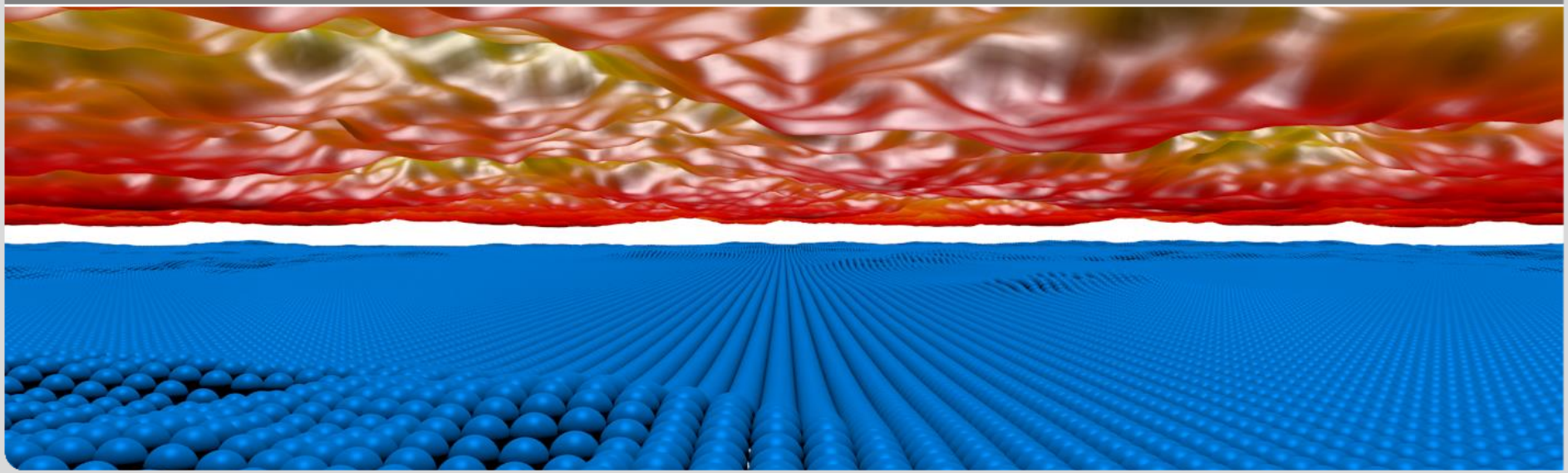
Karlsruhe Institute of Technology

IAM
Institute for Applied Materials

# Contact and cavitation: Computer models for tribological processes

**Lars Pastewka**
Karlsruhe Institute of Technology

**Warwick University**
Feb. 27, 2017



# Collaborators

**Bart Weber**

**Daniel Bonn**

**Tomislav Suhina**

**Fred Brouwer**

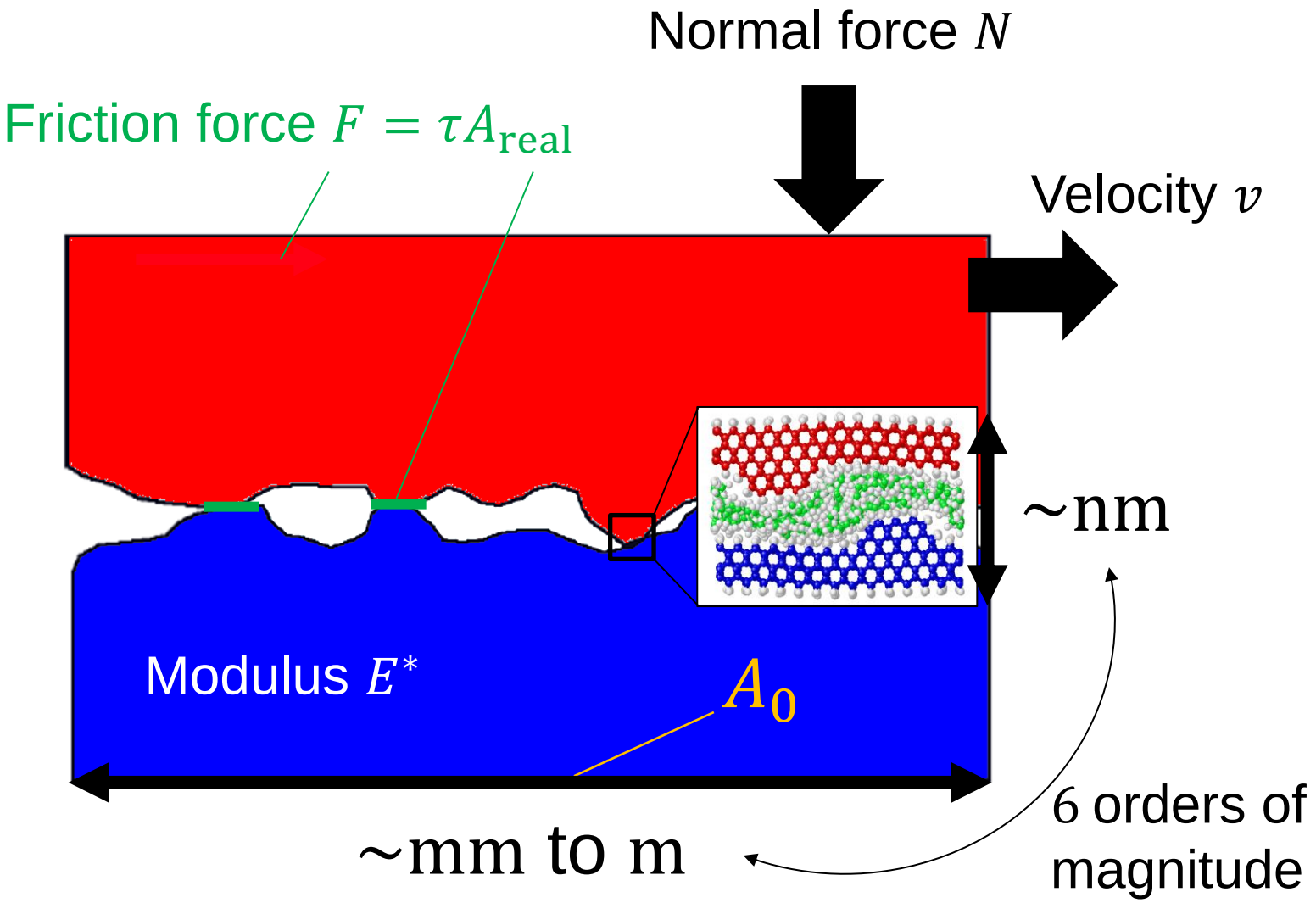
**Till Junge**
*(now at EPFL)*

**Daniele Savio**
*(now at Fraunhofer IWM)*

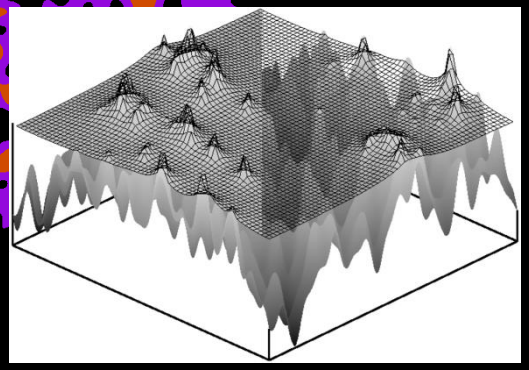
**Peter Gumbsch**

**Mark O. Robbins**

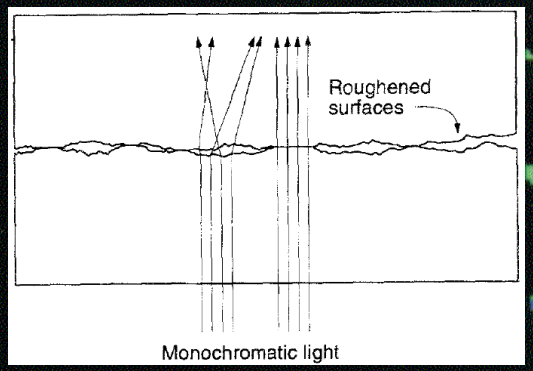
# Tribology


Normal force $N$
Friction force $F = \tau A_{\mathrm{real}}$
Velocity $v$
~nm
Modulus $E^*$
$A_0$
~mm to m
6 orders of magnitude

## Simulation



## Experiment




*Method:* Campana, Müser, *PRB* 74, 075420 (2006);
Pastewka, Sharp, Robbins, *PRB* 86, 075459 (2012)

Dieterich, Kilgore,
Pure and Applied Geophysics 143, 283 (1994)

# Computational methods


- Green‘s function for the elastic response

$$p(\vec{q}) = \frac{E^*}{2} q\, u(\vec{q}) \quad \Rightarrow \quad e = \frac{1}{2} \int \frac{d^2 q}{4\pi^2}\, p(\vec{q}) u(\vec{q})$$


Polonsky, Keer, *Wear* 231, 206 (1999)
Campaña, Müser, *Phys. Rev. B* 74, 075420 (2006)
Pastewka, Sharp, Robbins, *Phys. Rev. B* 86, 075459 (2012)

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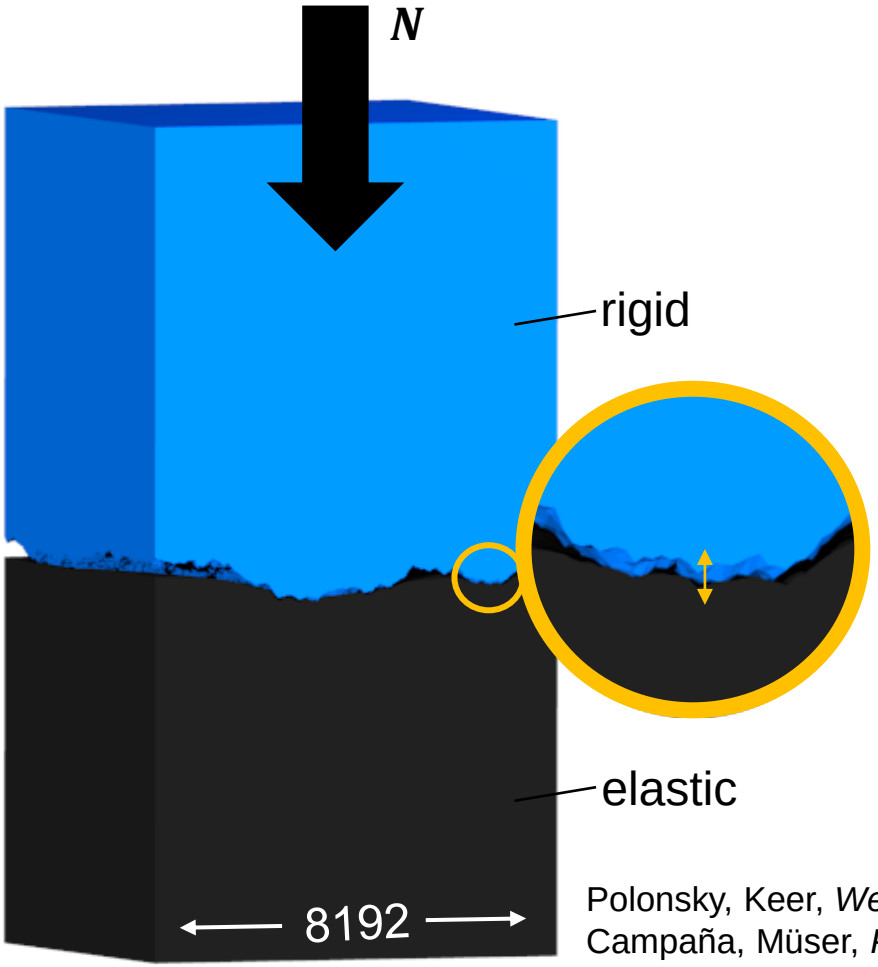
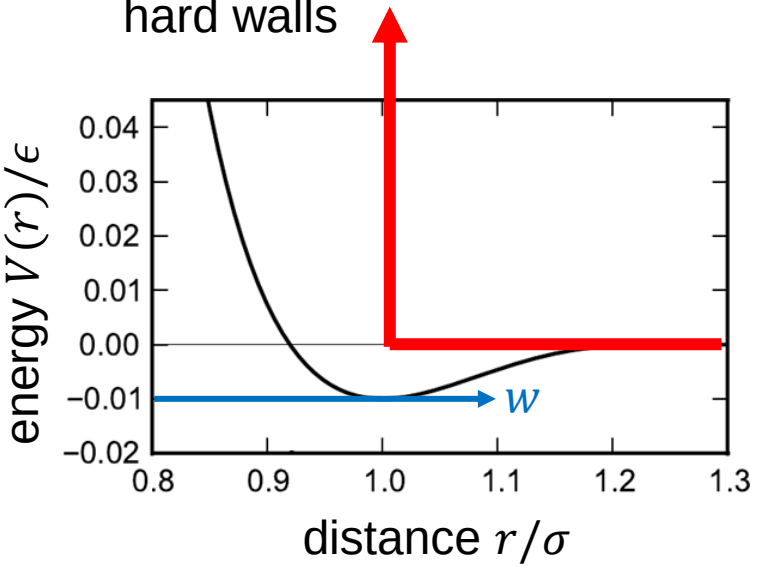
Pastewka, Sharp, Robbins, *Phys. Rev. B* 86, 075459 (2012)

