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**Instabilities and solid friction: from linear response to Coulomb friction**

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# **Instabilities and solid friction:** From viscous friction to Coulomb friction

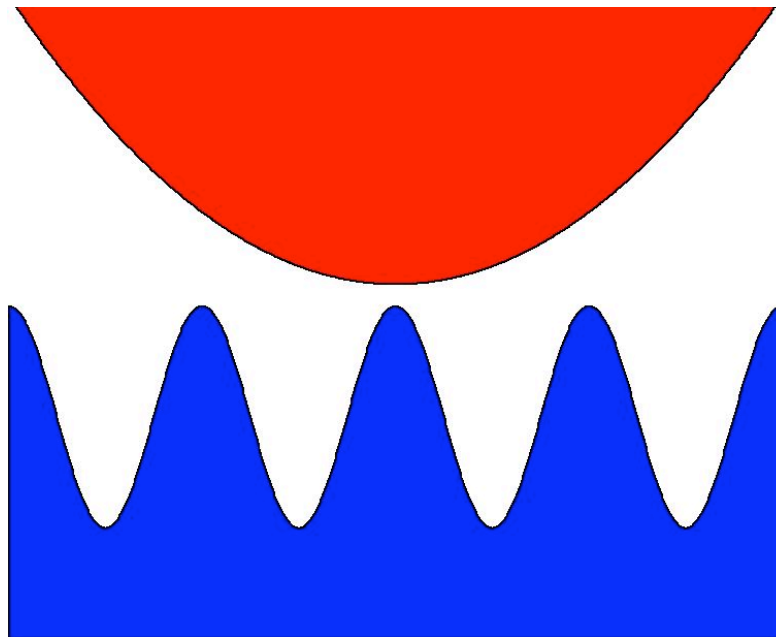
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# Background: Description of a simple tribo contact



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## simple tribo contact:

- no third bodies
- no plastic deformation

## strong interactions:

- within solids

## weak interactions:

- between substrate & slider

$x$  relative displacement of slider & substrate

any other *explicitly* kept variable

$u$  internal degrees of freedom (e.g. phonons)

# Background: Formal theory for simple tribo contact



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expand:  $V(x,u)$  around reference point  $x_{\text{ref}}$  and  $u_{\text{ref}} = 0$

$$V = V(x,0) + V_u(x_{\text{ref}},0) \cdot u + V_{xu}(x_{\text{ref}},0) \cdot (x-x_{\text{ref}}) \cdot u + \dots$$

$$\Rightarrow F = F(x,0) - V_{xu}(x_{\text{ref}},0) \cdot u(t)$$

deterministic force  
(explicit variables)

stochastic force:  $\Gamma(t)$   
(implicit/bath variables)

assume:  $x$  moves slowly compared to  $u$

phonons “equilibrate” at each value of  $x$

$\Rightarrow$   $\Gamma(t)$  satisfies fluctuation-dissipation theorem

# Background

## Eliminating “bath modes” in contacts



$$m\ddot{x}(t) = F(x) - m \int_{-\infty}^t dt' \gamma'(t-t') \dot{x}(t') + \Gamma(t) + F_{\text{ext}}(t)$$

$$\gamma'(\Delta t) = \frac{1}{2k_B T m} \langle \Gamma(t) \Gamma(t + \Delta t) \rangle_x$$

in our tribo system:  $\Gamma(t) = V_{xu}(x_{\text{ref}}, 0) \cdot u(t)$

$$\gamma'(x, \Delta t) = \sum_u \frac{|V_{xu}|^2}{2k_B T m} \langle u^*(\Delta t) u(0) \rangle_x$$

assuming time scale separation  $\rightarrow \approx \gamma(x) \cdot \delta(\Delta t)$

white noise  $\gamma(x) = \int d\Delta t \gamma'(x, \Delta t) \leftarrow$  inverse slip time  $\ll \omega_{\text{Debye}}$

see, e.g., Smith, Cieplak, Robbins, Phys. Rev. B **54**, 8252 (1996)

