SAND2019-3210PE

Friction and Fractals: Tribology using Molecular Simulation

Adam R. Hinkle

Sandia National Laboratories, Albuquerque, NM, USA

Schrödinger, New York, NY
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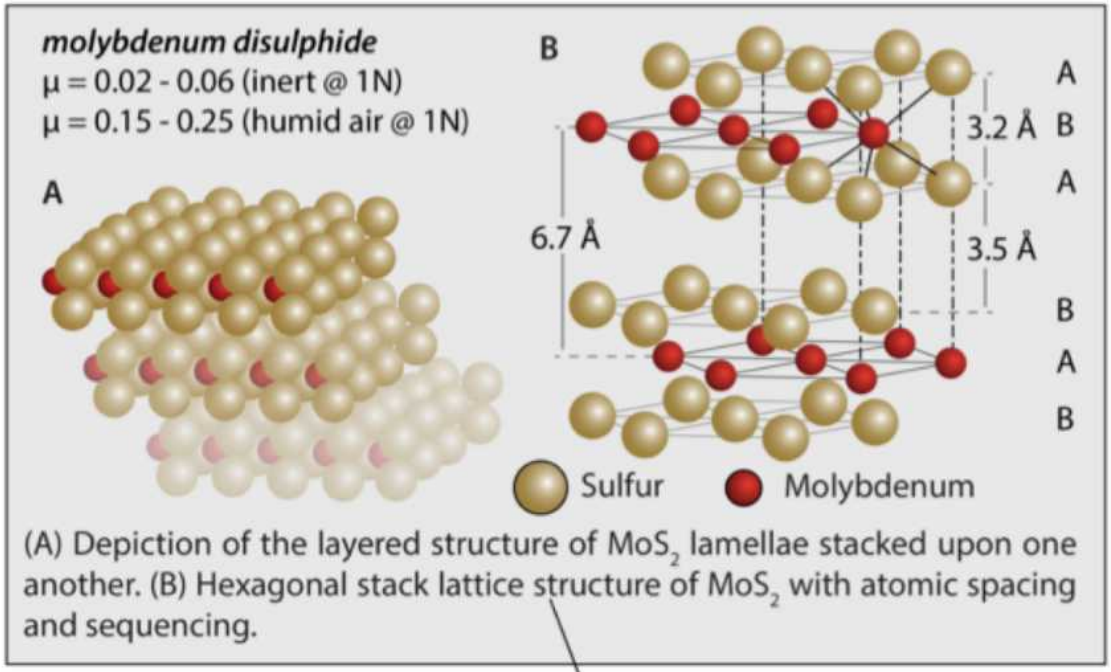
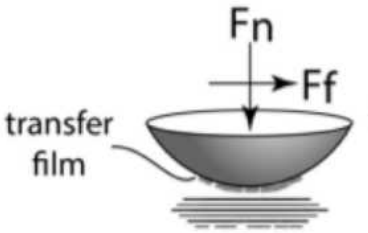
Part 1: Friction

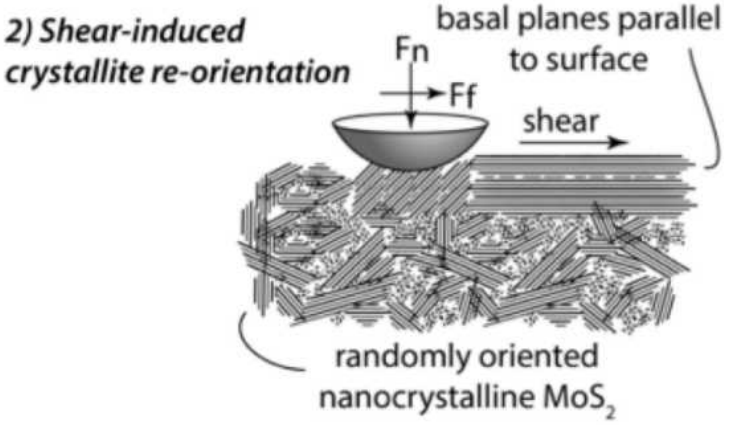
Molybdenum disulphide (MoS_2): Chemistry & sliding friction

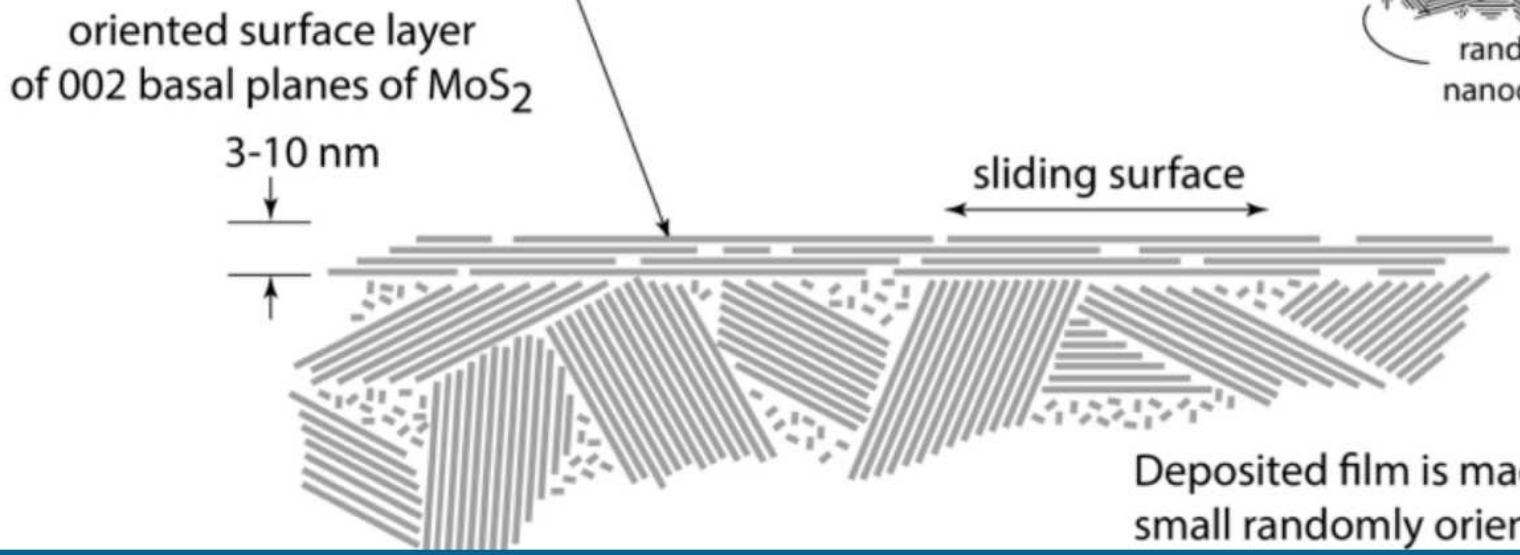


(A) Depiction of the layered structure of MoS_2 lamellae stacked upon one another. (B) Hexagonal stack lattice structure of MoS_2 with atomic spacing and sequencing.

Run-In Processes



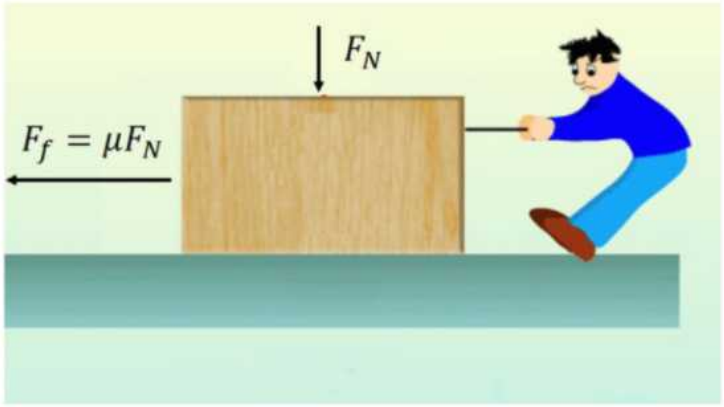




Deposited film is made of many small randomly oriented crystallites

Friction: Amontonian v. Non-Amontonian

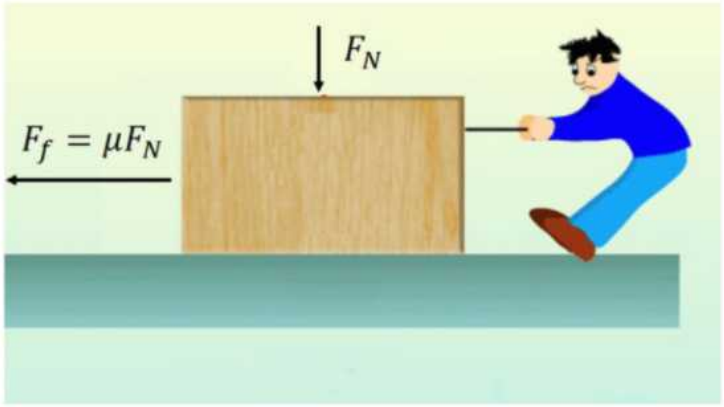
Amontonian Friction



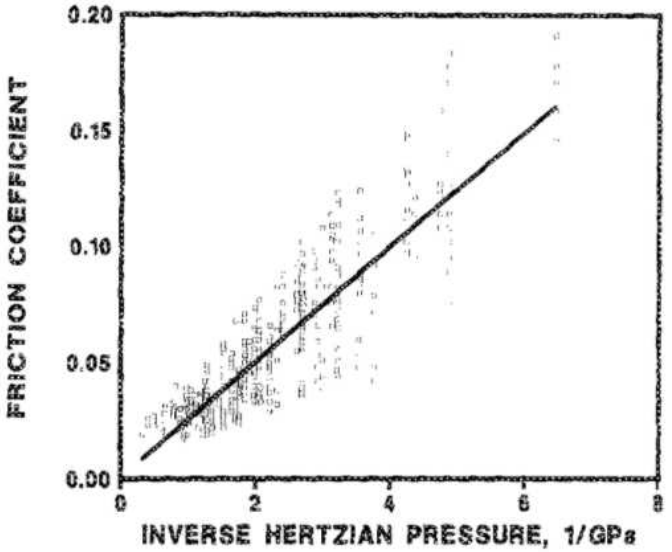
1. $\mu = \frac{F_f}{F_N}$
2. F_f does not depend on contact area
3. Kinetic Friction does not depend on sliding speed

Friction: Amontonian v. Non-Amontonian

Amontonian Friction



I.L. Singer et al., Appl. Phys. Lett. **50**, 995 (1990)



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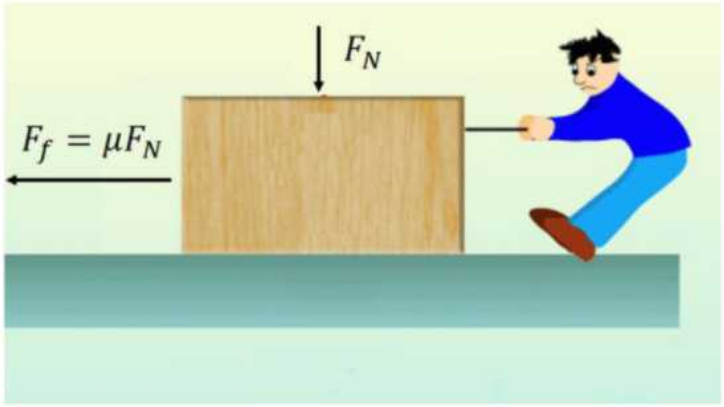