# Computational methods



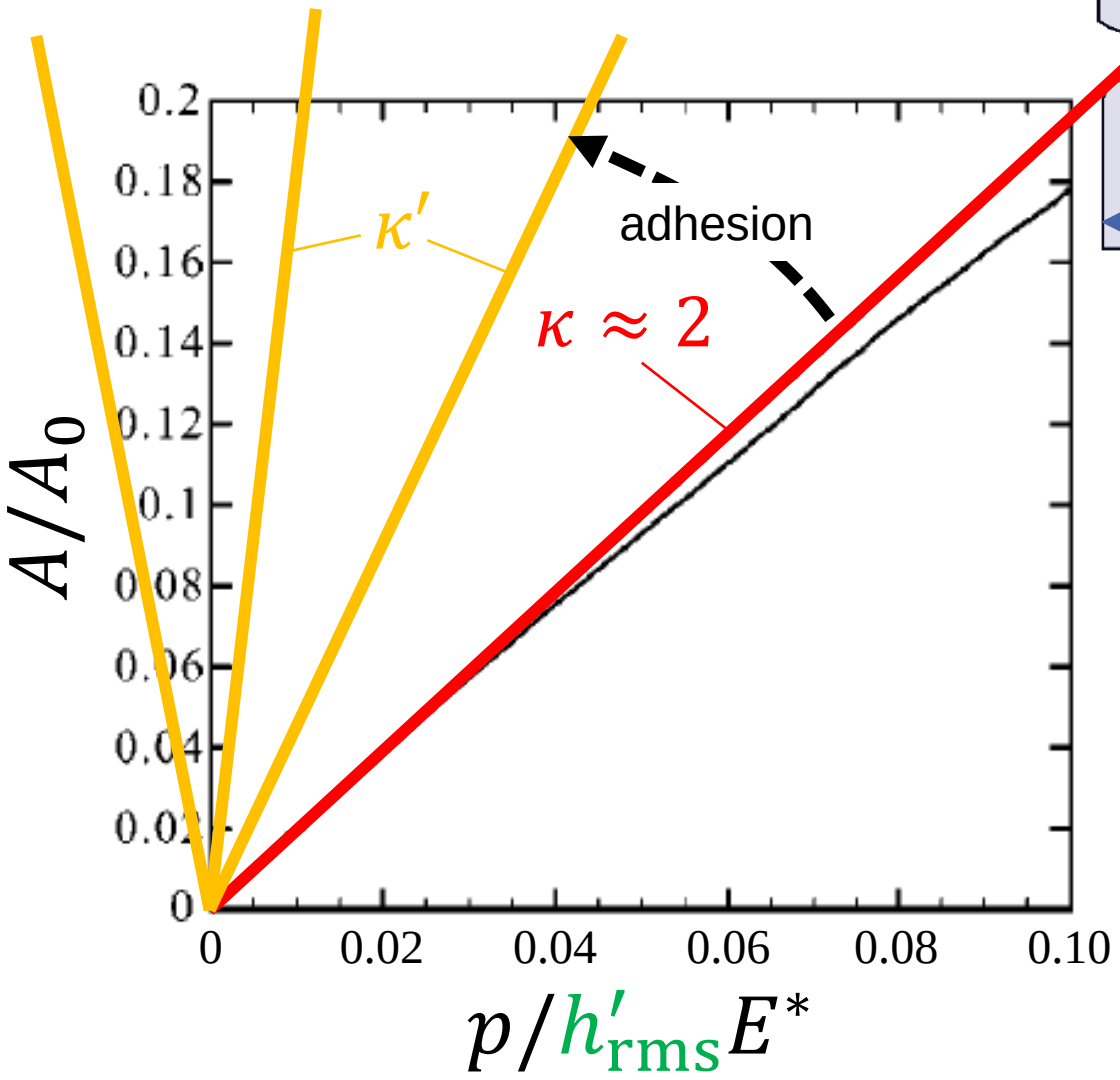

nonadhesive
continuum limit,
hard walls

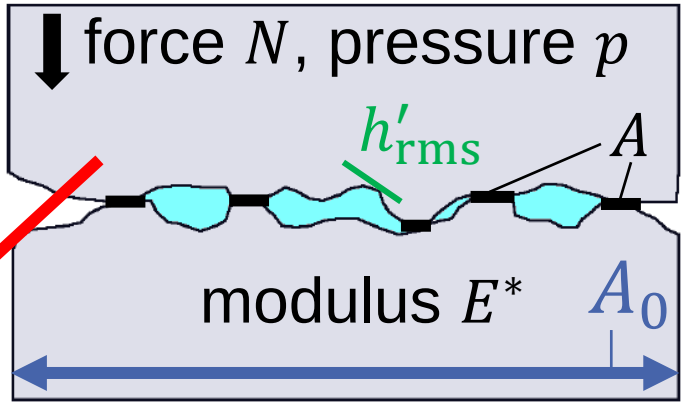



$w$: work of adhesion


Polonsky, Keer, *Wear* 231, 206 (1999)
Campaña, Müser, *Phys. Rev. B* 74, 075420 (2006)
Pastewka, Sharp, Robbins, *Phys. Rev. B* 86, 075459 (2012)

# Making contact



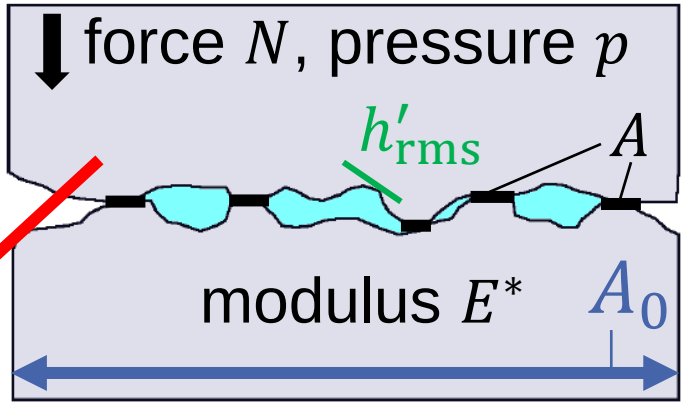



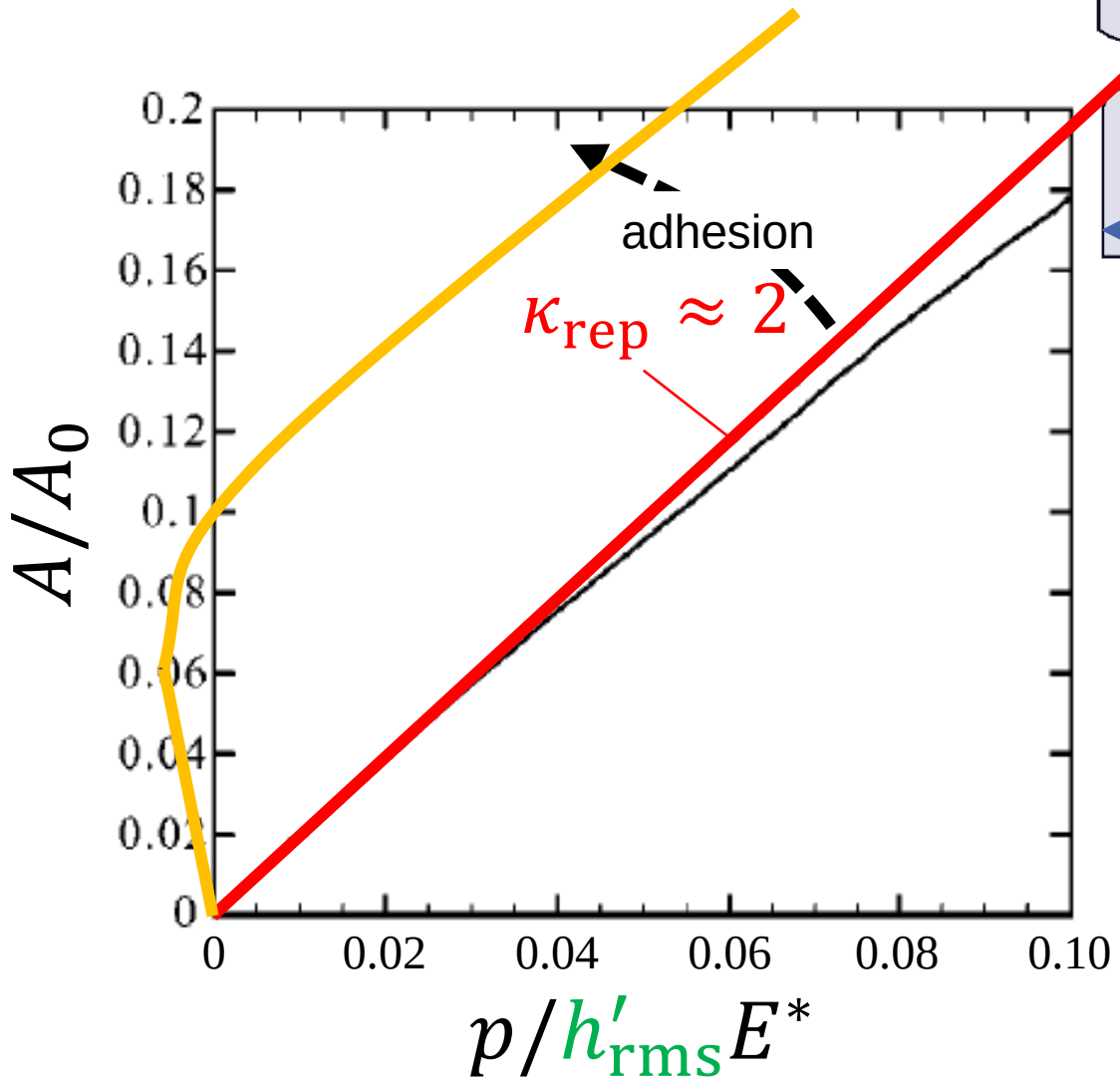

- $h'_{\mathrm{rms}}$ - amplitude of local slope fluctuations
- $E^*$ - elastic contact modulus
- $p = N/A_0$ – nominal pressure

*Nonadhesive calculation:*
e.g. Hyun, Pei, Molinari, Robbins, *Phys. Rev. E* 70, 026117 (2004)

*Analytical models:*
Bush, Gibson, Thomas, *Wear* 35, 87 (1975); Persson, J. Chem. Phys. 115, 3840 (2001)

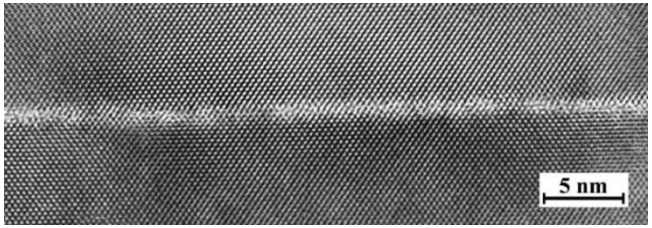
# Adhesive contact




- $h'_{\mathrm{rms}}$ - amplitude of local slope fluctuations
- $E^*$ - elastic contact modulus
- $p = N/A_0$ – nominal pressure

**Sticky if** $\frac{w}{E^* a_0} = \frac{\ell_a}{a_0} \geq 0.5 h'_{\mathrm{rms}}$

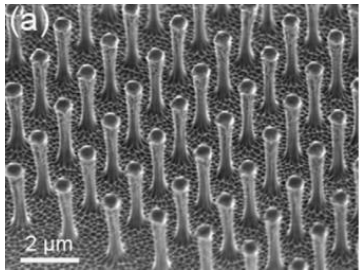



Reznicek, Scholz, Senz, Gösele, *Mater. Chem. Phys.* 81, 277 (2003)