Friction on adsorbed monolayers,  $u$  = internal modes of layer

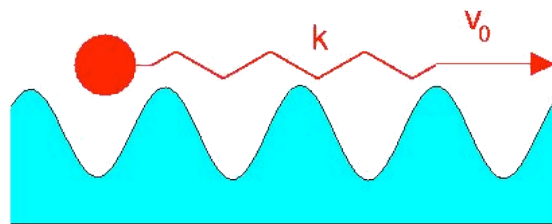
# Background

## Eliminating “bath modes” in contacts



$$m\ddot{x} = F - m\gamma(x)\dot{x} - F_{\text{ext}}(x, t) + \Gamma(x, t)$$

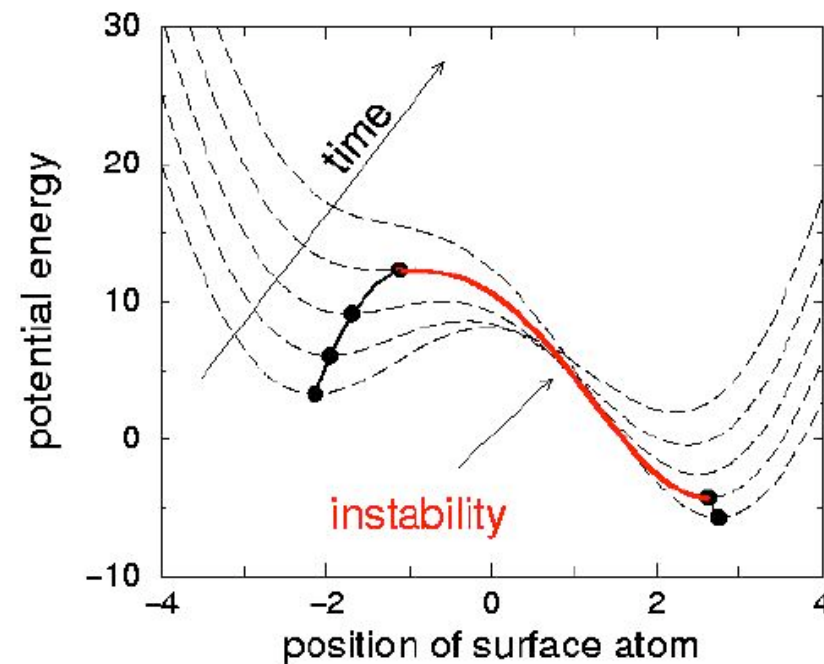
e.g.  $m\ddot{x} = V_0 \sin x - m\gamma\dot{x} - k \cdot (x - vt) + \Gamma(t)$



if  $V''$  exceeds  $k$   
 $\Rightarrow F_k$  is finite and relatively  
 independent of  $\gamma$

$$F_k = \Delta E / \Delta a$$

Prandtl-Tomlinson model



# Prandtl Tomlinson model

## Role of damping

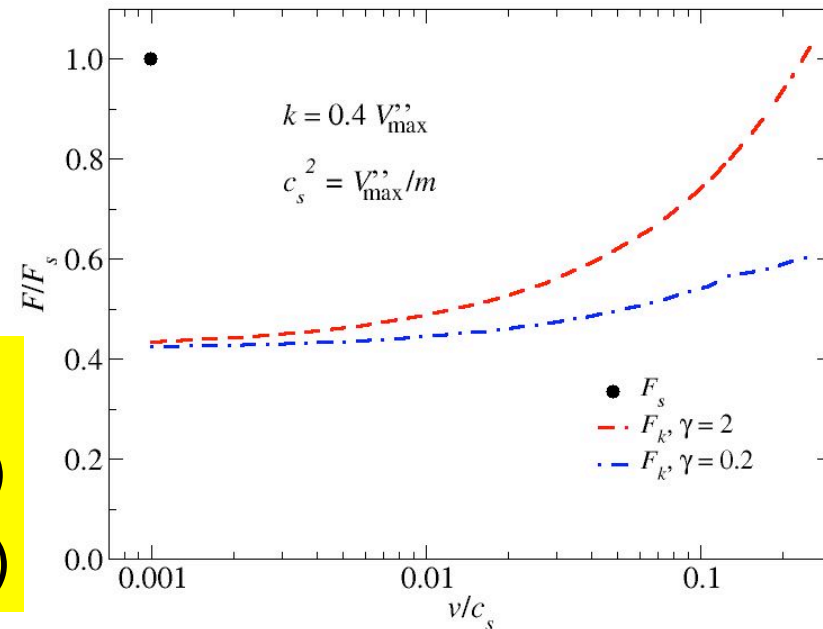


For *bi-stable* potentials:  
 $F_k$  barely depends on  $\gamma$   
(at “relevant” velocities  $v$ )

Prandtl (1928)

$\sim \text{const} + T \ln v$  ( $v$  large,  $T$  small)

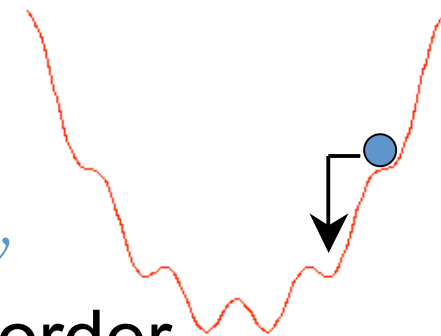
$\sim v \exp(E/k_B T)$  ( $v$  small,  $T$  large)



For *multi-stable* potentials:

$F_k$  can depend on  $\gamma$

- (always) discontinuous in both  $\gamma$  and  $v$
- (usually) non-monotonic in both  $\gamma$  and  $v$
- dependence reduced/eliminated by disorder





## What is the nature/magnitude of the **dissipation**?

- usually **irrelevant**  
**unless** significant heating, adsorbed layers,  
superlubric or other viscous systems

## What is the nature of the **instabilities**?

- dislocation motion / plastic deformation
- third bodies (boundary lubricants)
- chemical reactions including hybridization changes
- phase transformations
- elastic instabilities (incommensurations)



# Damping vs. instabilities (1)

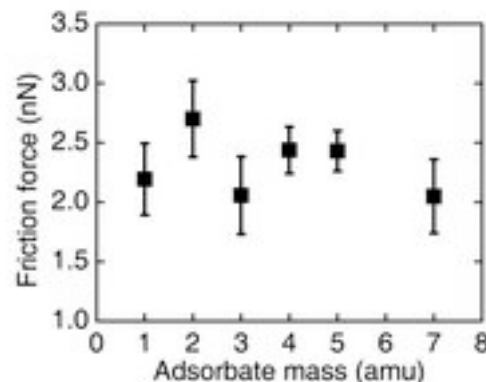


R. J. Cannara et al., Science **318**, 780 (2007):

We compared H- and D-terminated single-crystal diamond and silicon surfaces, and in all cases the hydrogenated surface exhibited higher friction. [ $\sim 30\%$ ]

What does linear response say about  $m$ -dependence of  $\gamma$ ?

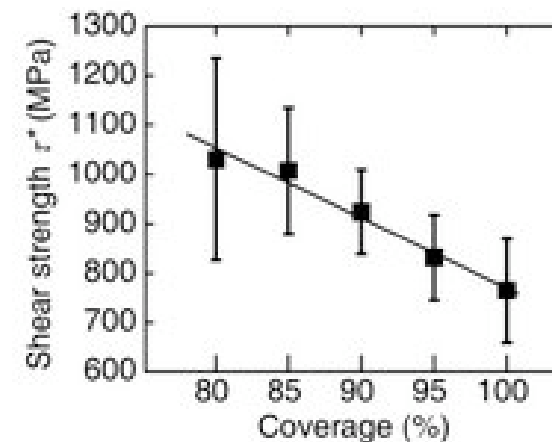
- attempt frequency  $\sim 1/\sqrt{m}$
  - momentum exchange  $\sim m$
- }  $\gamma \sim \sqrt{m}$  How can small damping lead to large friction?



if nothing but isotope mass is changed

Easier H desorption  
- small  $\Delta E$   
- large  $\nu$

Mo, Müser, Szulfarska,  
Phys Rev B (in press)



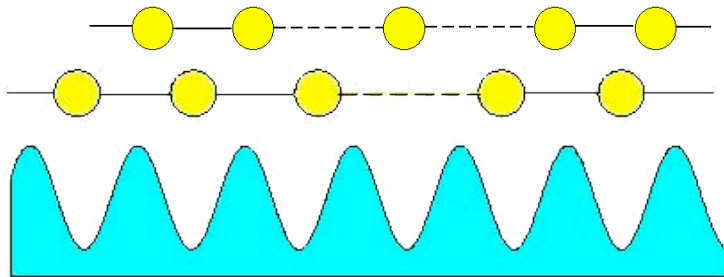
## Damping vs. instabilities (2)



T. Filleter et al., Phys. Rev. Lett. **102**, 086102 (2009):

The friction on SiC is greatly reduced by a single layer of graphene and reduced by another factor of 2 on bilayer graphene.

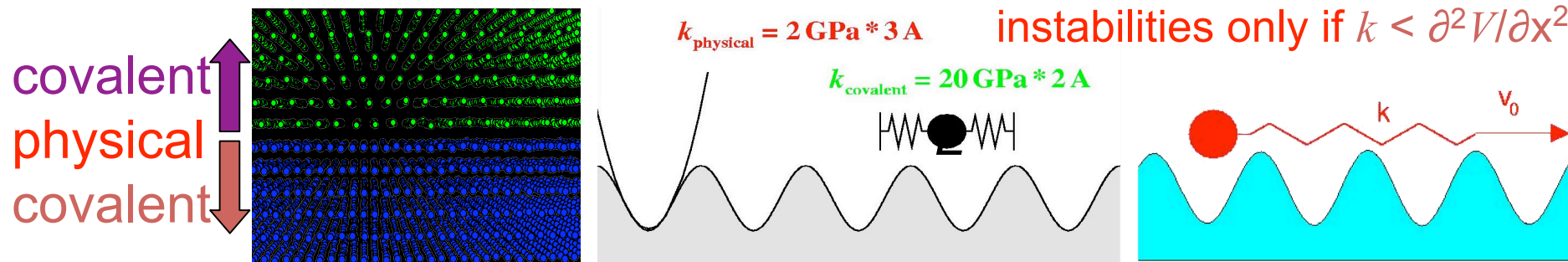
If slip / pinning occurs at the substrate,  
then single layer likely to be “deformed” &  
second layer changes energetics of instability