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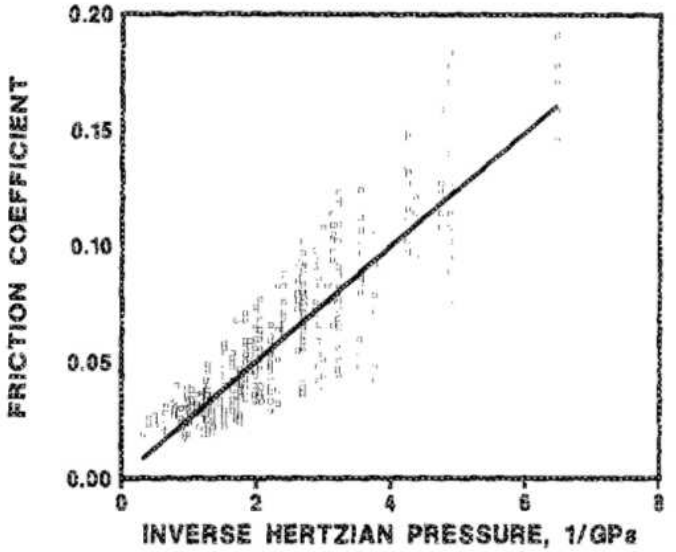
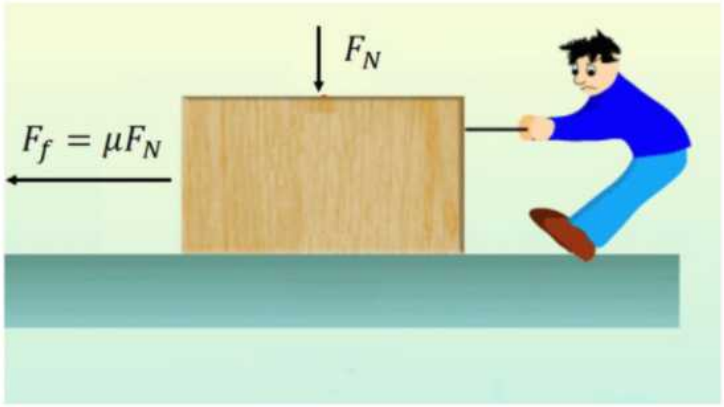


$$S = S_o + \alpha P, \text{ where } P = F_N / A_{\text{real}}$$

Friction: Amontonian v. Non-Amontonian

Amontonian Friction



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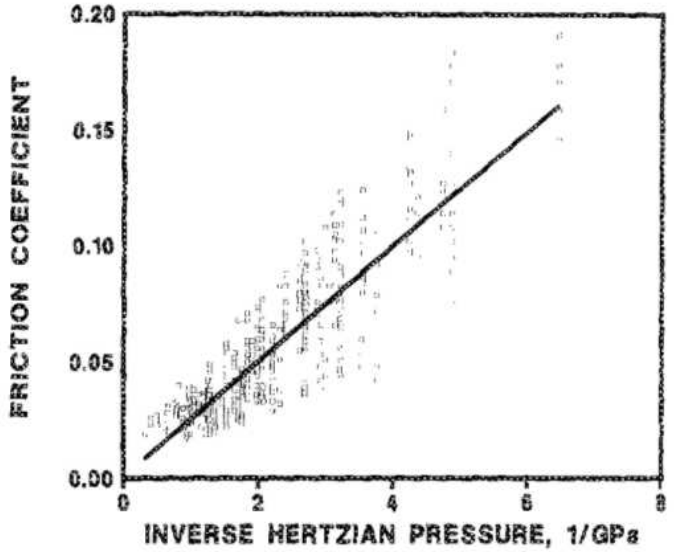
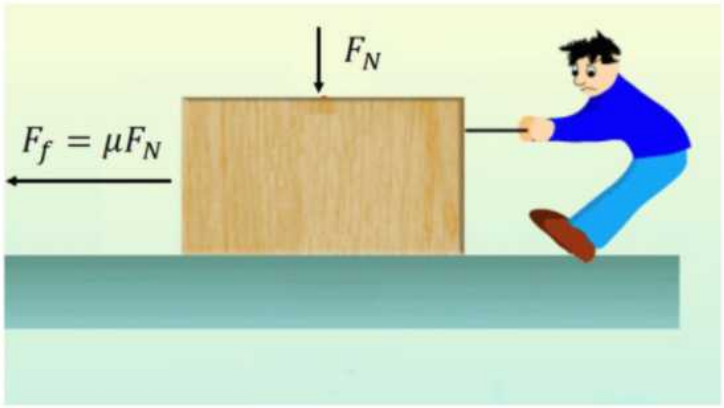


$$S = S_o + \alpha P, \text{ where } P = F_N / A_{\text{real}}$$

$$F_f = S_o A_{\text{real}} + \alpha F_N$$

Friction: Amontonian v. Non-Amontonian

Amontonian Friction



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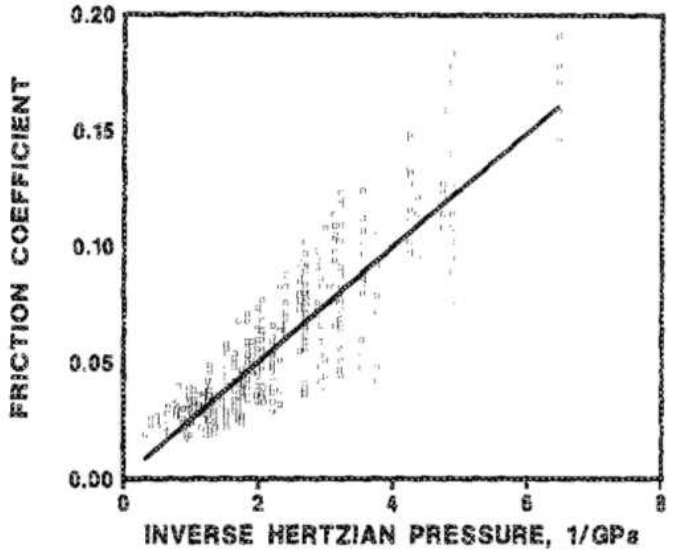


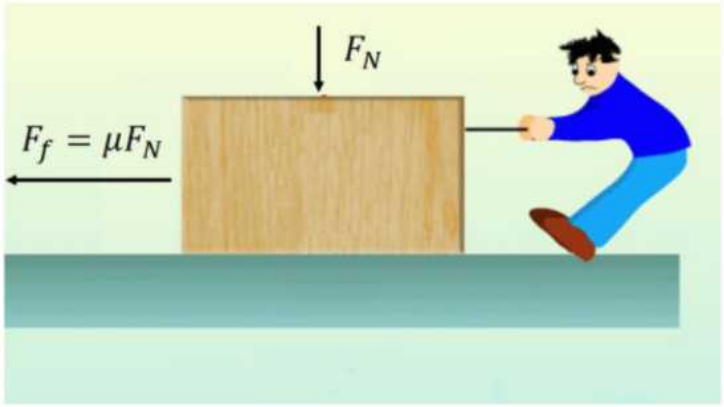
$$S = S_o + \alpha P, \text{ where } P = F_N / A_{\text{real}}$$

$$F_f = S_o A_{\text{real}} + \alpha F_N$$

$$\mu = \alpha + S_o / P$$

Friction: Amontonian v. Non-Amontonian

Amontonian Friction



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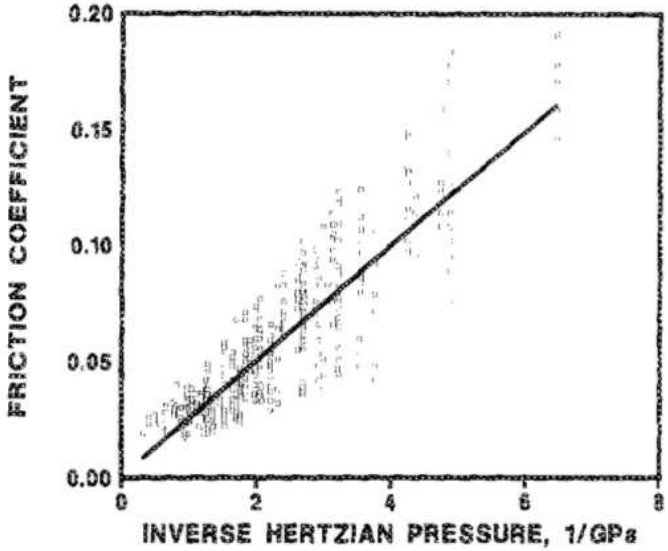


$$S = S_o + \alpha P, \text{ where } P = F_N / A_{\text{real}}$$

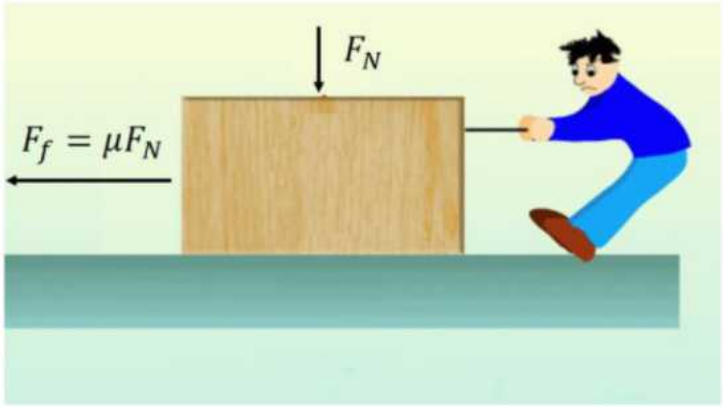
$$F_f = S_o A_{\text{real}} + \alpha F_N$$

$$\mu = \alpha + S_o / P$$

$$\approx \frac{S_o}{P} = S_o \pi \left(\frac{3R}{4E} \right)^{\frac{2}{3}} F_N^{-\frac{1}{3}}$$

Friction: Amontonian v. Non-Amontonian

Amontonian Friction



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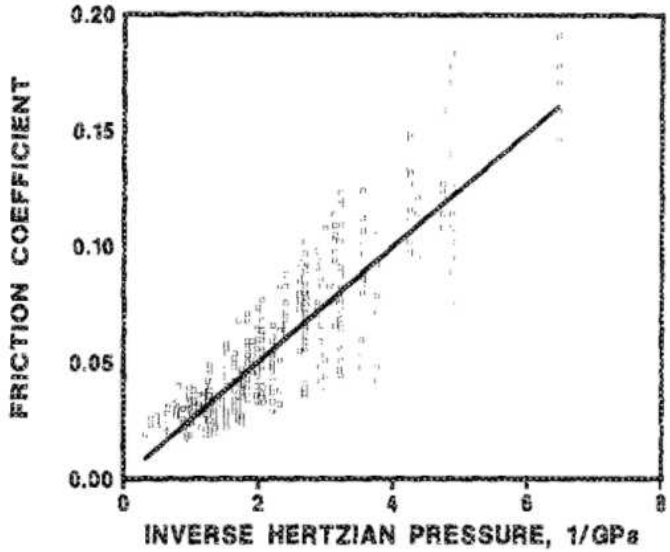

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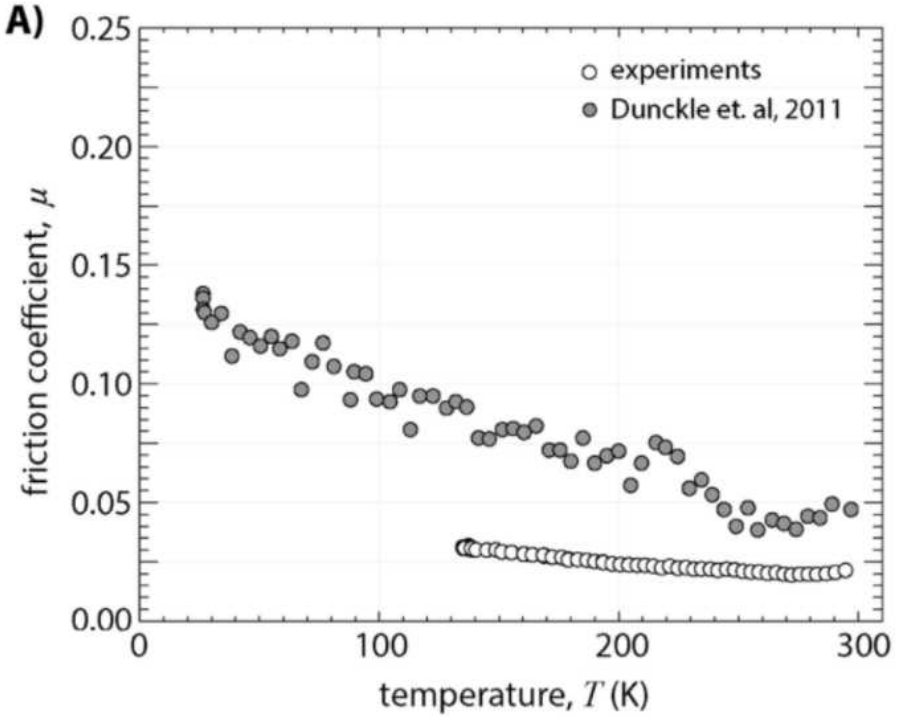
$$F_f = S_o A_{\text{real}} + \alpha F_N$$