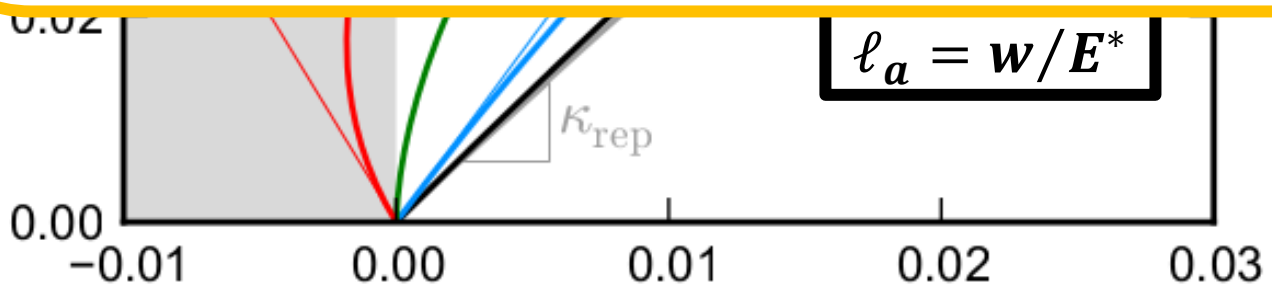
$h'_{\mathrm{rms}} < 10^{-3}$

Dahlquist criterion:
$E^* < 0.1$ MPa


Hansen, Autumn, *PNAS* **102**, 385 (2005)

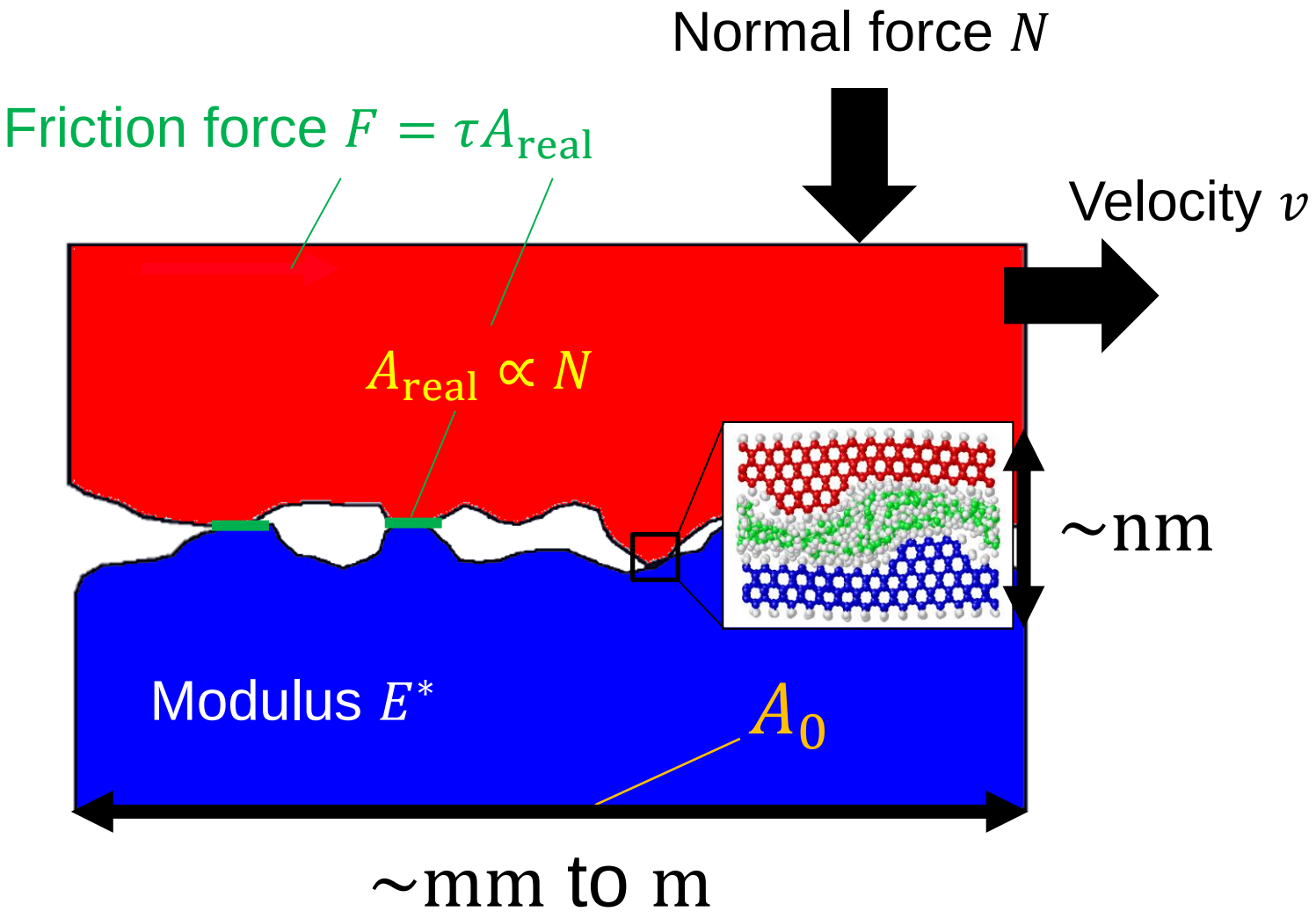



Jeong, Suh, *Nano Today* 4, 335 (2009)



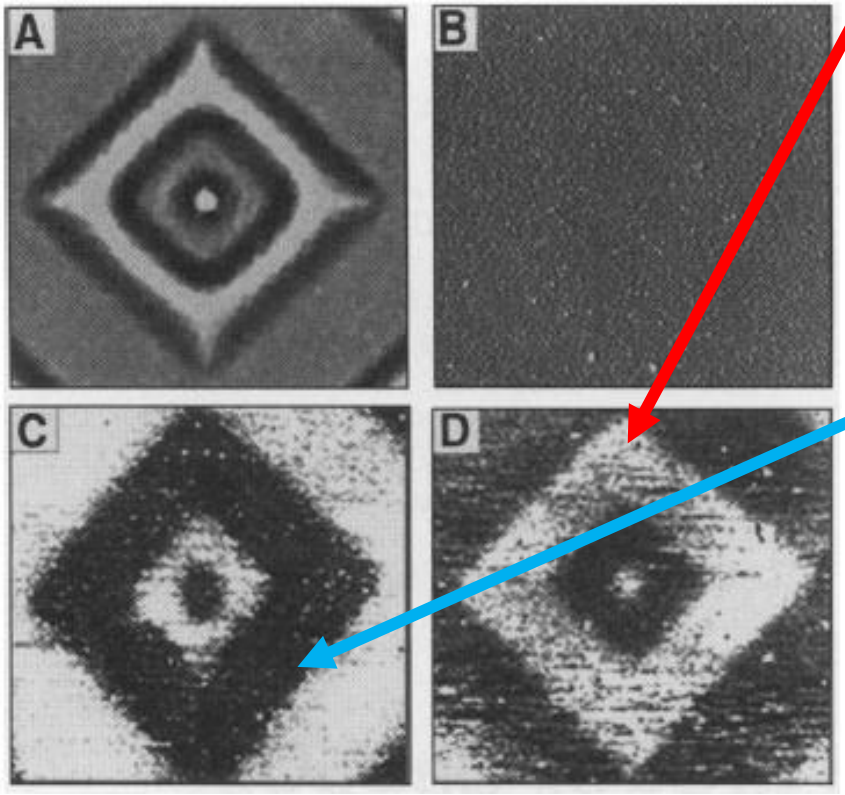

Pastewka, Robbins, *PNAS* 111, 3298 (2014)

# Amontons‘ law: $F = \mu N$



# Chemical roughness

## SAMs on Au

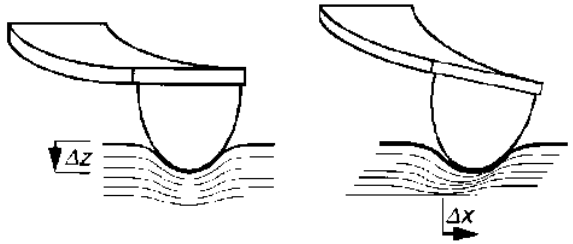



Frisbie, Rozsnyai, Noy, Wrighton, Lieber, *Science* 265, 2071 (1994)

## PS-PVP copolymer

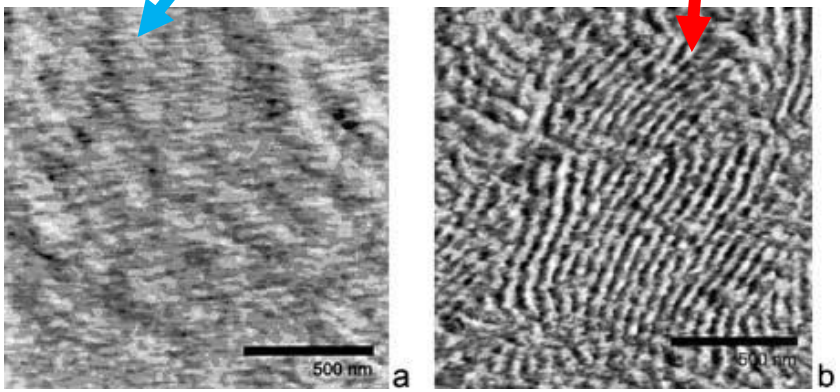
COOH-functionalized tip

(hydrophilic/oleophobic)



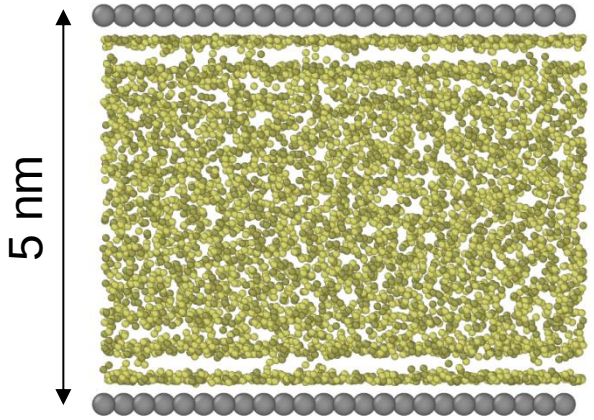

CH3-functionalized tip

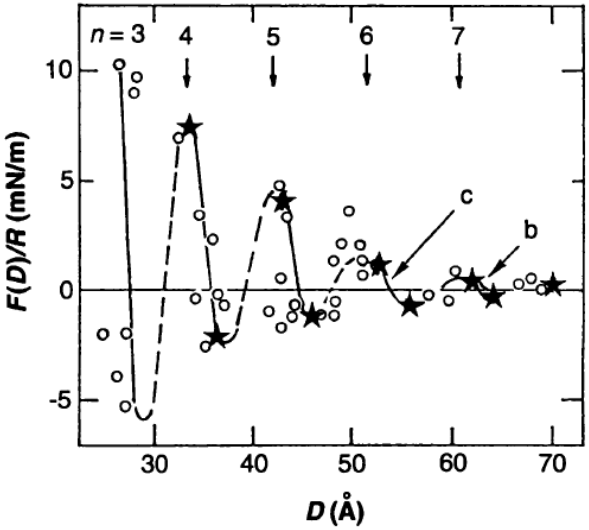
(hydrophobic/oleophilic)



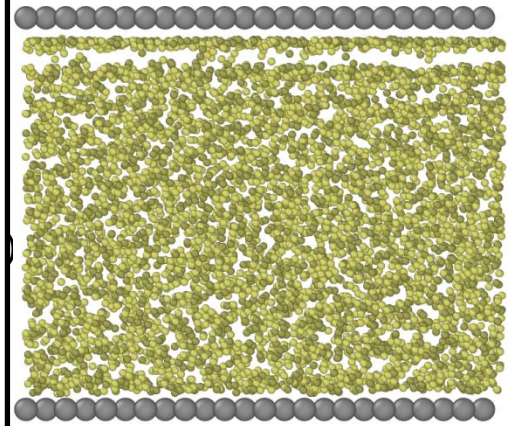

Werts, van der Vegte, Grayer, Esselink, Tsitsilianis, Hadziiannou, *Adv. Mater.* 10, 452 (1998)

# Wetting and non

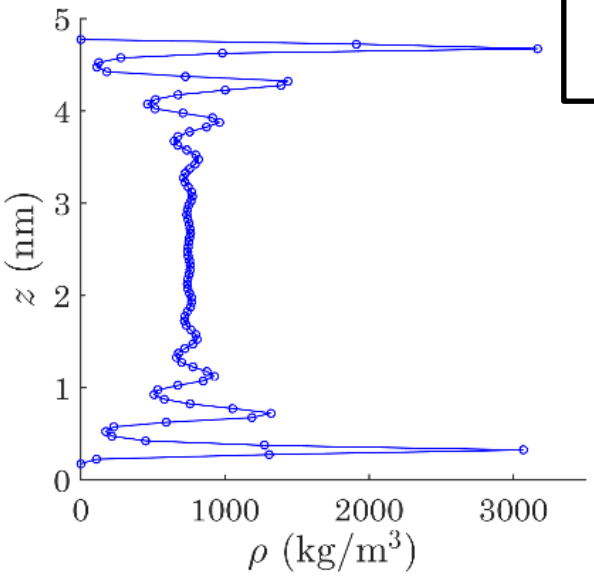


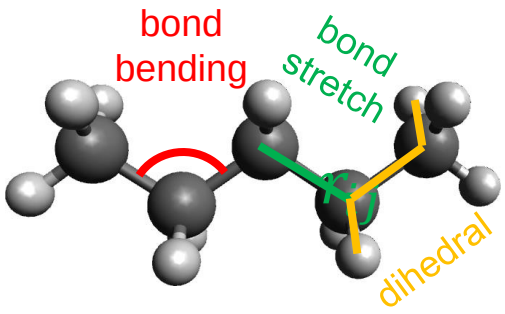




Mica in OMCTS,
Klein, Kumacheva,
*Science* 269, 816 (1995)