There is an effect of dimensionality  
of object on pinning (friction)

Müser, Europhys Lett **66**, 97 (2001)

# Elastic instabilities and dimensionality

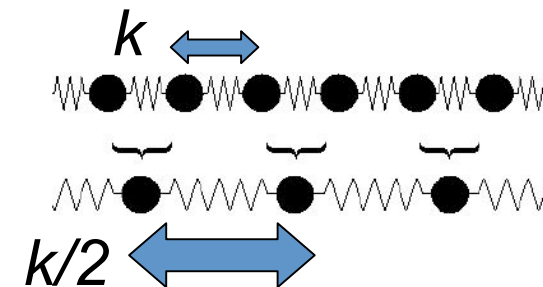


If on local scale:  $k_{\text{bulk}} > k_{\text{interf}}$  then on large scale:  $k'_{\text{bulk}} < k'_{\text{interf}}$  ?

Need to analyze how  $k$  changes with size:

1d linear chain

$$k_L = \frac{L_{\text{atomic}}}{L} k_{\text{atomic}}$$



2d elastic sheet:  $k_L = k_{\text{atomic}}$  (no resistance to bending)

3d solid:  $k_L = L^{1/2} k_{\text{atomic}}$

What is the nature/magnitude of the dissipation?

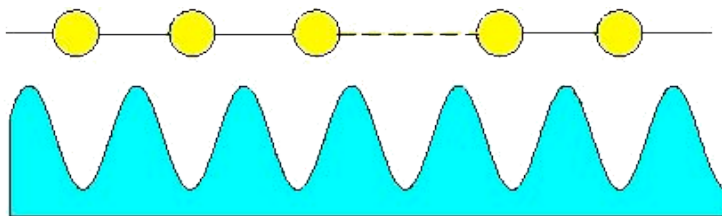
What is the nature of the **instabilities**?

- dislocation motion / plastic deformation of bulk
- third bodies
- chemical reactions including hybridization changes
- phase transformations

- **elastic instabilities**

Hammerberg et al., Physica D **123**, 330 (1998)

Frenkel Kontorova model captures early time behavior of friction process & low-dimensional systems (graphene?)



Müser, Tribol. Lett. **10**, 15 (2001)

**If interactions in atom-based models are tuned to produce elastic instabilities, irreversible processes such as cold-welding and wear occur.**

# Elastic wrinkle instabilities

## Examples



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# Elastic wrinkle instabilities

## Preliminary results (1)



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# Elastic wrinkle instabilities

## Preliminary results (2)



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Force  
0

$a$  ↑ ↑  
time/  
slid distance

# Elastic wrinkle instabilities

## Preliminary results (3)



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# Conclusions



In order to rationalize **kinetic** (solid/Coulomb) friction, we need to unravel the **instabilities** in the system.

not for yet for public exposure

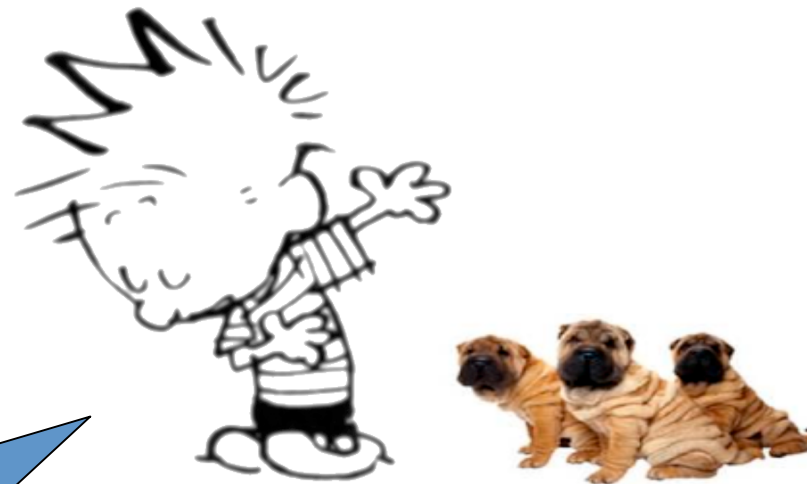
- friction of **graphite lamella**: stiffness-effect

**It's the thickness that matters**

- **isotope effect** in friction due to stability of D atoms?



**That's it.**



**Thanks for  
your attention!**