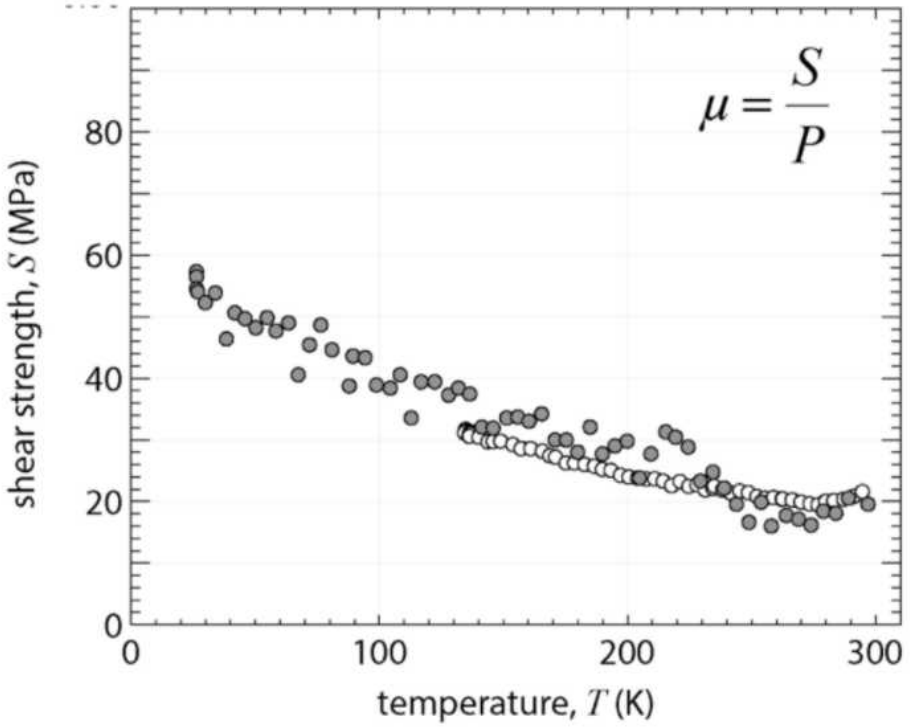
$$\mu = \alpha + S_o / P$$

$$\approx \frac{S_o}{P} = S_o \pi \left(\frac{3R}{4E} \right)^{\frac{2}{3}} F_N^{-\frac{1}{3}}$$

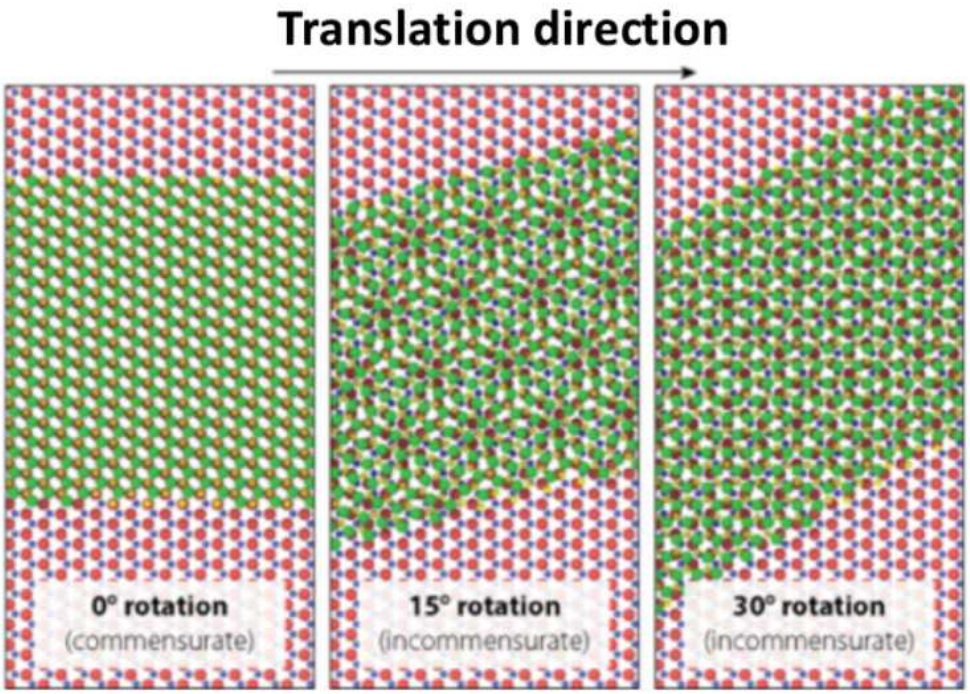
$$S_o = 25 \text{ MPa}$$

T-dependence $\mu = \mu(T, P)$ and $S = S(T)$ via MoS_2 Friction Experiments





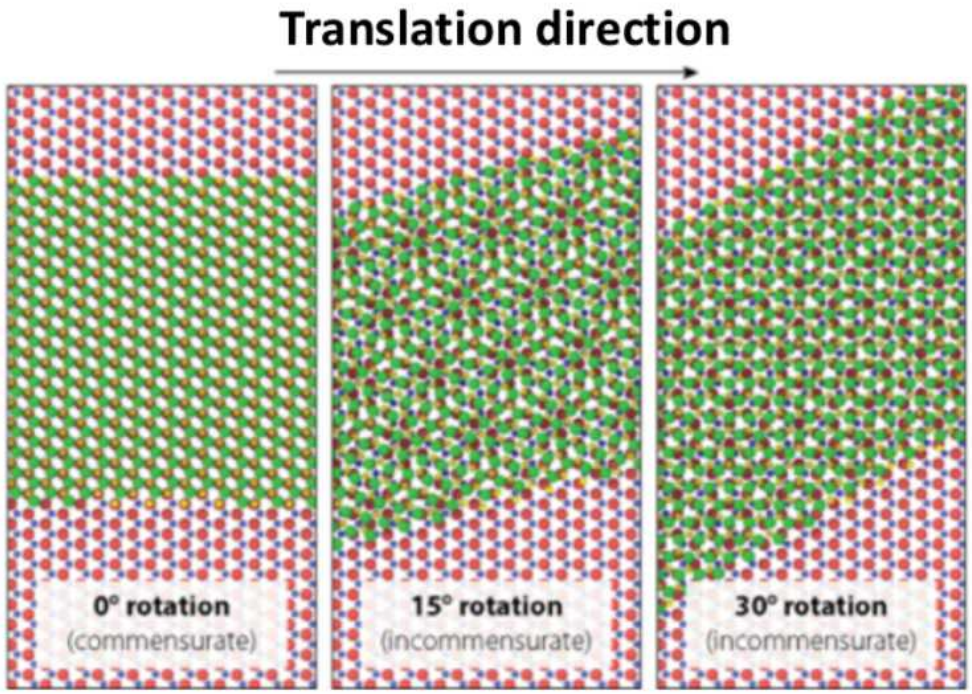
Nudged Elastic Band Calculations and Commensurate Sliding



commensurate
egg shell

incommensurate
egg shell

Nudged Elastic Band Calculations and Commensurate Sliding



commensurate
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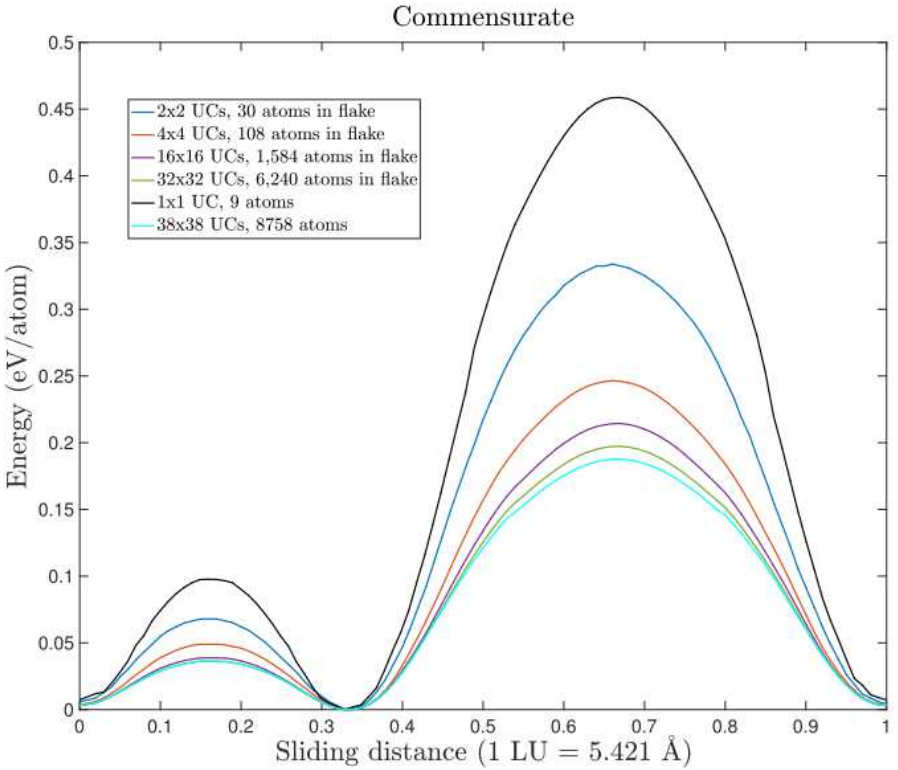
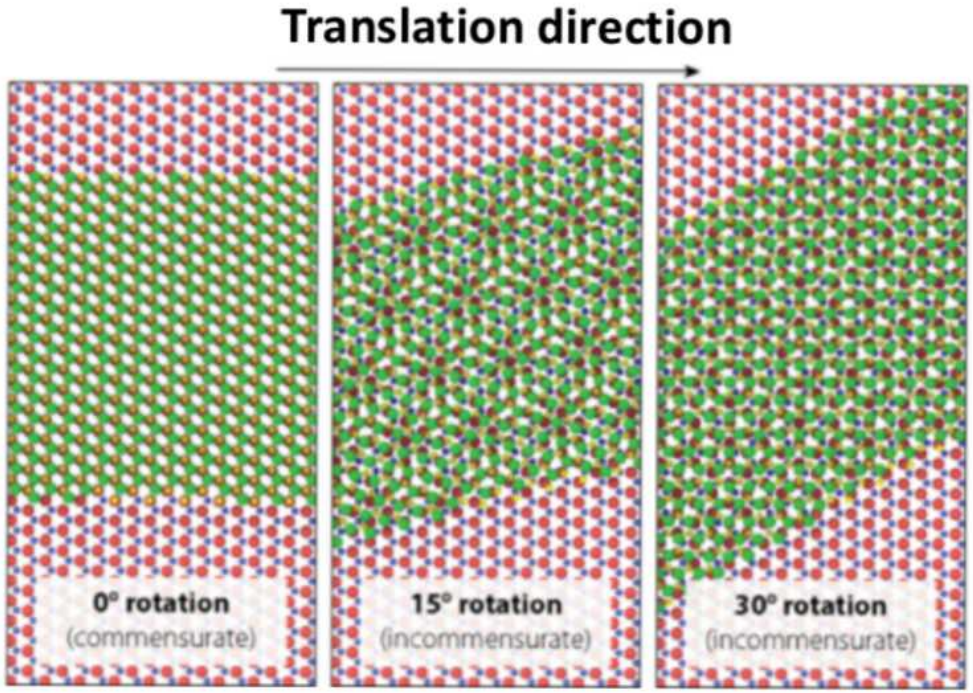
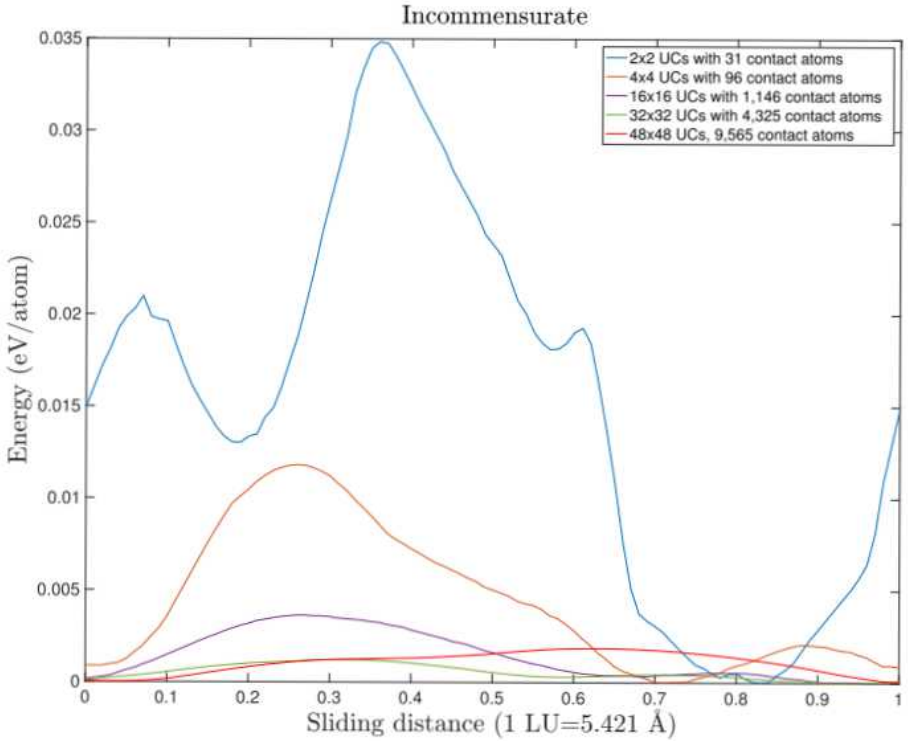