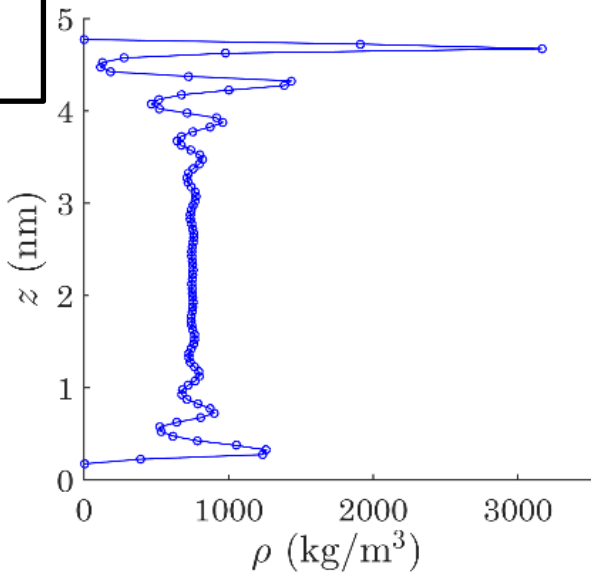


Wetting/oleophilic

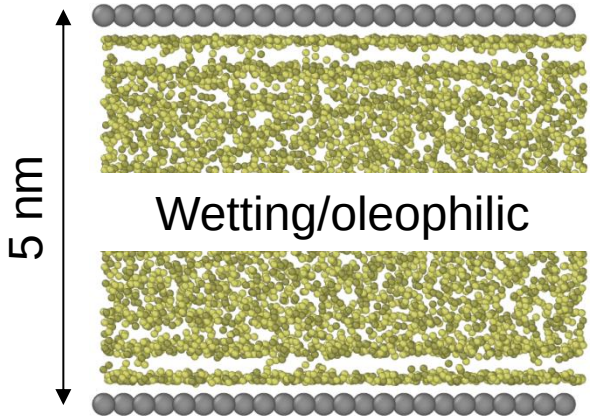



Non-wetting/oleophobic

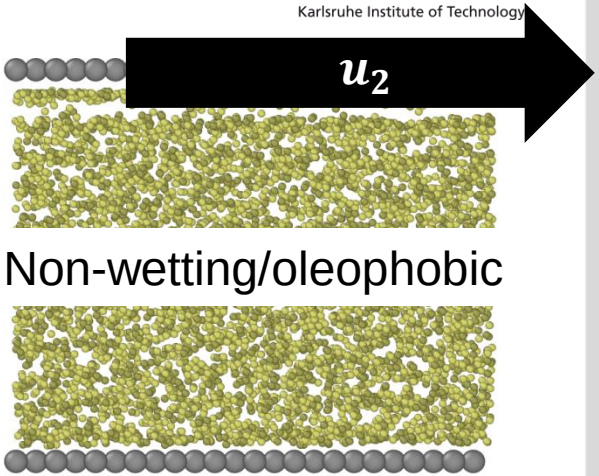


# Slip length

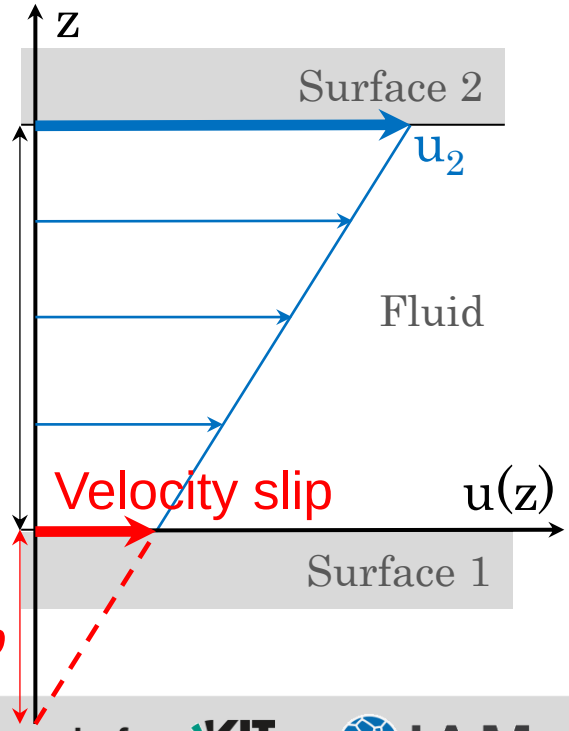



**Velocity jump** at the **wall-fluid interface**

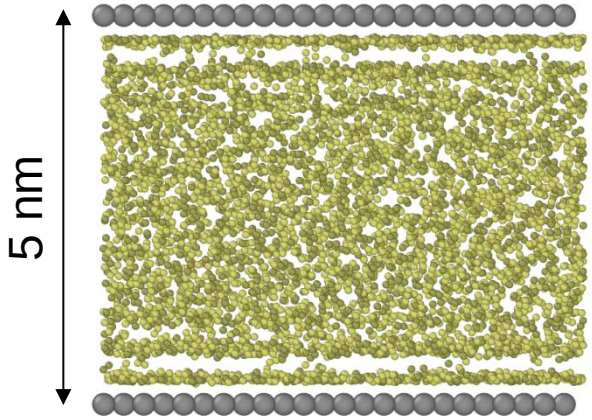
$$b = \frac{u(z=0)}{\partial u/\partial z|_{z=0}}$$



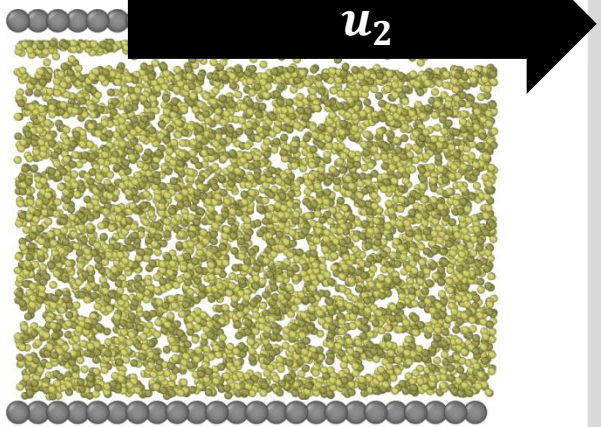

| Surface | Fluid | h (nm) | b (nm) |
|---|---|---|---|
| Photores. coated glass [Cheng, 2002] | $C_{16}H_{34}$ | 50 | 25 |
| Thiol coated gold [Baudry, 2001] | Glycerol | 300 | 40 |
| Fusso coated glass [Ponjavic, 2014] | PB1300 | 100 | 519 |

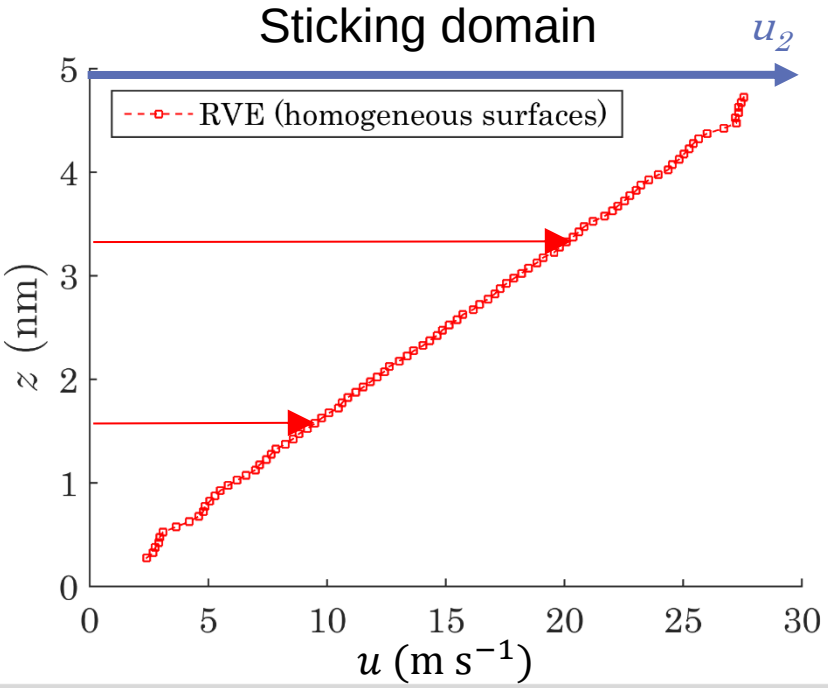


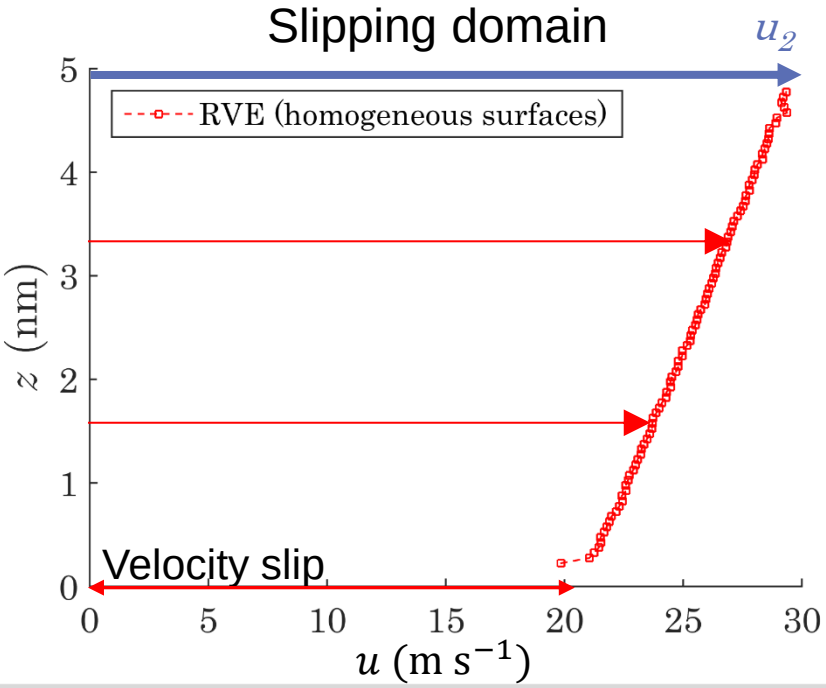
# Slip length in molecular dynamics



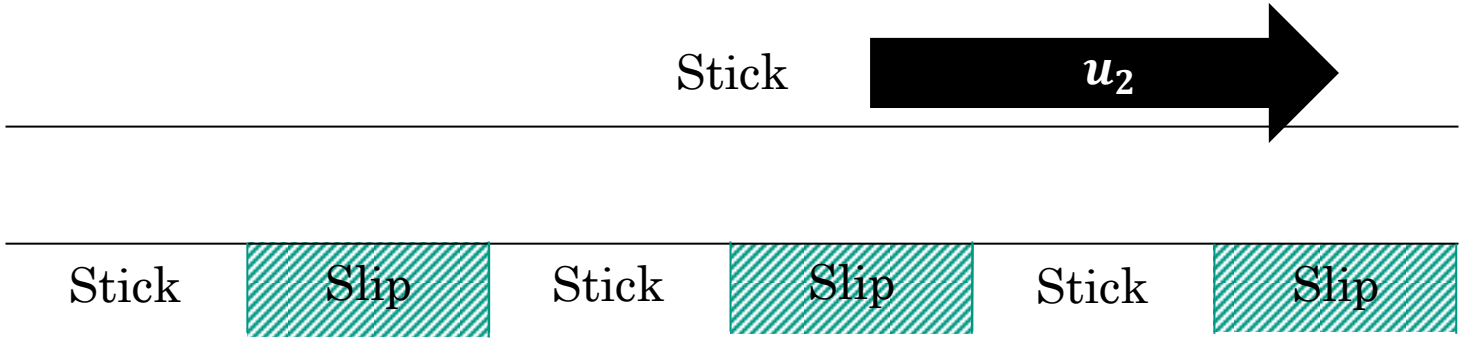

- n-pentane ($C_5H_{12}$), gold (111) surfaces
- $h$ = 5 nm, $u_2$ = 30 m/s, $P_{ext}$ = 250 MPa

