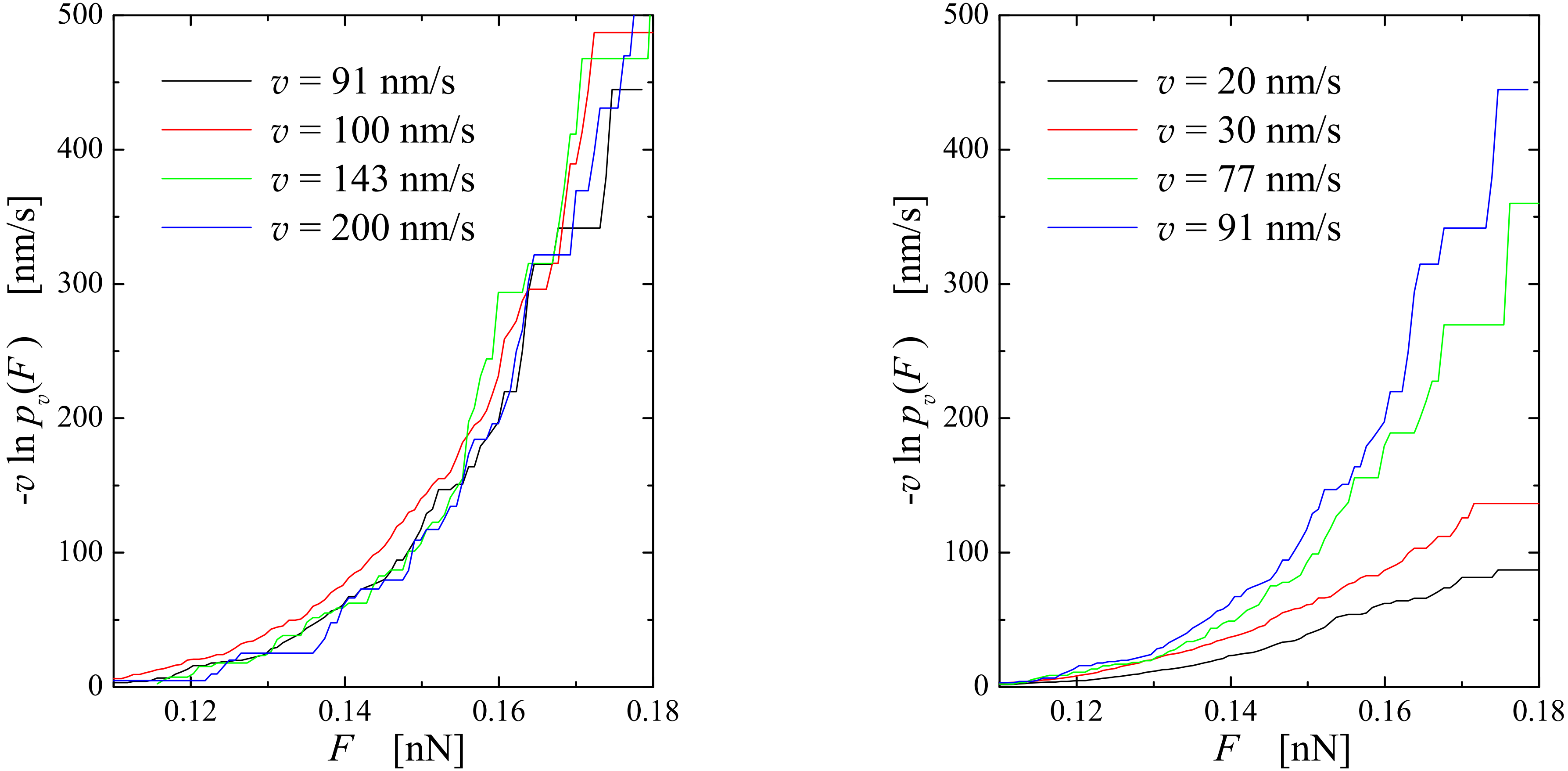

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Summary

- first theoretical explanation of “plateaux” in $\bar{F}(v)$
- prediction of non-monotonic $\bar{F}(v)$ upon further increasing v
- dynamics dominated by deformations of tip apex and contact region
- inertia effects are small (overdamped dynamics)
- damping and noise due to tip apex are crucial
- single-step rate description breaks down at **small** v