Rotation Barrier





commensurate
egg shell

incommensurate
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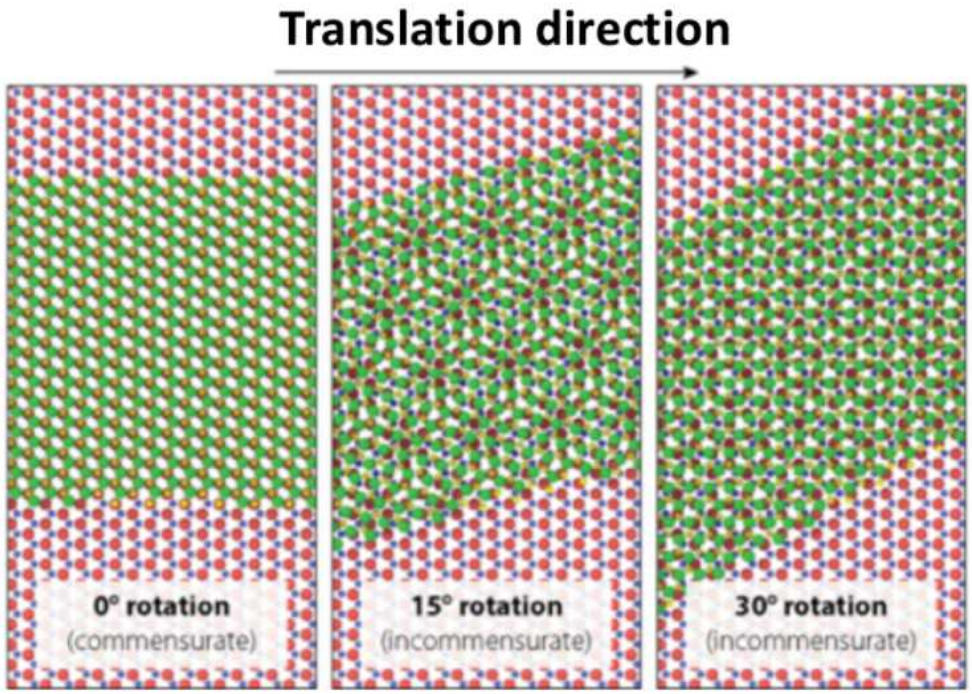
Incommensurate Barrier



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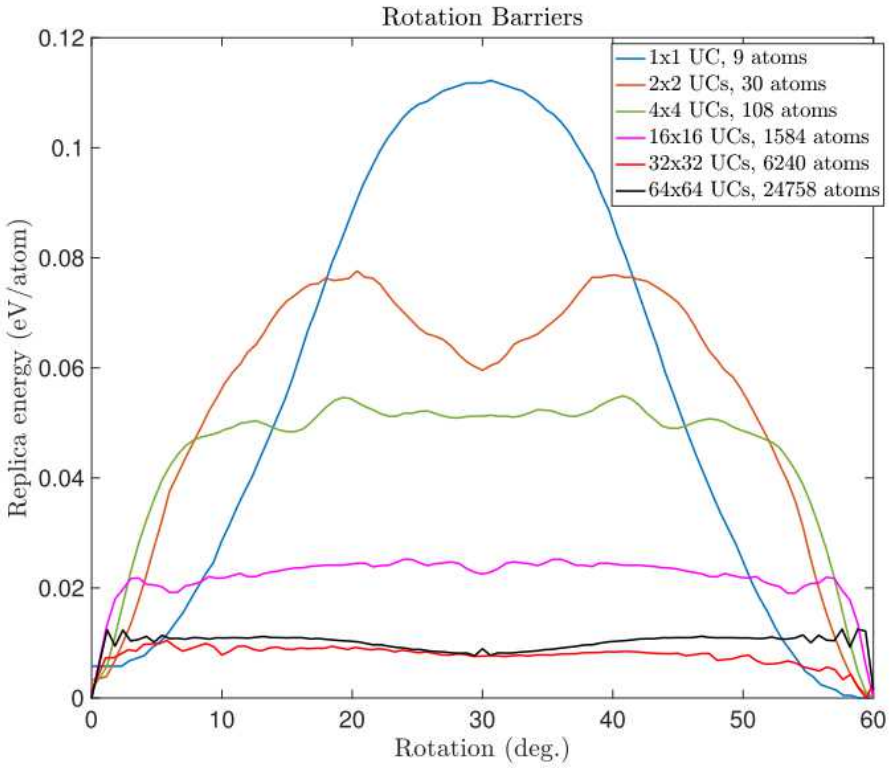
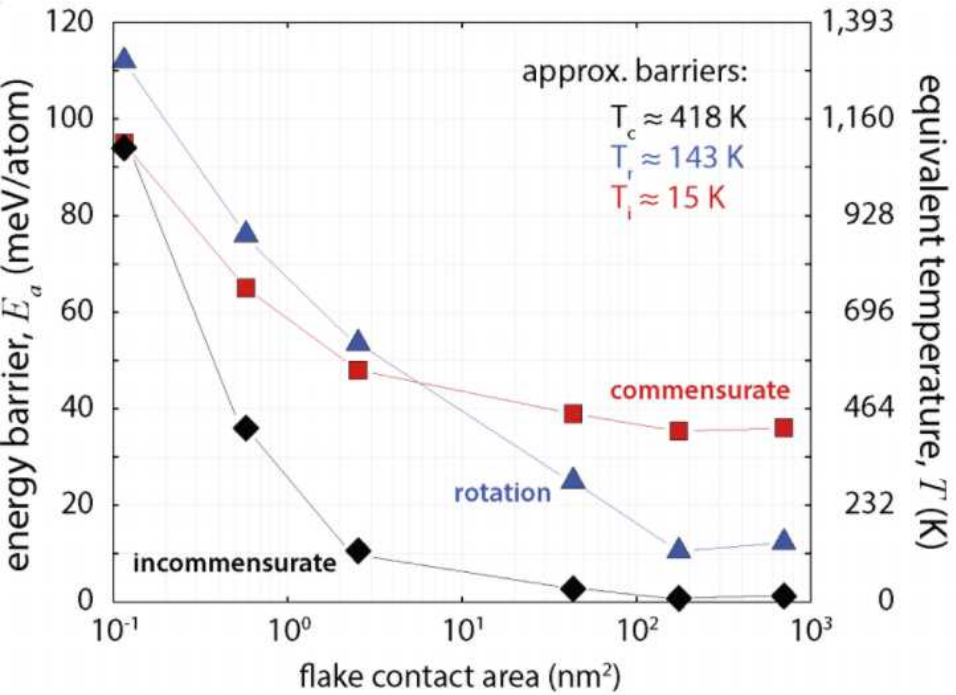


A Toy Model in terms of energy barriers (mechanisms to sliding)



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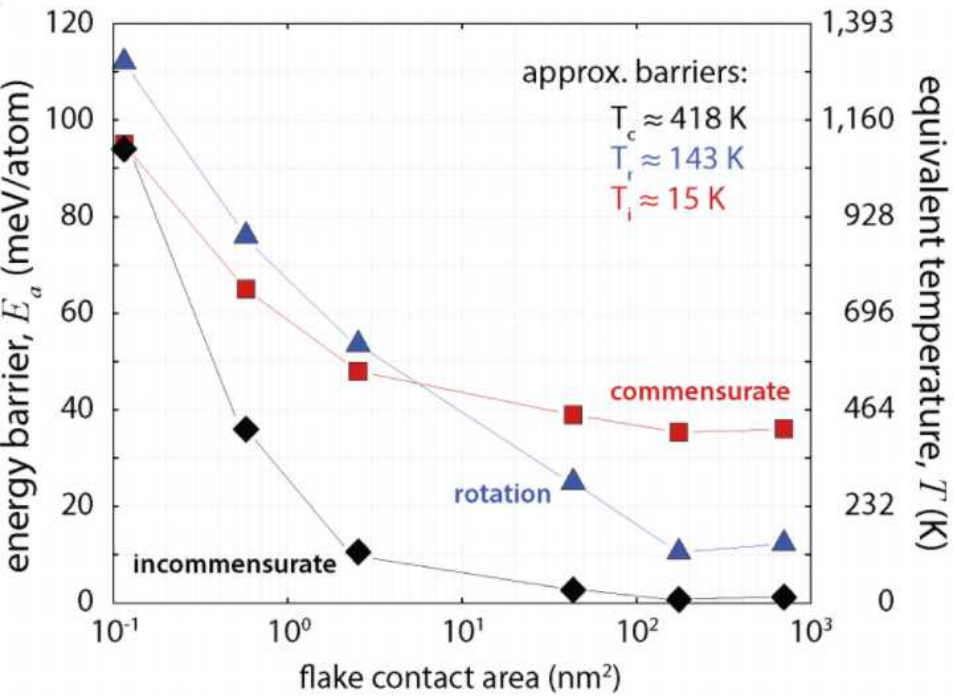


The probability and failure to overcome a barrier n

$$p_n = A \exp\left(\frac{-\Delta E_n}{k_B T}\right)$$

$$f_n = 1 - p_n$$

The probability to slide and fail to slide (friction):

$$p_{slide} = p_r p_i + f_r p_c$$

$$f_{slide} = 1 - p_{slide}$$

$$= 1 - (p_r p_i + f_r p_c)$$

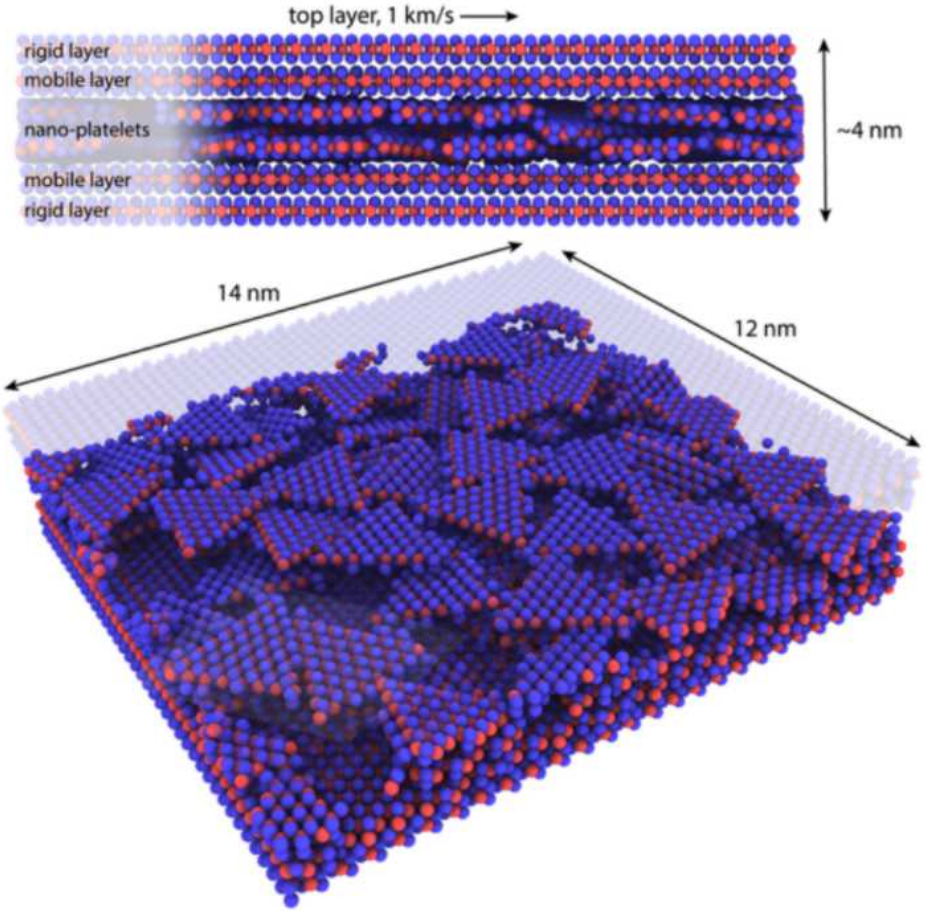
The model and scaled data from $S(T) = S_L f_{slide}(T)$