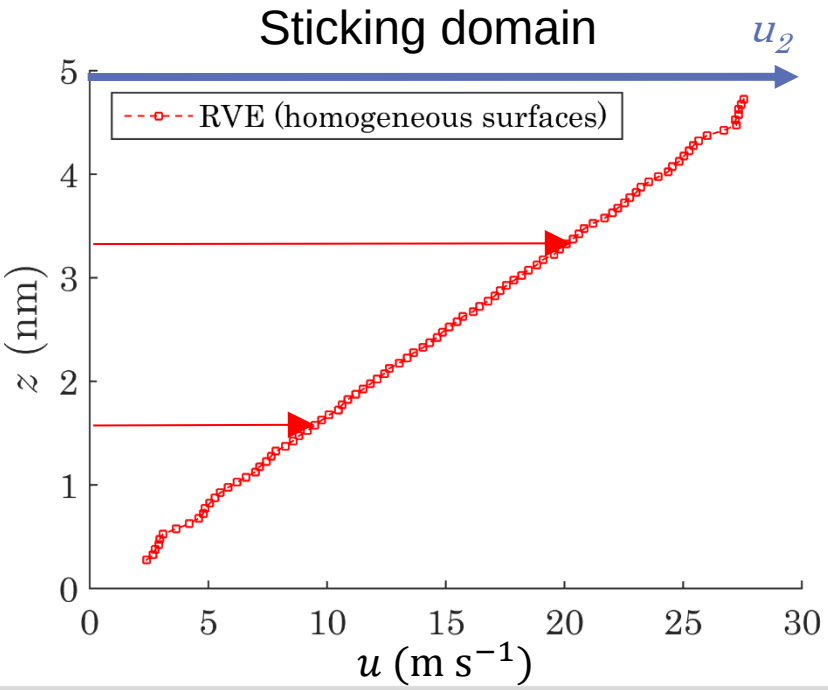


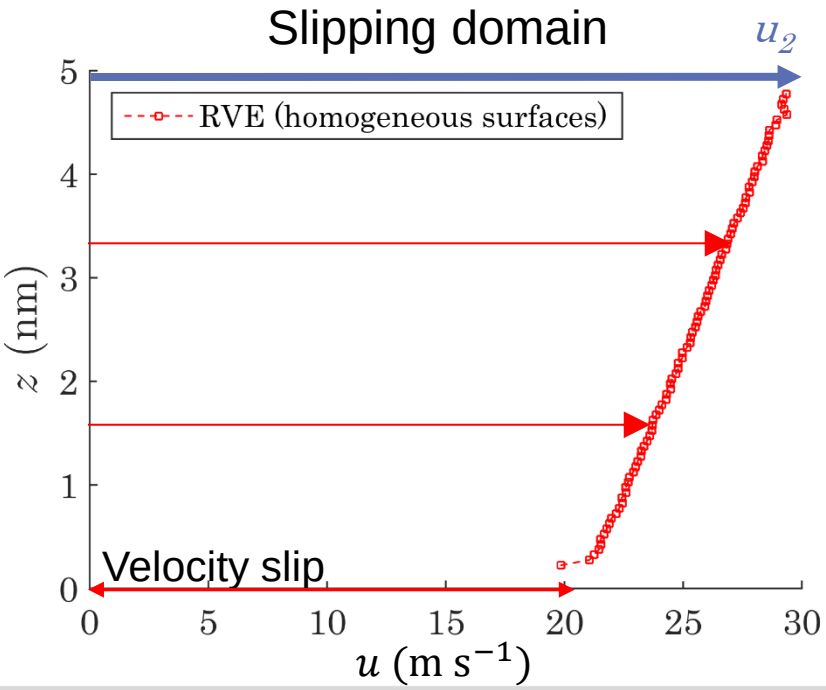



# Heterogeneous surfaces



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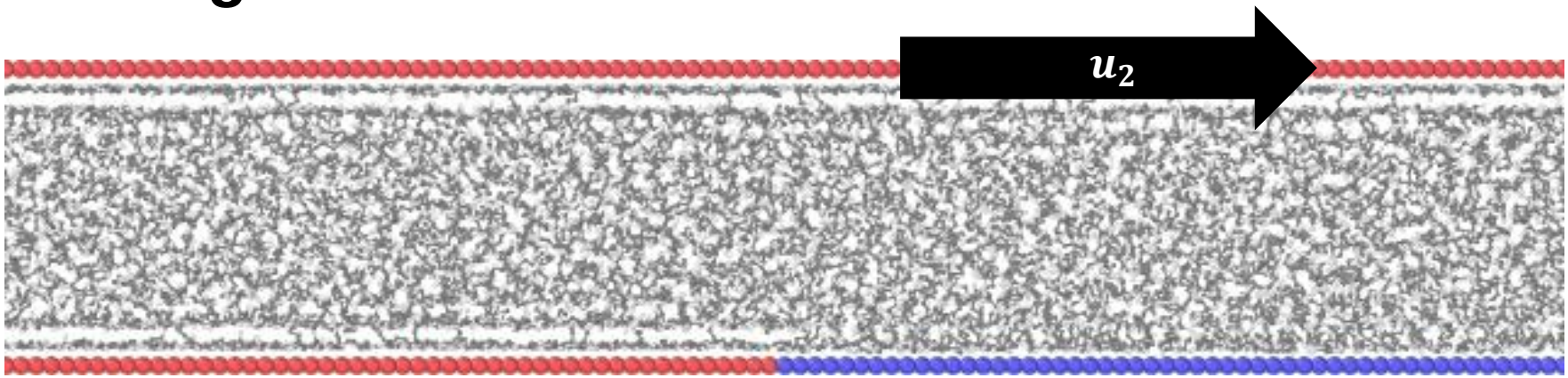


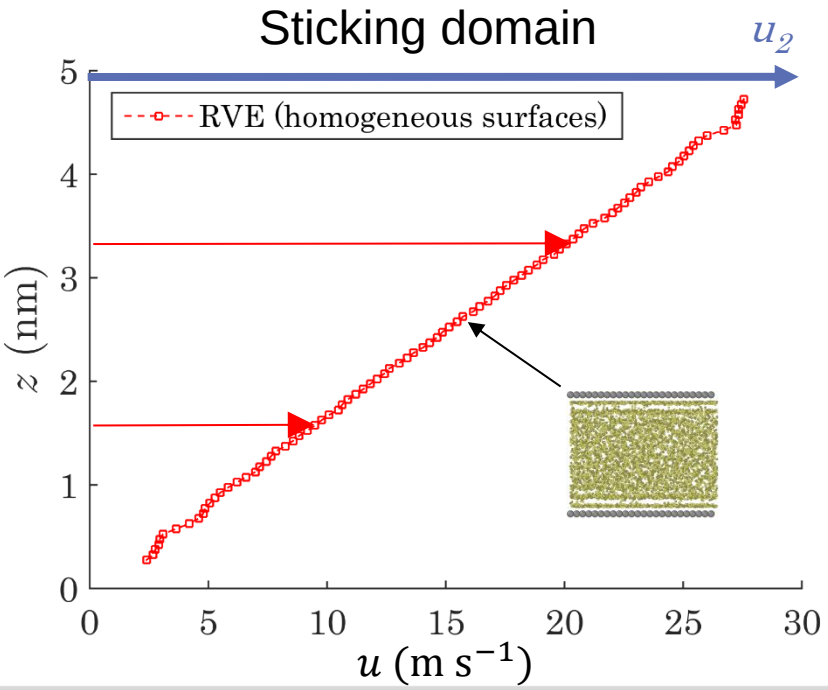


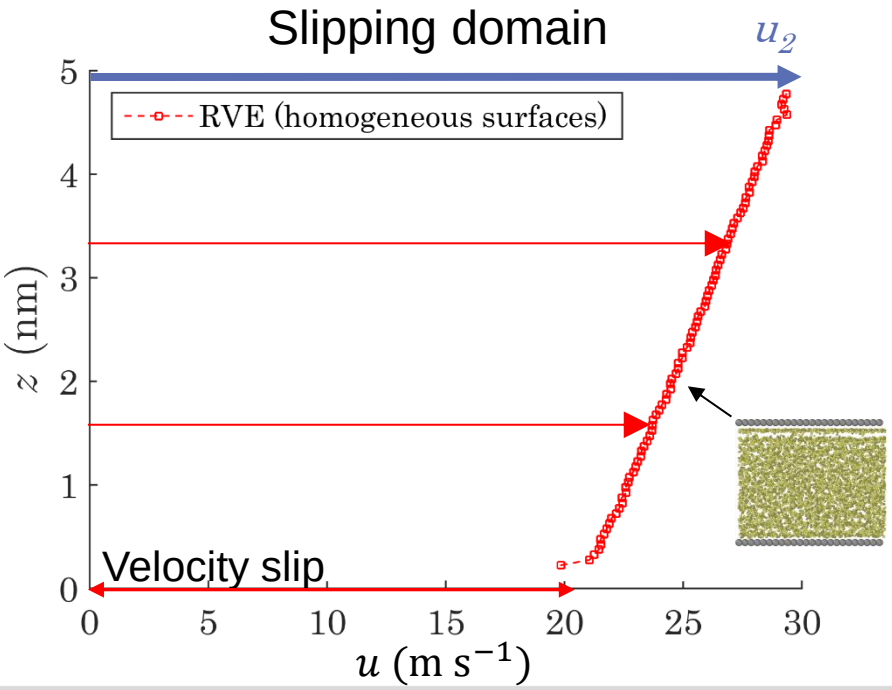

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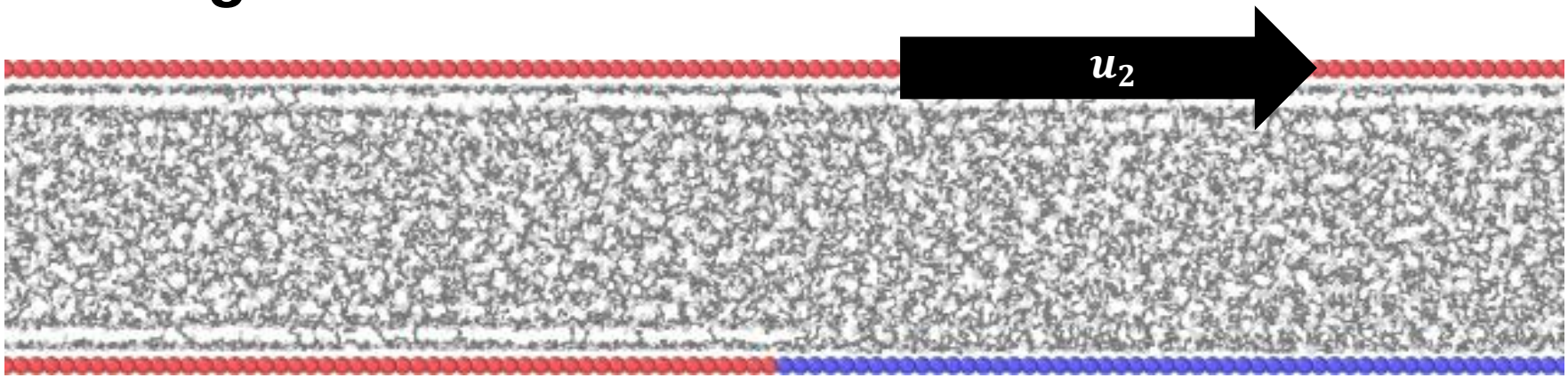
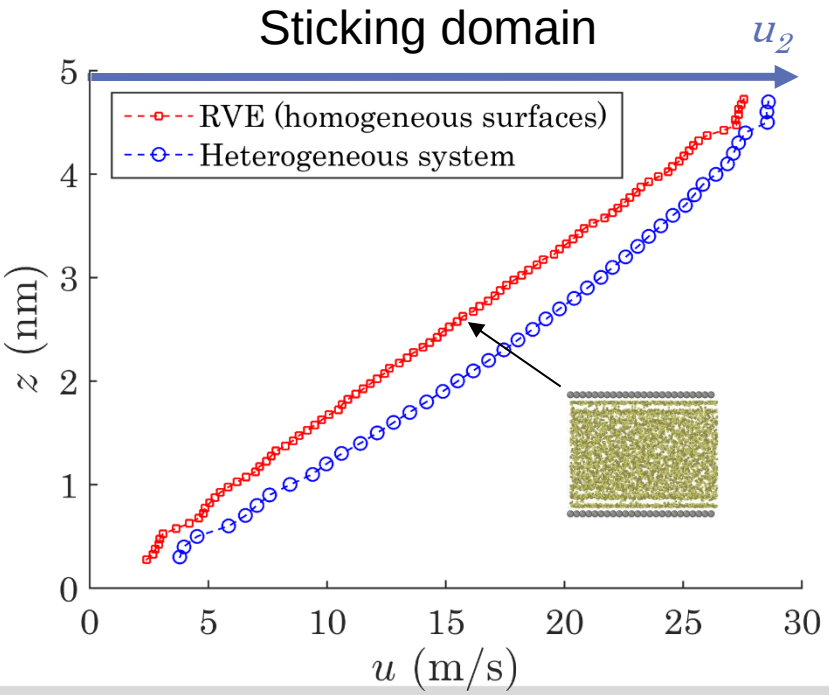
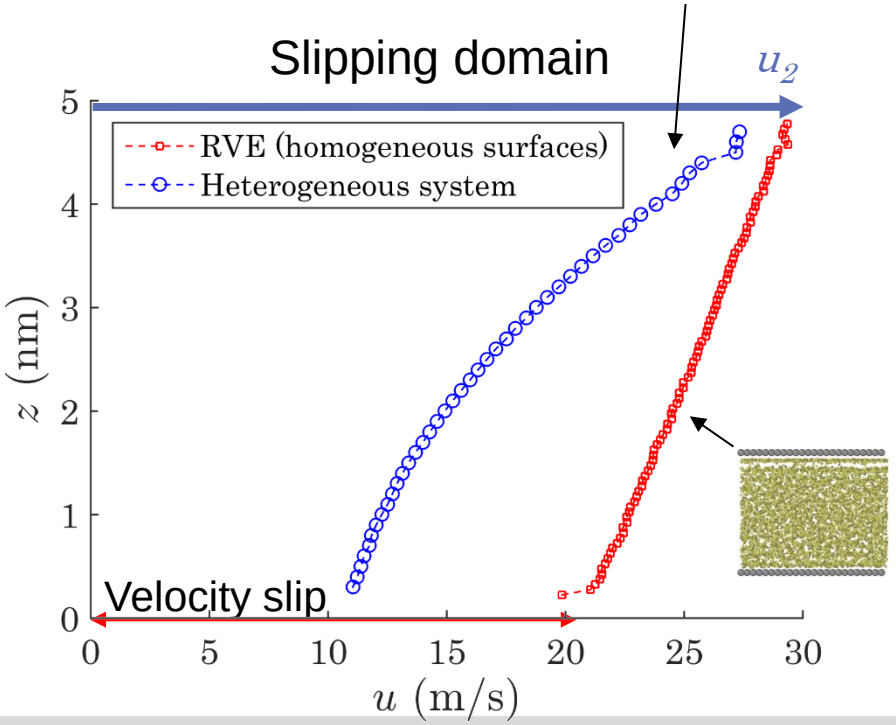


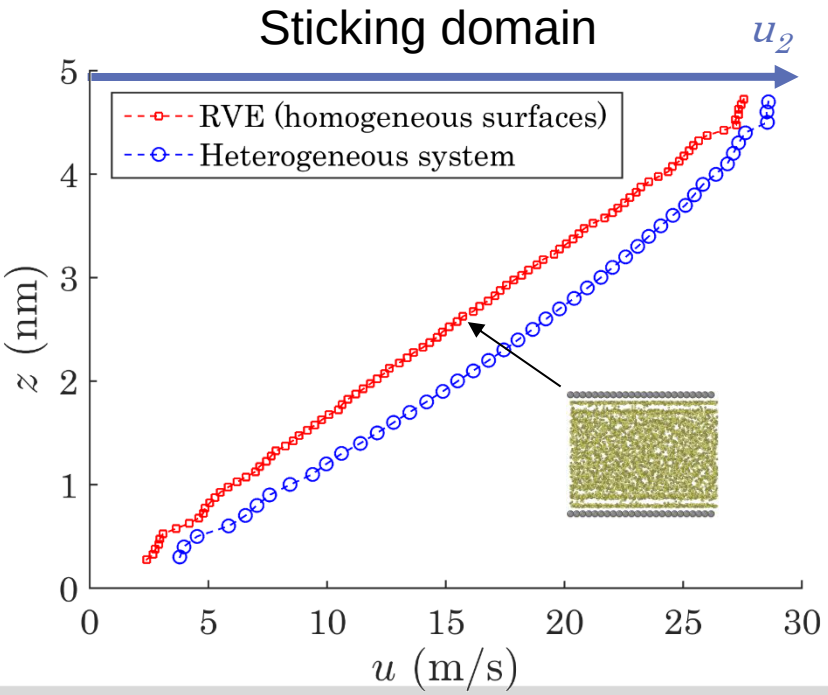



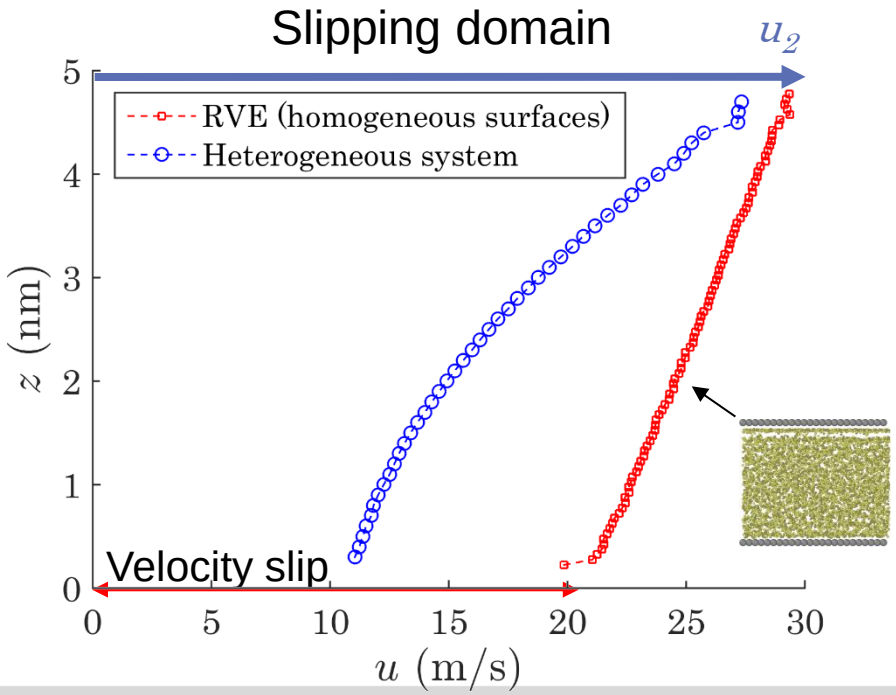



# Heterogeneous surfaces

- Hydrodynamic model (Reynolds eq. + slip)

$$u(z) = u_2\left(\frac{z+b(x)}{h+b(x)}\right) + \frac{1}{2\eta}\left(z^2 - \frac{z+b(x)}{h+b(x)}h^2\right)\frac{\partial P}{\partial x}$$



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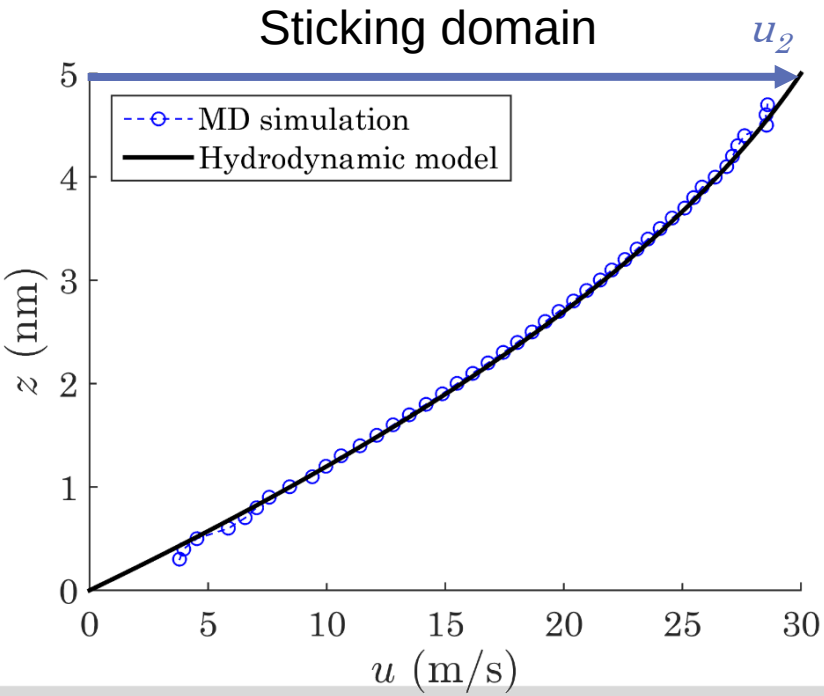
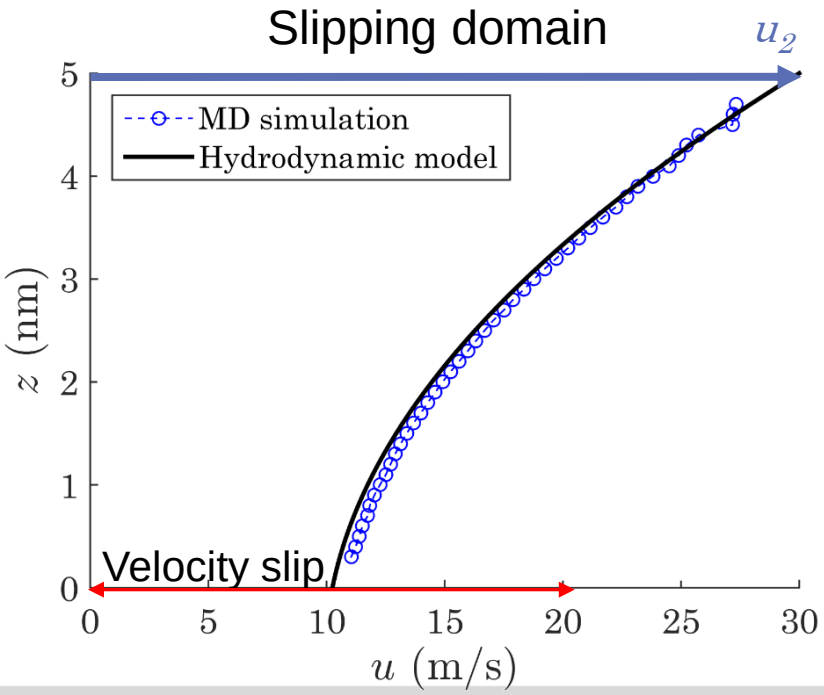
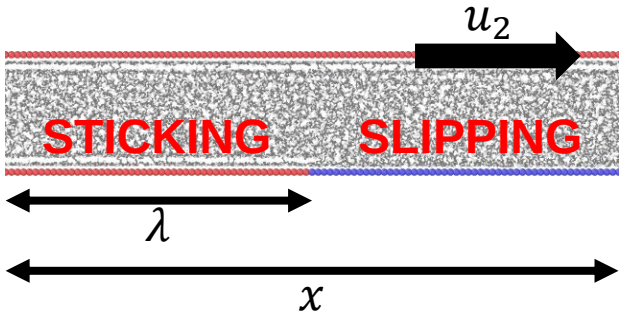
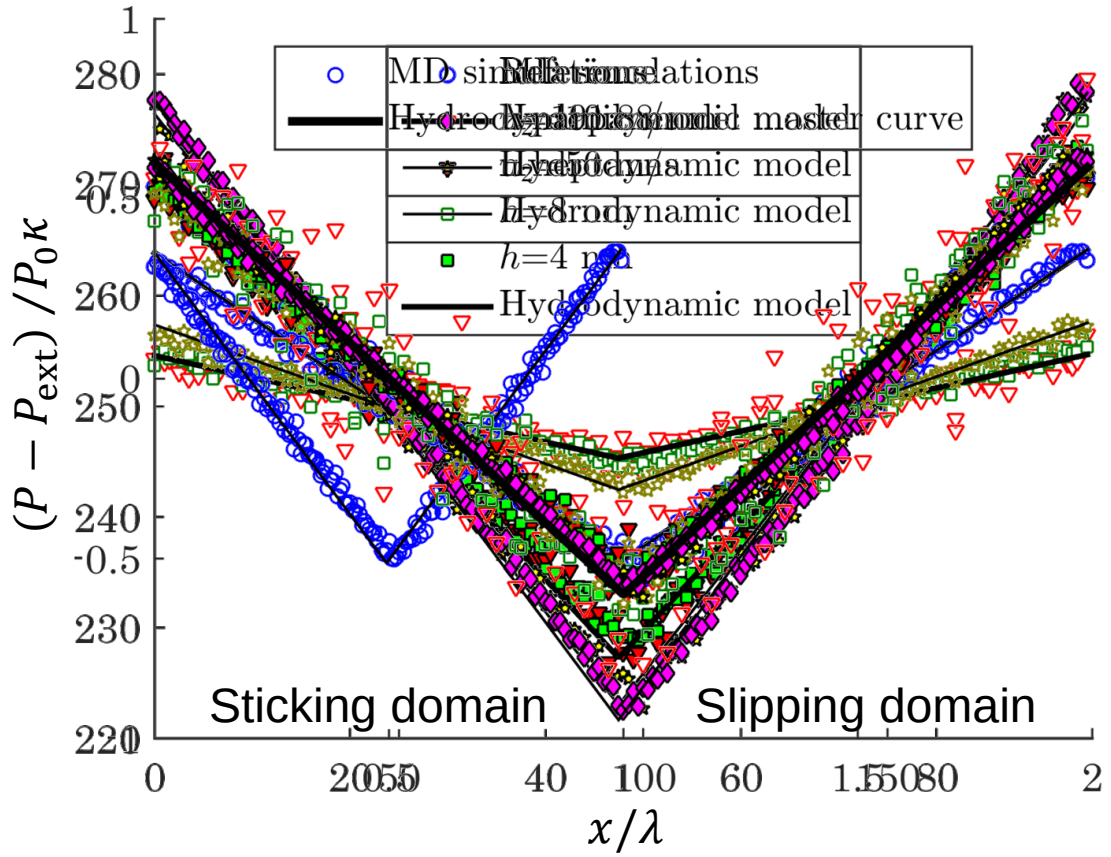