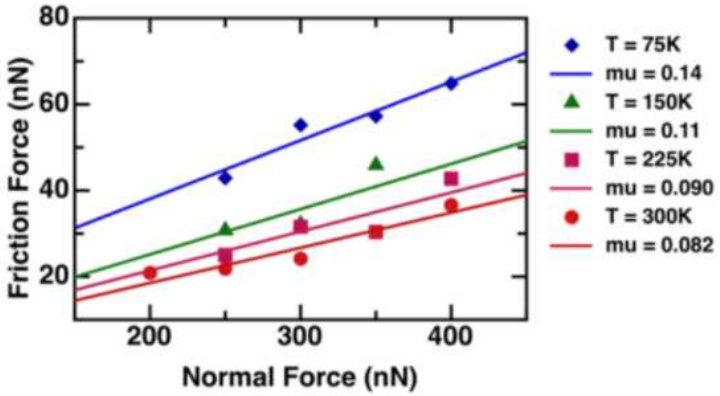
$$S(T) = S_L f_{slide}(T)$$

$$S(T) = S_L \left(1 - \exp\left(-\frac{\Delta E_i + \Delta E_r}{k_B T}\right) - \exp\left(-\frac{\Delta E_c}{k_B T}\right) + \exp\left(-\frac{\Delta E_r + \Delta E_c}{k_B T}\right)\right)$$

What is S_L?

MD ReaxFF Simulations

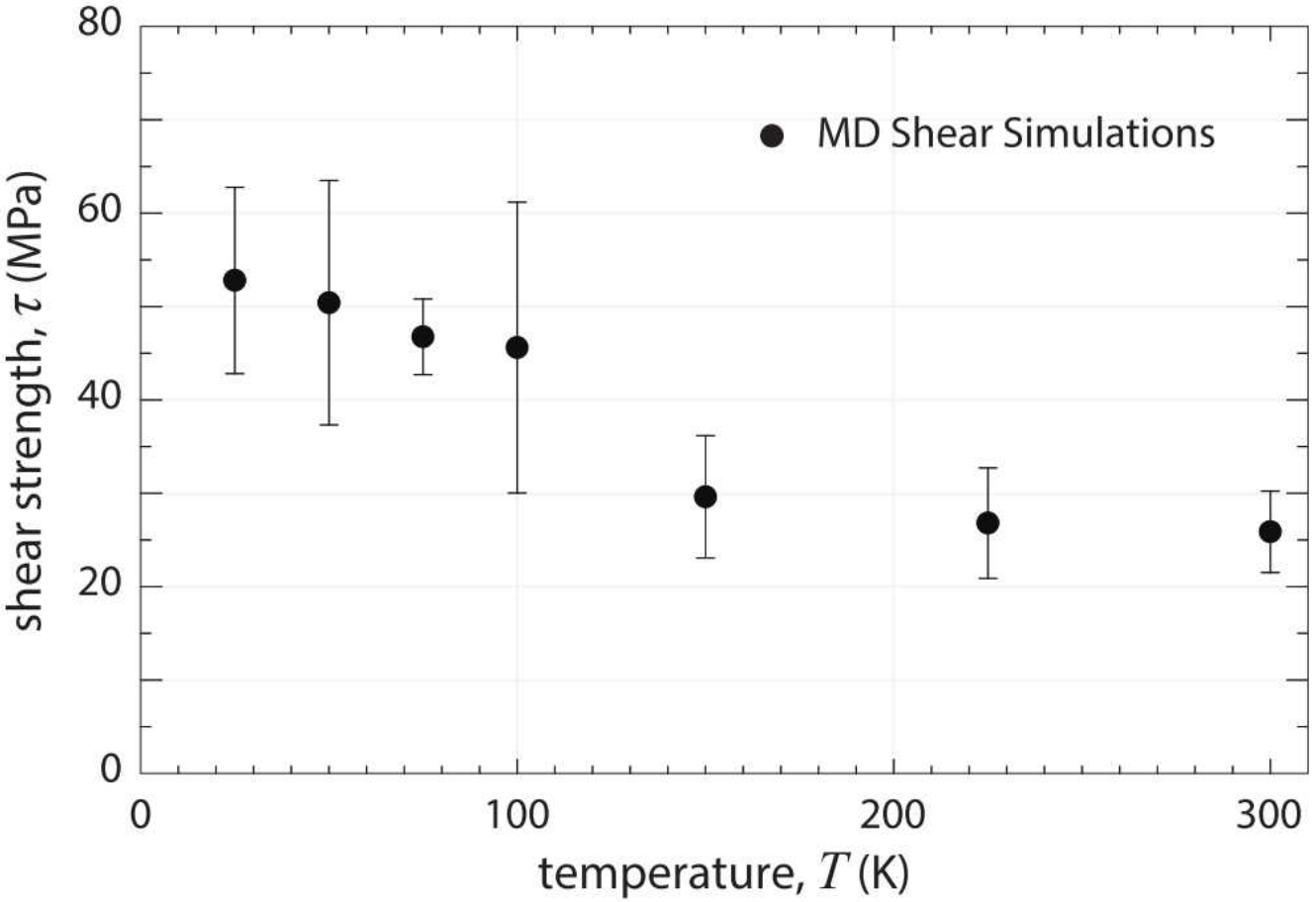




- Six normal forces used at each temperature
- $\mu = \frac{\mathrm{d}F_f}{\mathrm{d}F_N}$
- Data set of $S(T)$ from MD simulations

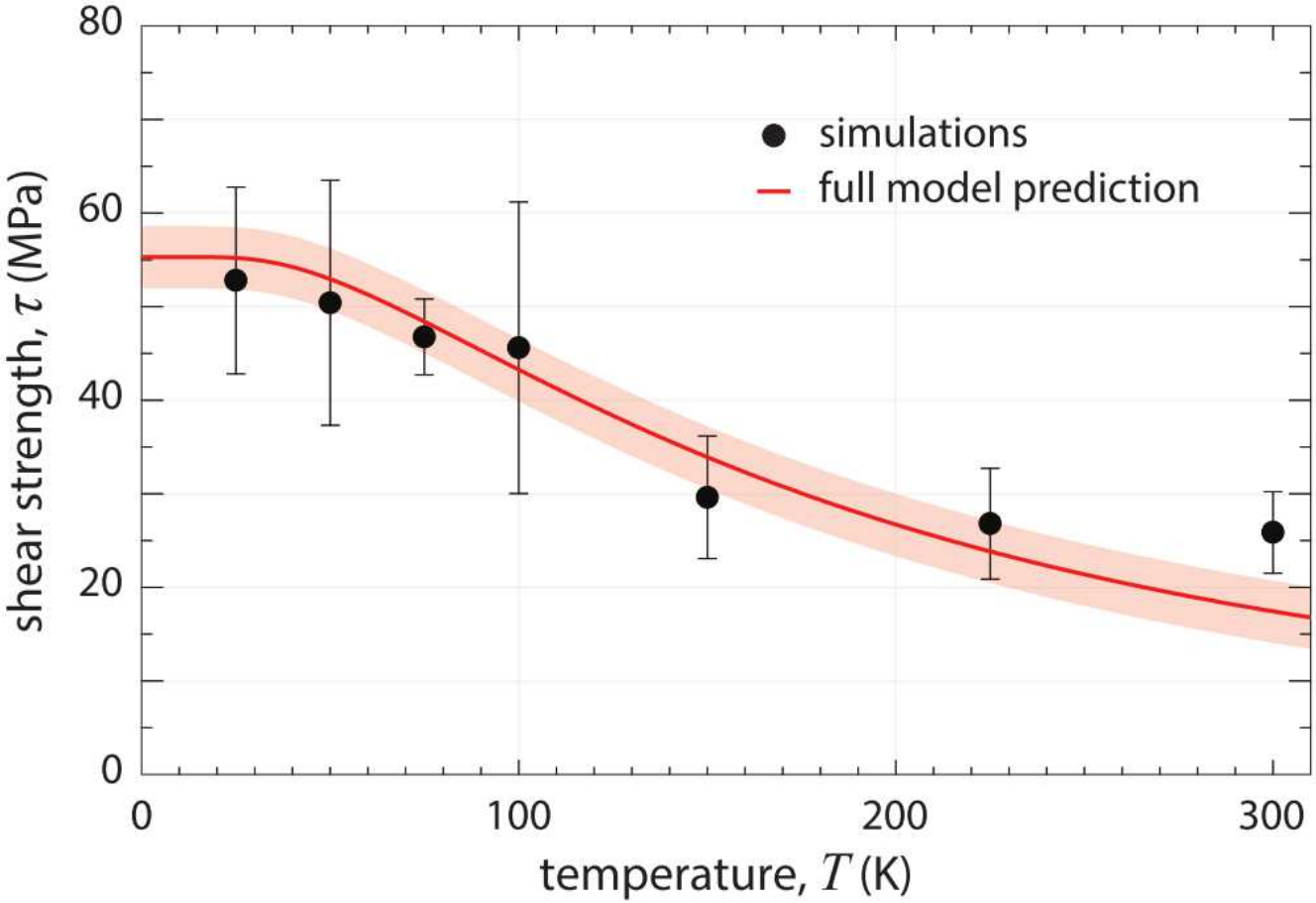
The model and data from $S(T) = S_L f_{slide}(T)$

$$S(T) = S_L \left(1 - \exp\left(-\frac{\Delta E_i + \Delta E_r}{k_B T}\right) - \exp\left(-\frac{\Delta E_c}{k_B T}\right) + \exp\left(-\frac{\Delta E_r + \Delta E_c}{k_B T}\right)\right)$$



The model and data from $S(T) = S_L f_{slide}(T)$

$$S_L = 55.3 \text{ MPa}$$



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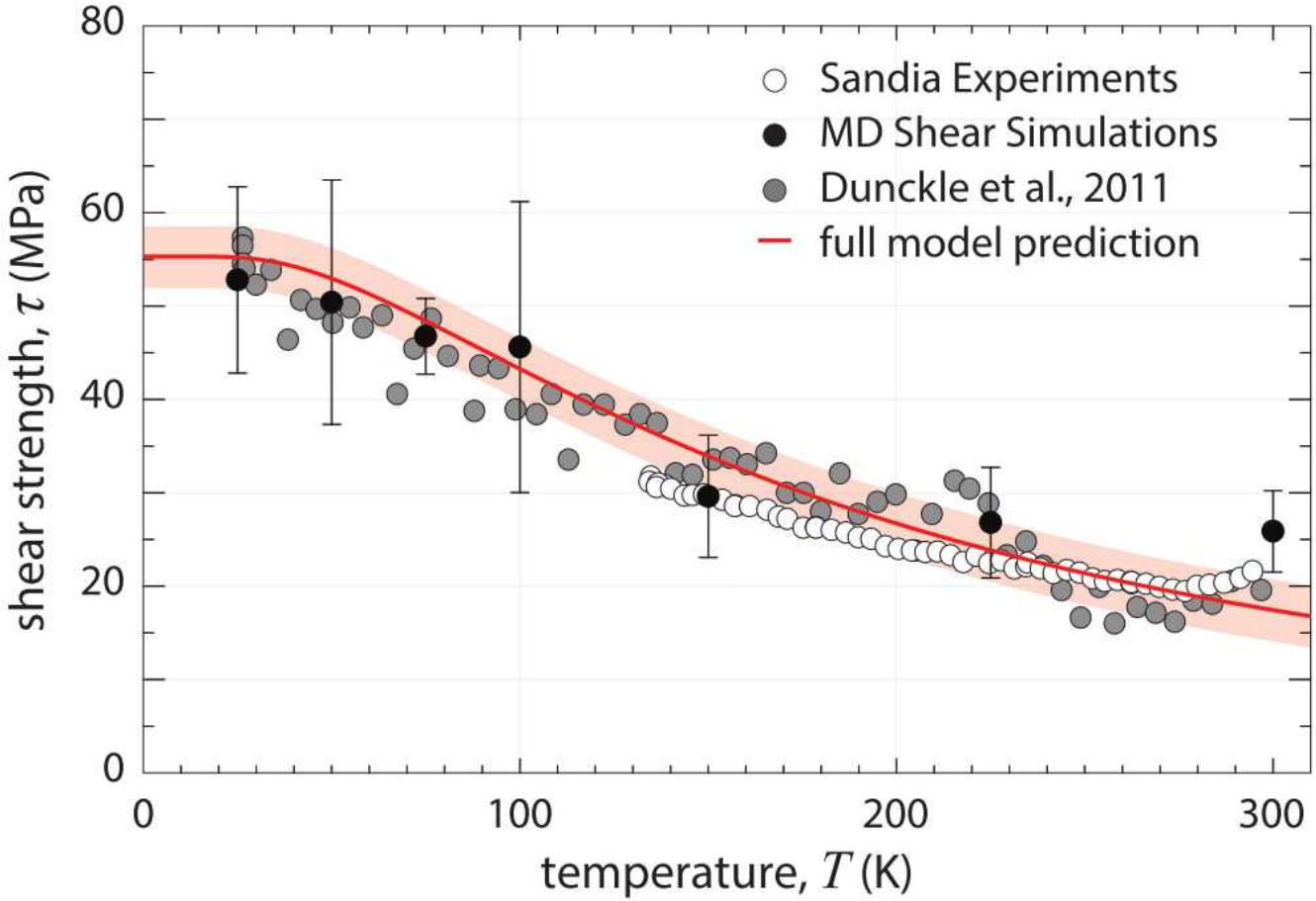
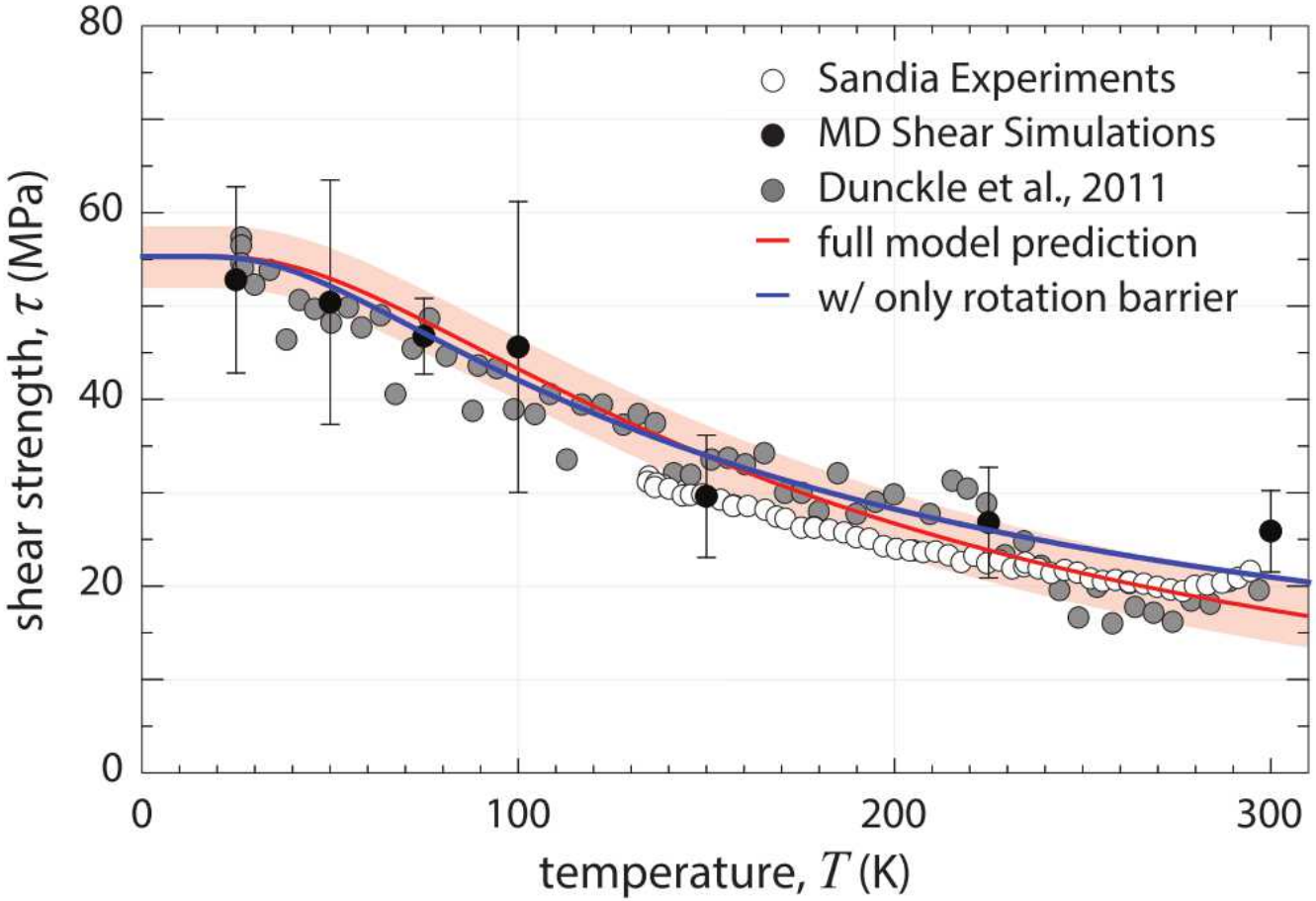


The model and data from $S(T) = S_L f_{slide}(T)$

$$S(T) = S_L \left(1 - \exp\left(-\frac{\Delta E_r}{k_B T}\right)\right)$$



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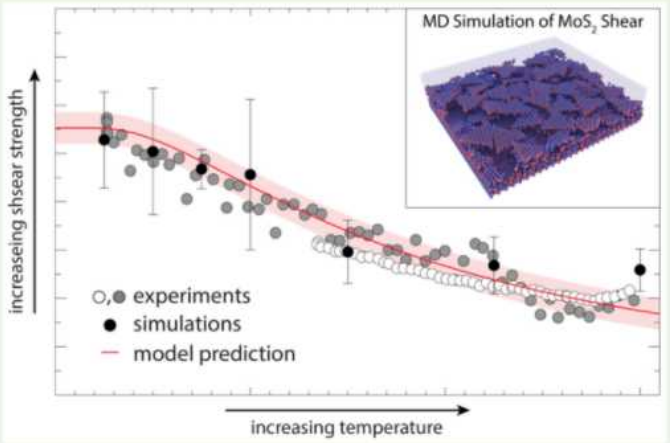
Atomistic Origins of Temperature-Dependent Shear Strength in 2D Materials

John F. Curry,[†,‡] Adam R. Hinkle,[†,‡] Tomas F. Babuska,[†,§] Mark A. Wilson,[†] Michael T. Dugger,[†] Brandon A. Krick,[§] Nicolas Argibay,[*,†] and Michael Chandross[*,†]

[†]Material, Physical and Chemical Sciences Center, Sandia National Laboratories, Albuquerque, New Mexico 87123, United States
[§]Department of Mechanical Engineering & Mechanics, Lehigh University, Bethlehem, Pennsylvania 18015, United States

ABSTRACT: We present a model that predicts the macroscale temperature-dependent interfacial shear strength of 2D materials like MoS_2 based on atomistic mechanisms and energetic barriers to sliding. Atomistic simulations were used to systematically determine the lamellar size-dependent rotation and translation energy barriers, that were used to accurately predict a broad range of experimental data. This framework provides insight about the origins of characteristic shear strengths of 2D materials.



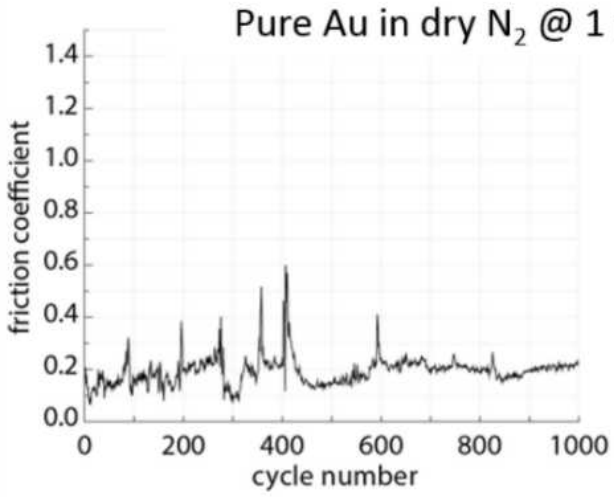
KEYWORDS: *2D materials, MoS_2, molybdenum disulfide, nudged elastic band, superlubricity, molecular dynamics, activation energy, temperature*

Acknowledgements

- Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

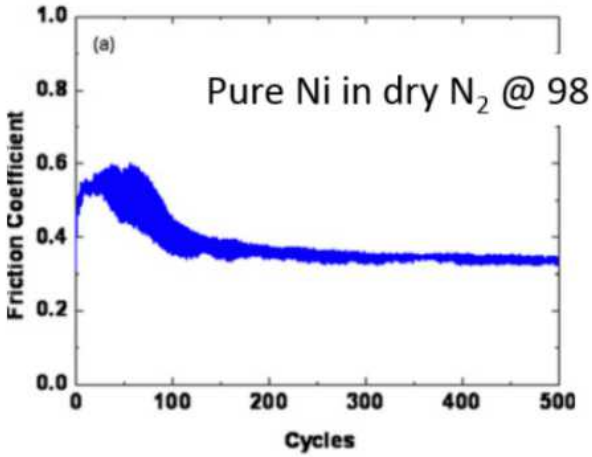
- James Batteas, Texas A&M, Karin Dahmen, UIUC

Evidence of low friction in soft, bare, pure metals

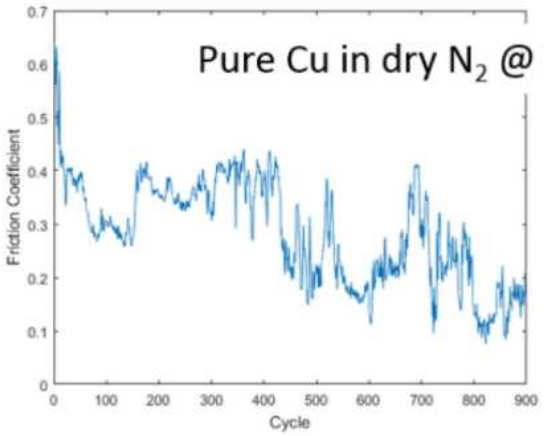


"when surfaces are cleaned in a good vacuum, the sliding friction... becomes vanishingly small." Bowden & Hughes, *Nature* 1938.