# Pressure along channel

- **Pressure excursions** under shearing
- Amplitude increases with shear rate, fluid viscosity, system length



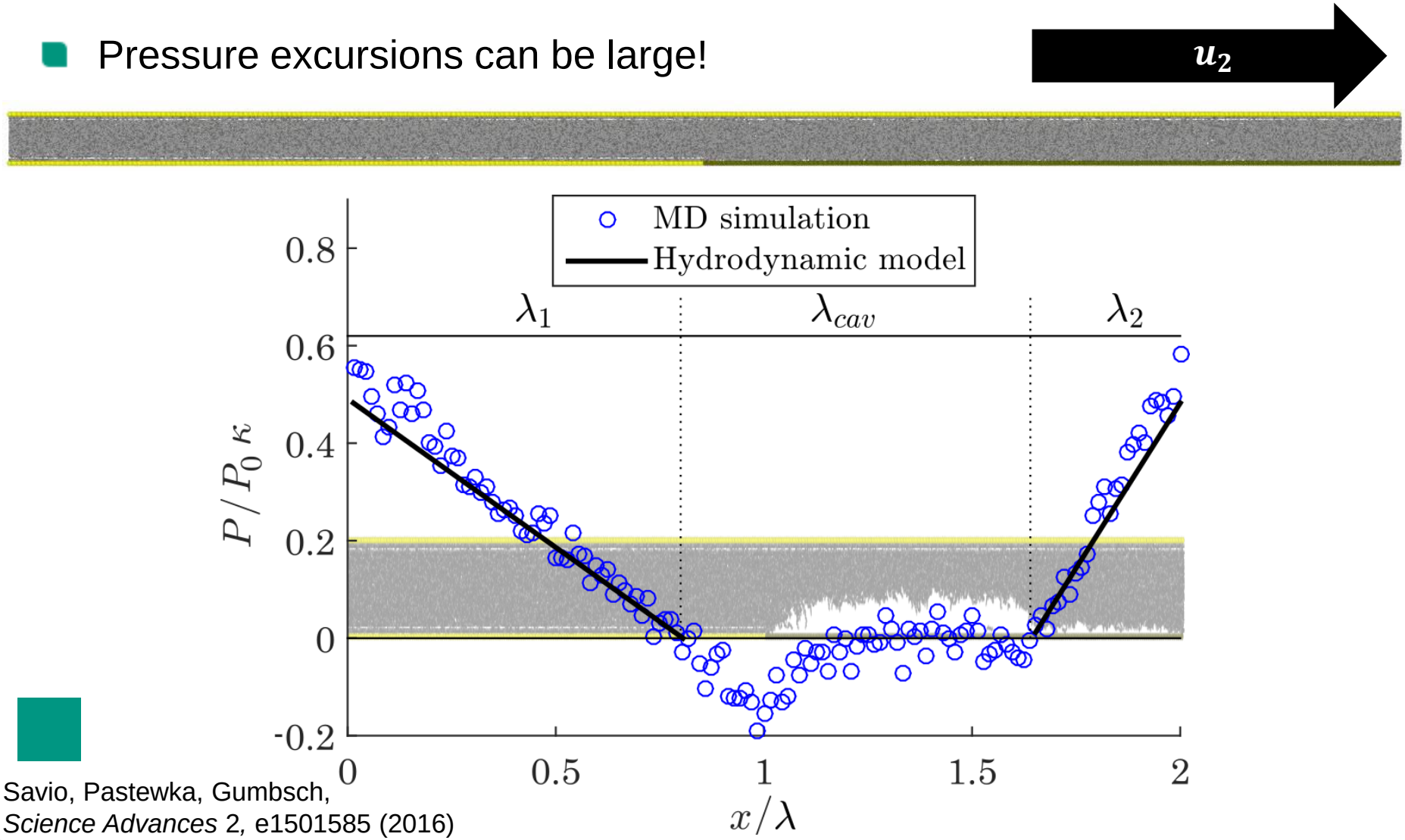




- Reference
  - $u_2 = 30\ \mathrm{m\ s^{-1}}$
  - $h = 5\ \mathrm{nm}$
  - n-pentane

Savio, Pastewka, Gumbsch,
*Science Advances* 2, e1501585 (2016)

# Pressure can drop to zero ➔ cavitation

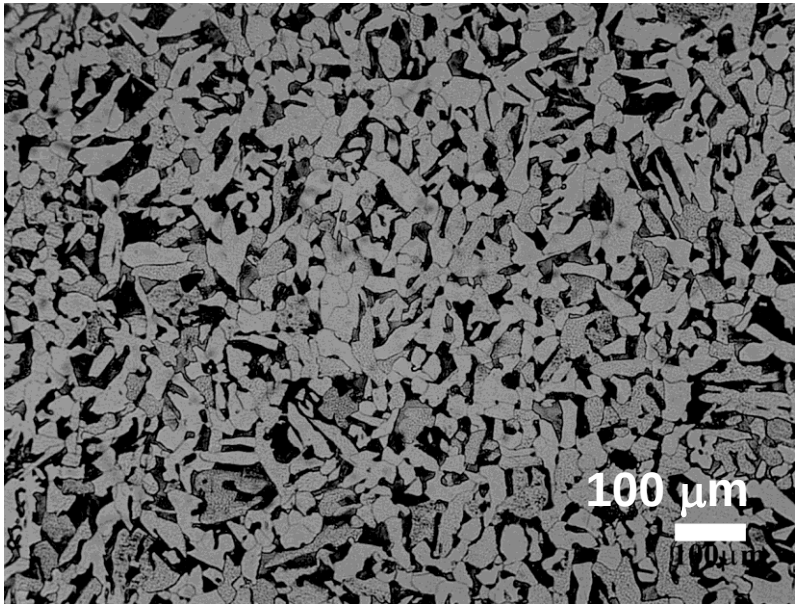
- Pressure excursions can be large!




Savio, Pastewka, Gumbsch,
*Science Advances* 2, e1501585 (2016)

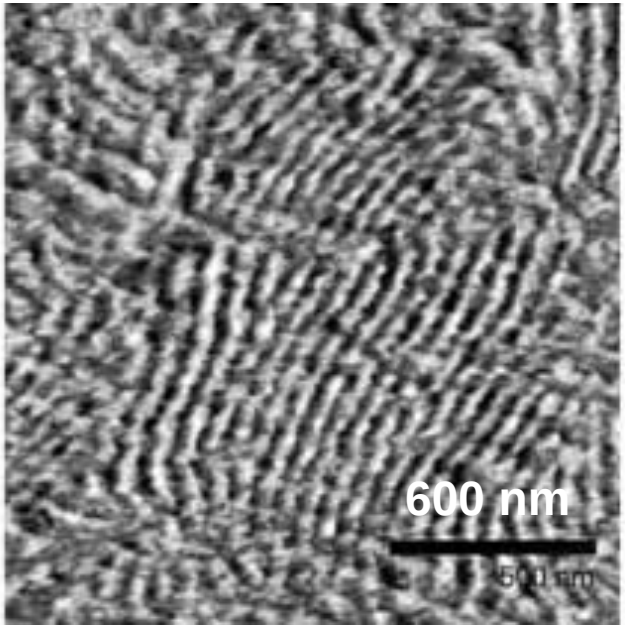
# Roughness

## Steel




US Department of Energy Report
WSRC-MS-2000-00282

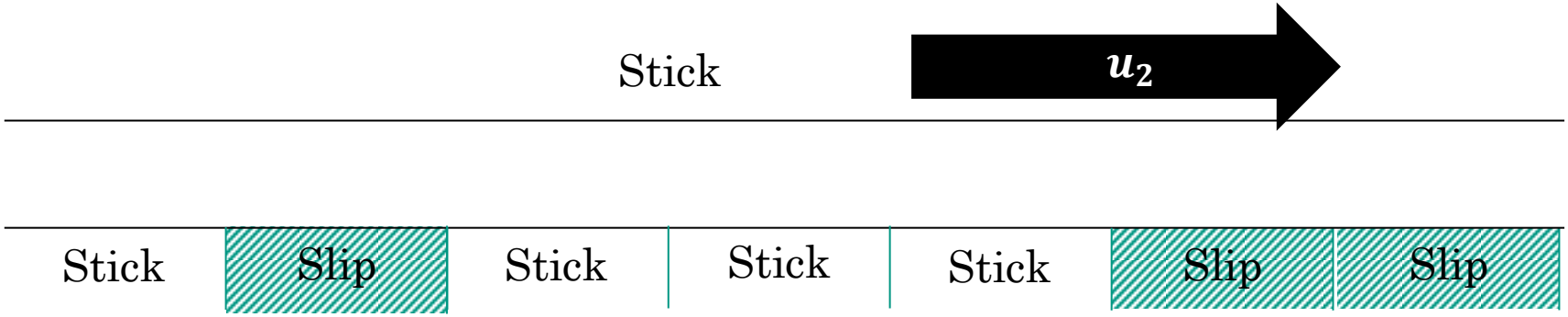
## PS-PVP block copolymer



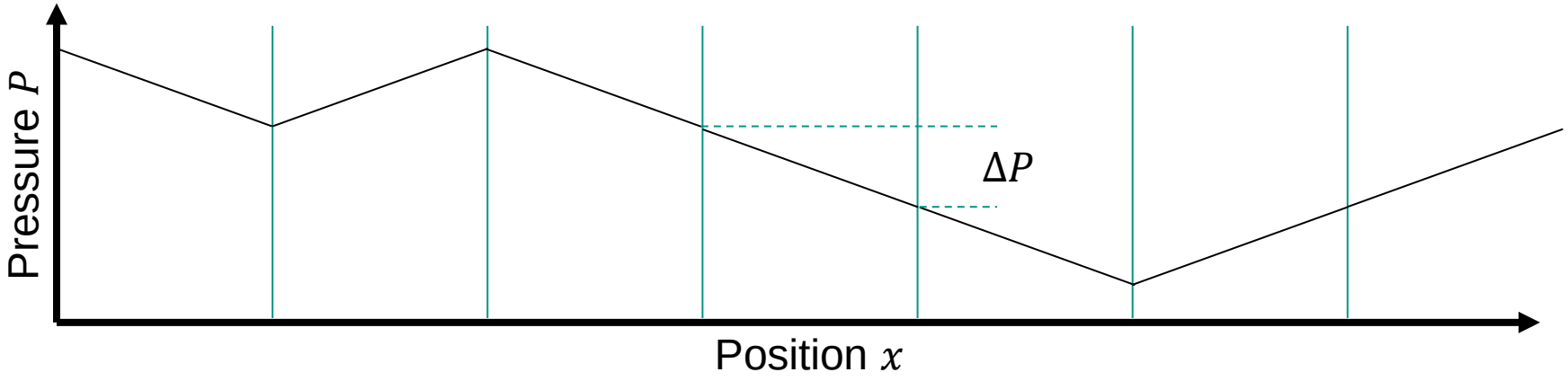

Werts, van der Vegte, Grayer, Esselink, Tsitsilianis, Hadziiannou, *Adv. Mater.* 10, 452 (1998)