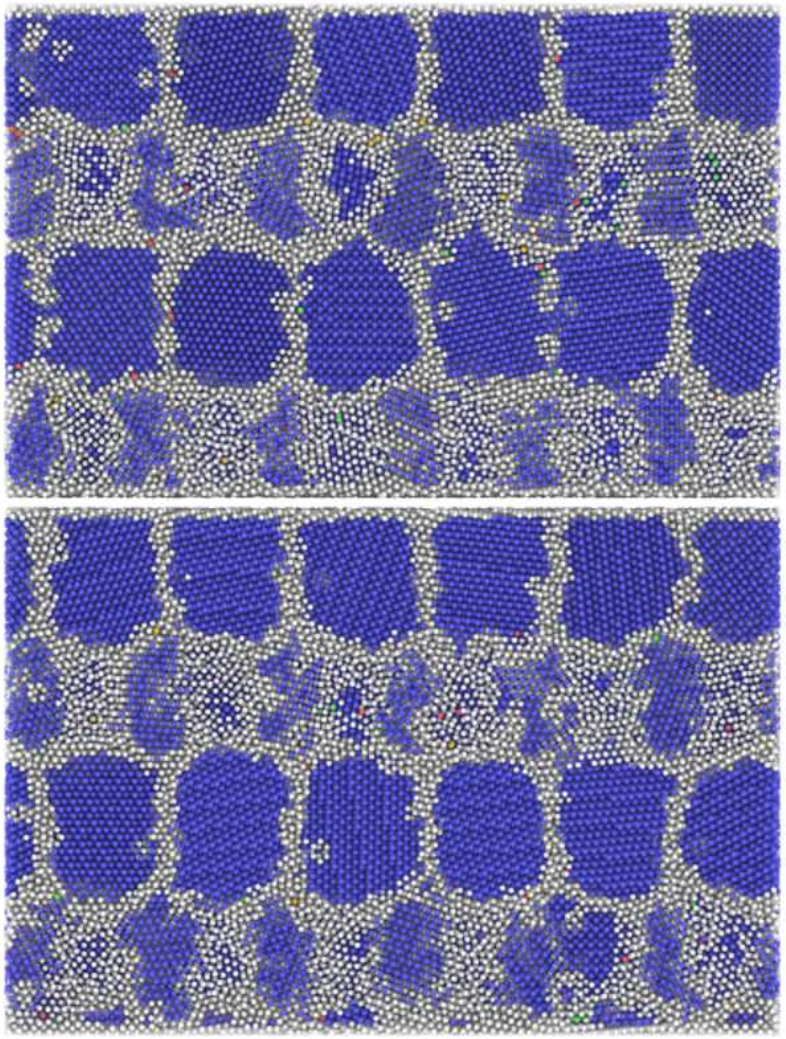
"It was found quite unexpectedly that with some metals, very low friction less than 0.10 was observed." Tamai, *J. Appl. Phys*. 1961

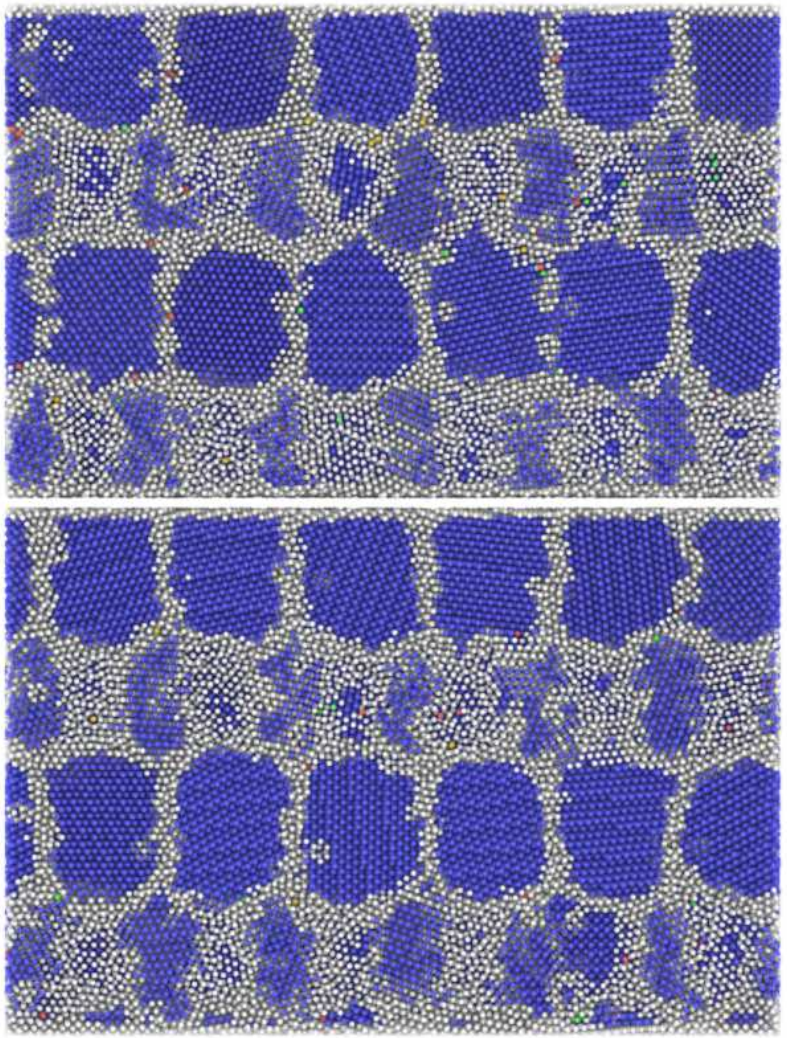


Prasad, *Scripta Mat.* 2011

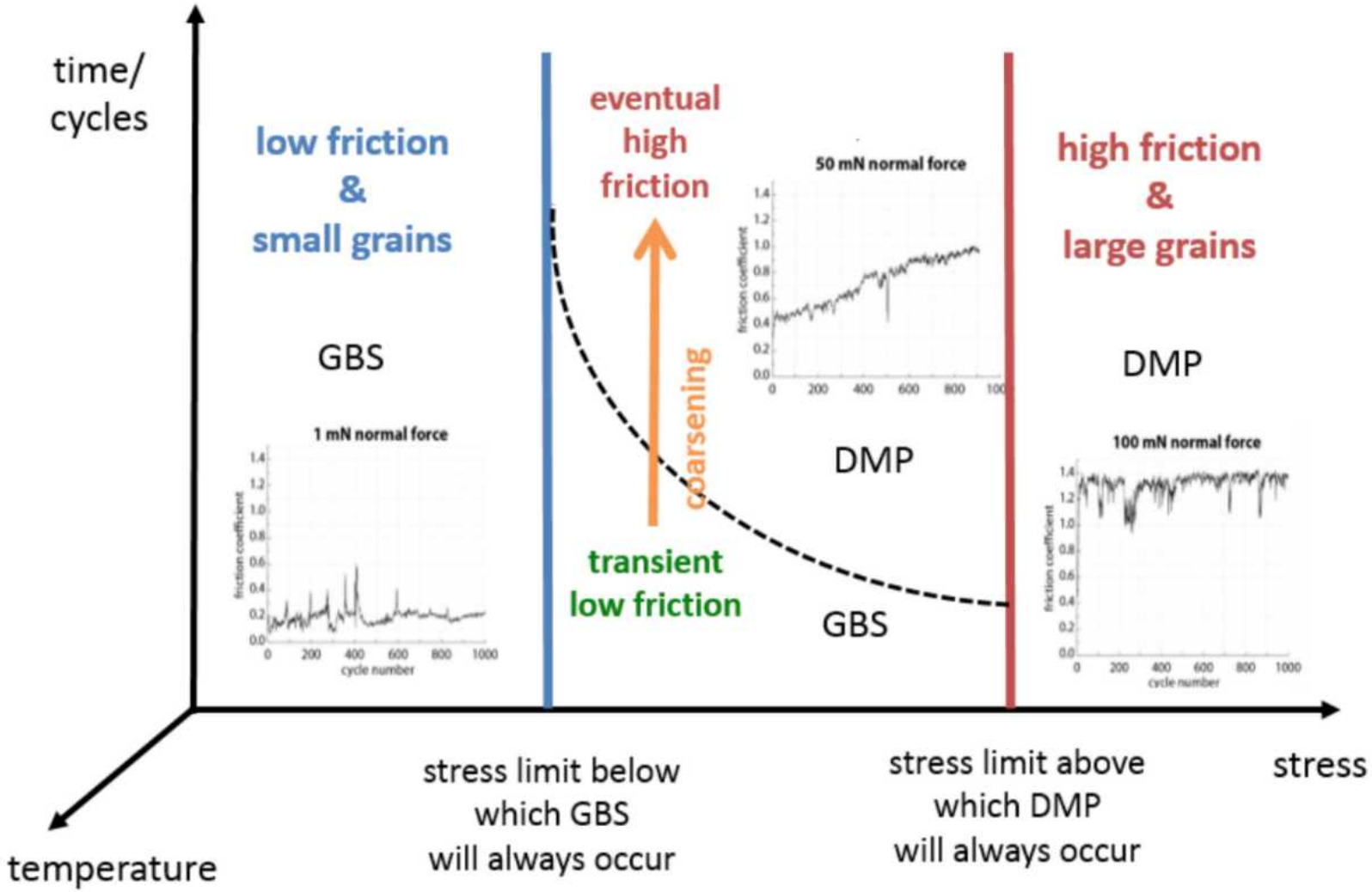


Sliding friction of BCC Tantalum slabs





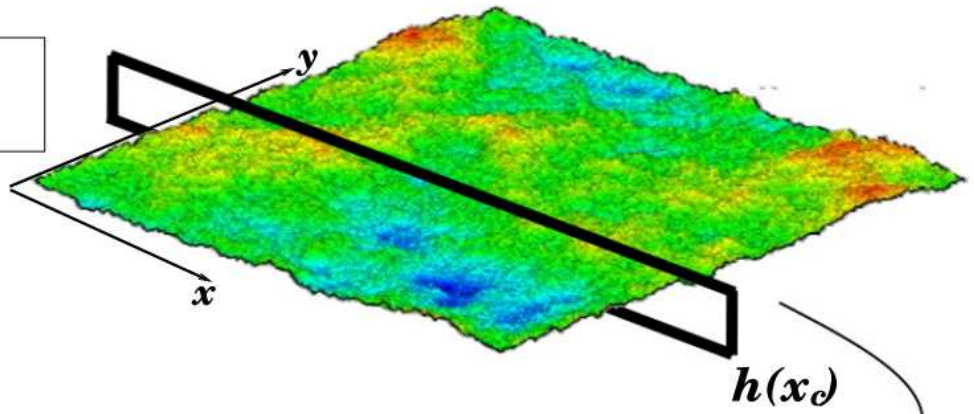
Generalized friction map for (FCC) metals J. Mater. Sci. 52:2780 (2017)

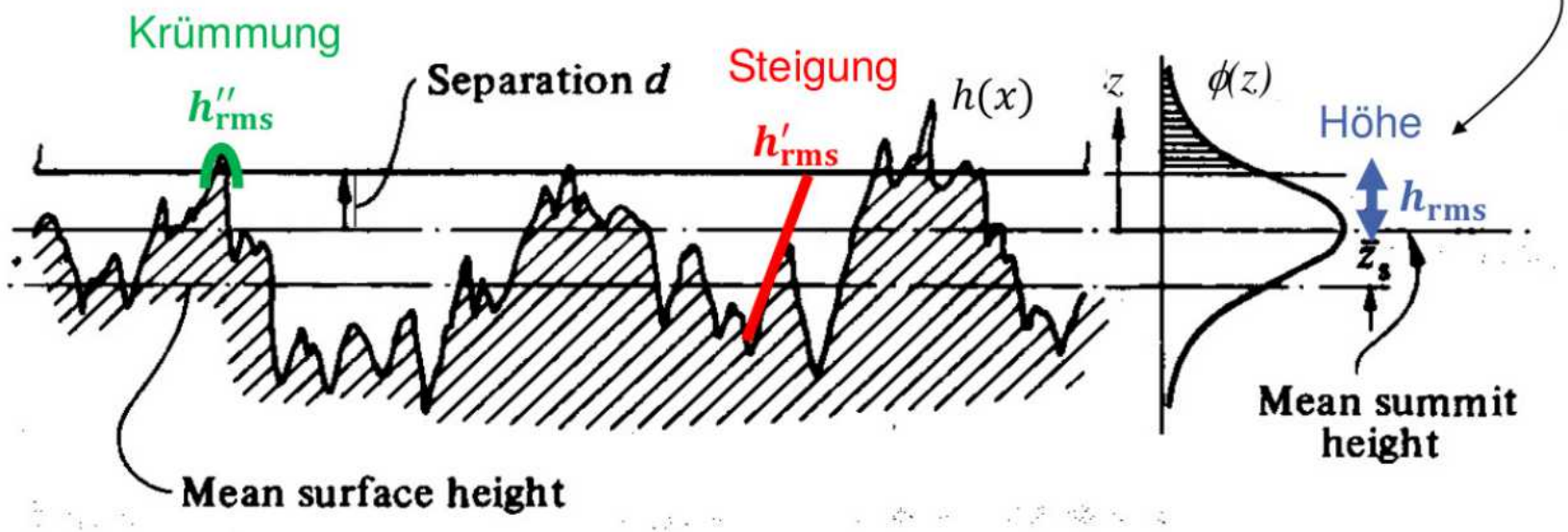


Part 2: Fractals

Surface topography and roughness

Height Profile $h(x,y)$





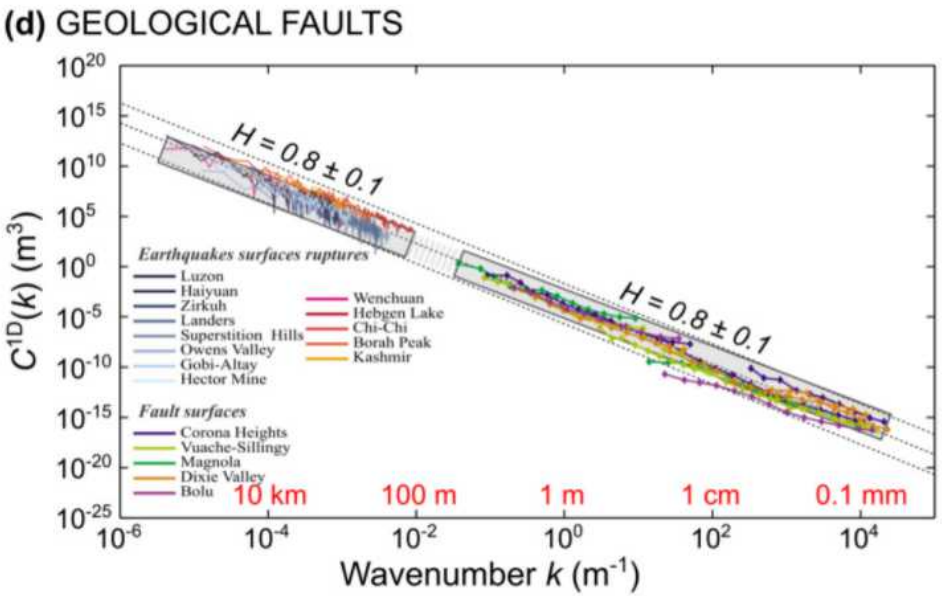
$$h''_{rms} = \frac{1}{2}\sqrt{\langle(\nabla^2 h)^2\rangle} \qquad h'_{rms} = \sqrt{\langle|\nabla h|^2\rangle} \qquad h_{rms} = \sqrt{\langle h^2\rangle}$$