# Roughness

- Simple roughness model: random arrangement of slip/no-slip domains




- Linear pressure drop/increase over domain



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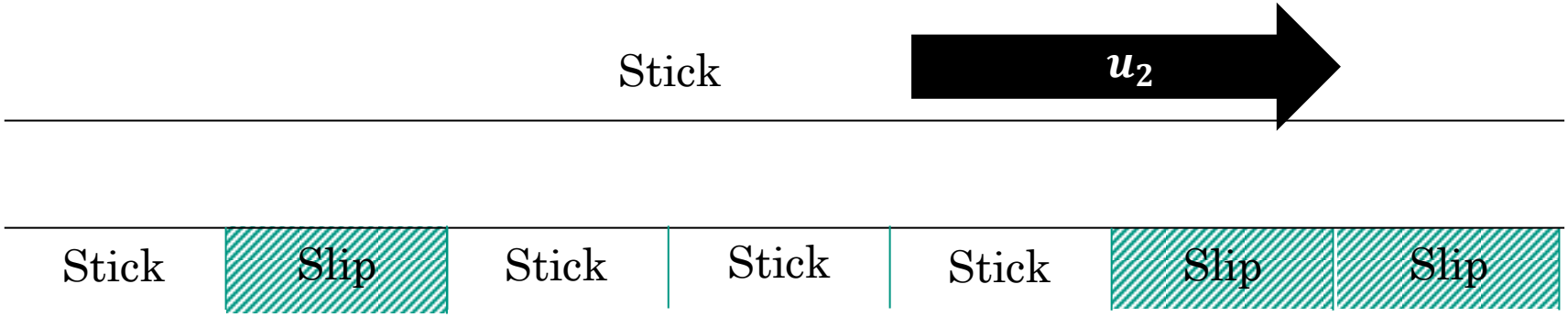
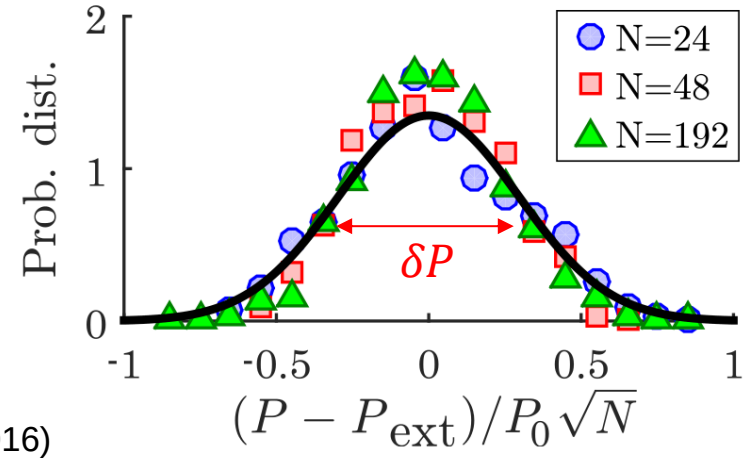
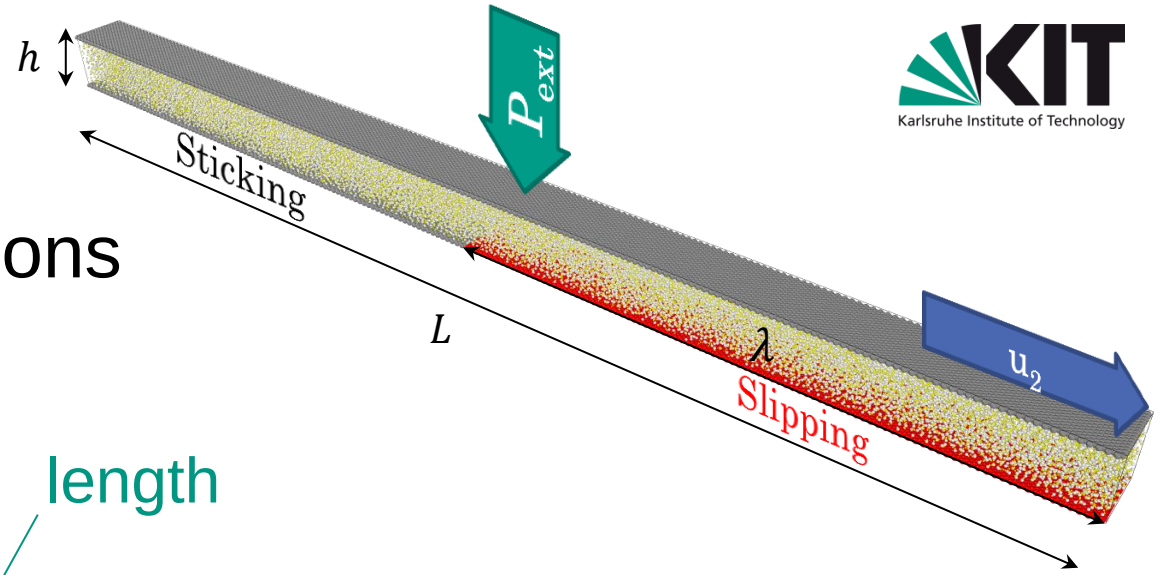



- Linear pressure drop over domain ➔ Random walk of overall pressure




Savio, Pastewka, Gumbsch,
*Science Advances* 2, e1501585 (2016)

# Pressure




- Pressure excursions scale as

viscosity length

$$\delta P \propto \eta u_2 L/h^2$$ regular patterns

$$\delta P \propto \eta u_2 \sqrt{L\lambda}/h^2$$ random patterns

velocity pattern width film thickness

Savio, Pastewka, Gumbsch,
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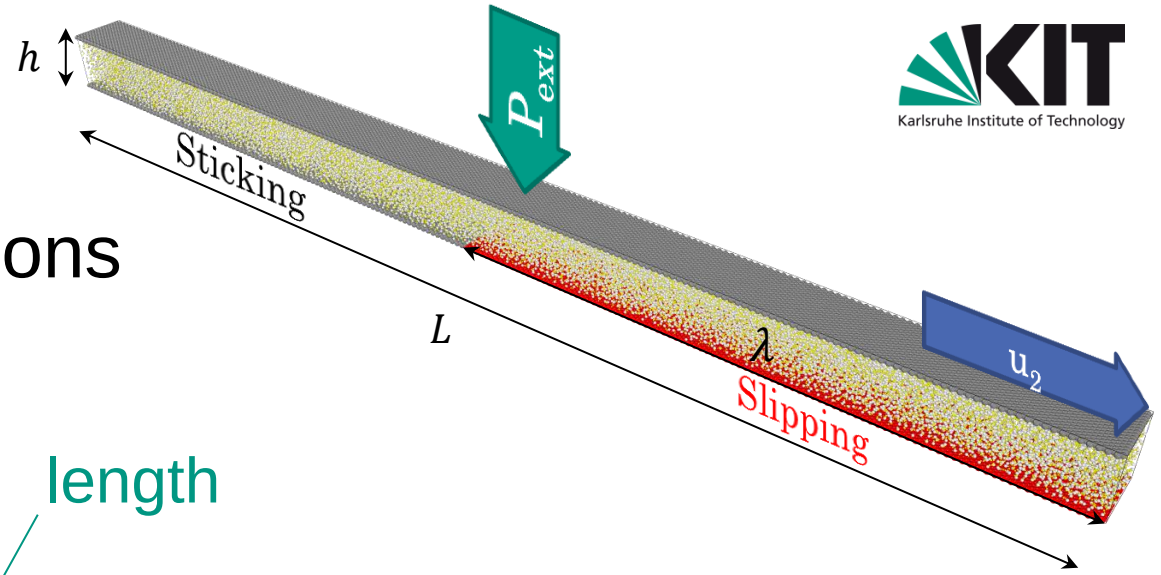
# Pressure

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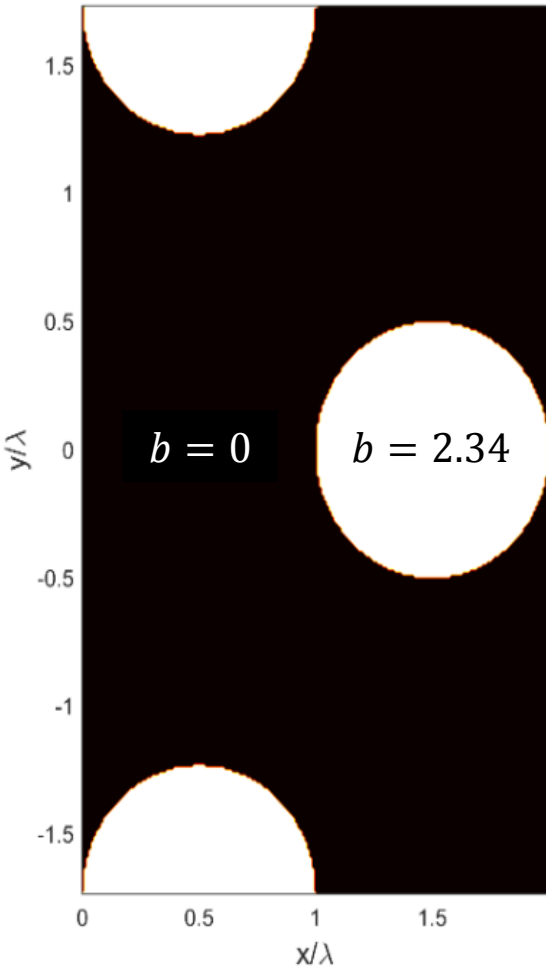
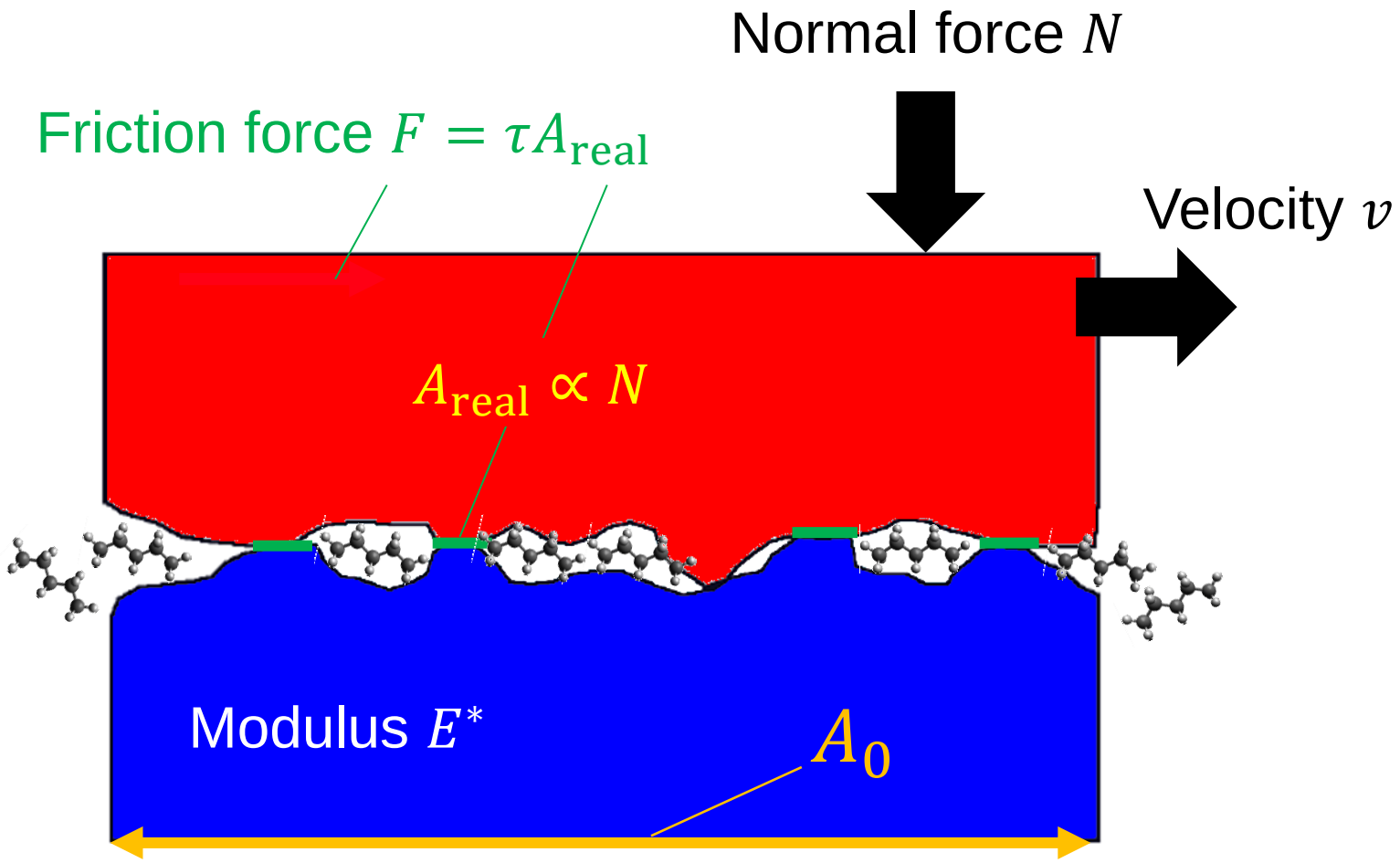
# 2D patterned surfaces



# Tribology


Normal force $N$
Friction force $F = \tau A_{\mathrm{real}}$
Velocity $v$
$A_{\mathrm{real}} \propto N$
Modulus $E^*$
$A_0$

# Thank you for your attention!





DAAD



## Collaborators

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