Greenwood, Williamson, *Proc. Roy. Soc. Lond. A* 295, 300 (1966)

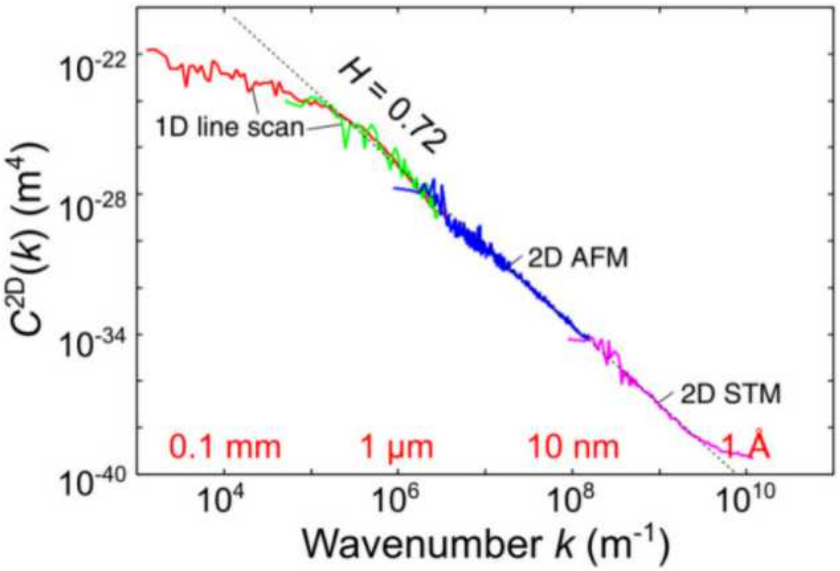
Self-affine system

$$C(\boldsymbol{q}) = \frac{1}{(2\pi)^2} \int d^2x \ \langle h(\boldsymbol{x}), h(\boldsymbol{x} + \delta\boldsymbol{x}) \rangle e^{-i\boldsymbol{x}\cdot\boldsymbol{q}}$$

$C(q) \sim q^{-2(1+H)}$ where H ranges from 0 - 1



T. Candela et al., J. Geophys. Res. Solid Earth 117, 1 (2012)

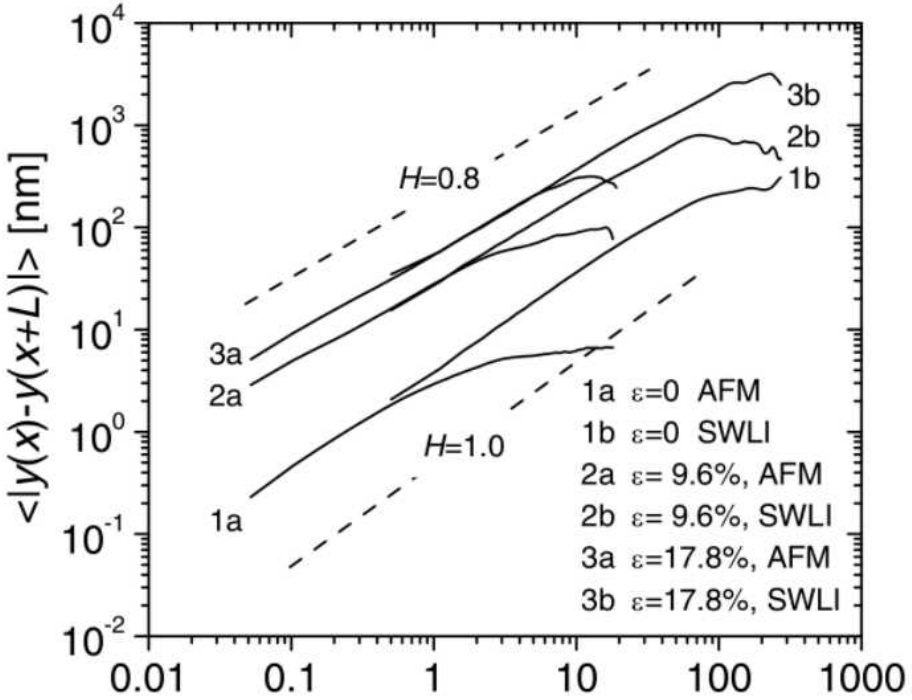


B.N.J. Persson, Tribol. Lett. 54, 99 (2014)

A common origin in plastic deformation? Quantify?

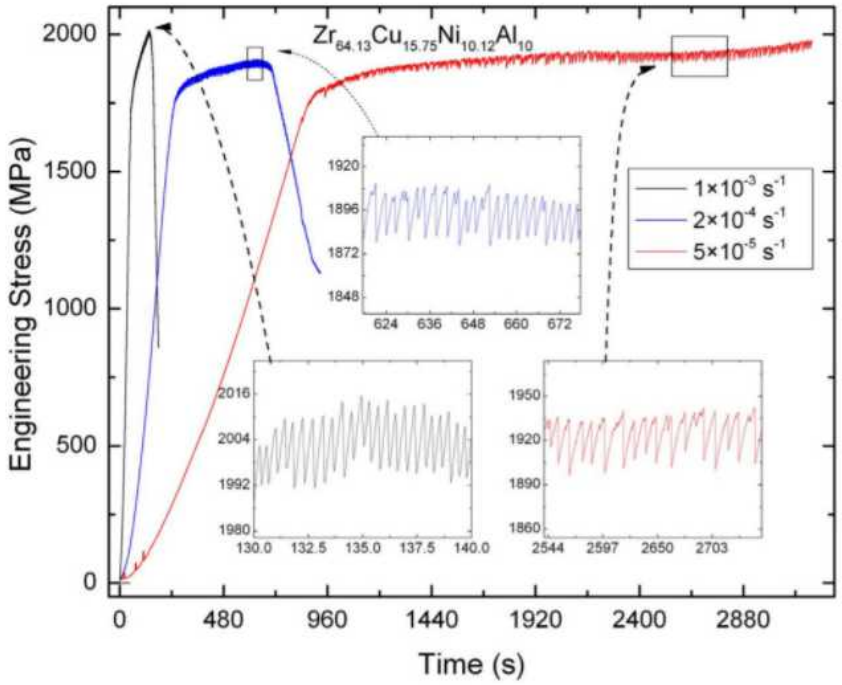
Plasticy and self-affine scaling

Experiments of polycrystalline Cu and single–crystal KCl



M. Zaiser et al. Phy. Rev. Lett. 93 (2004)
J. Schwerdtfeger et al., J. Stat. Mech. (2007) L04001

Experiments of metallic glasses



Antonaglia, J. et. al. Sci. Rep. 4, 4382(2014)

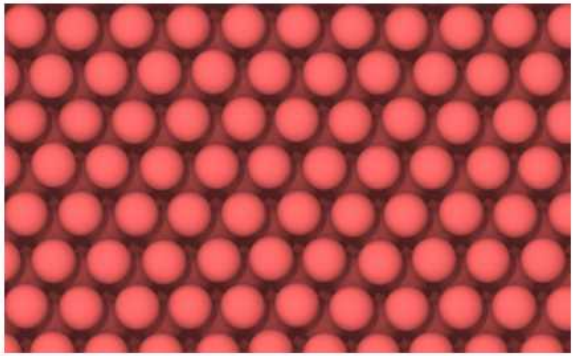
1D ONLY

NO ATOMISTIC STUDIES

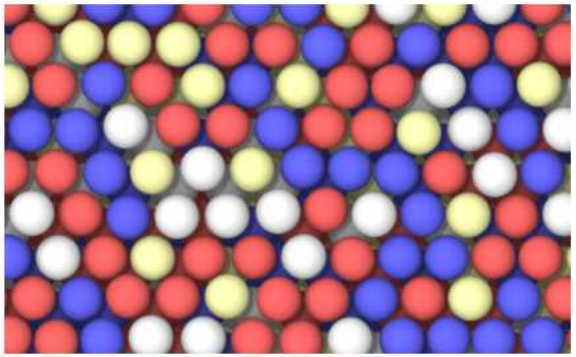
NO ATOMISTICS OF ROUGHNESS & SELF AFF.

NO EXPERIMENTS OF ROUGHNESS & SELF AFF.

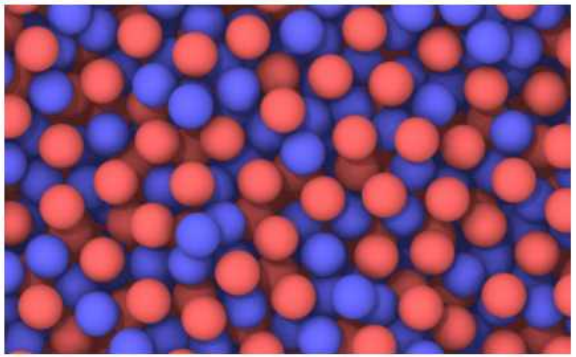
Bi-axial compression of Au(111), H.E. Alloy, and CuZr glass



Au



NiCoFeTi



CuZr

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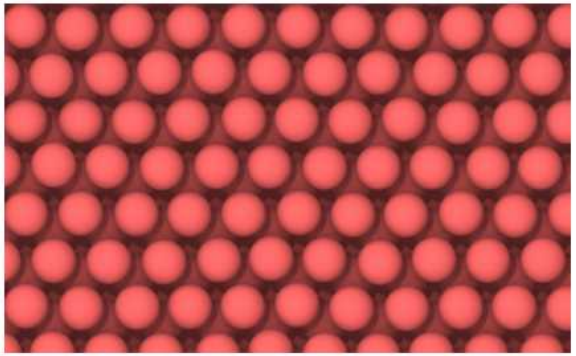
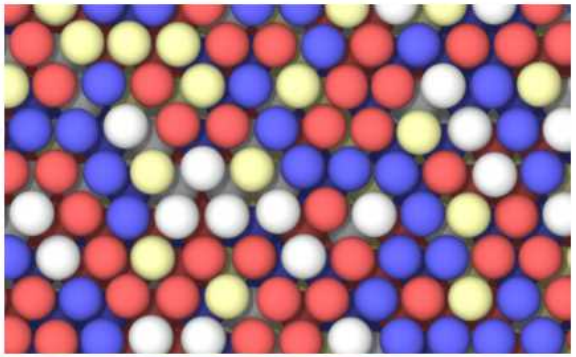


Au



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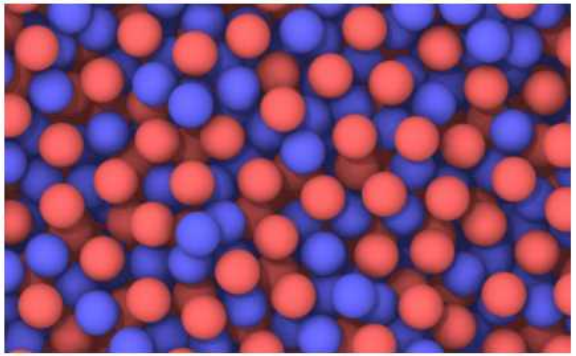
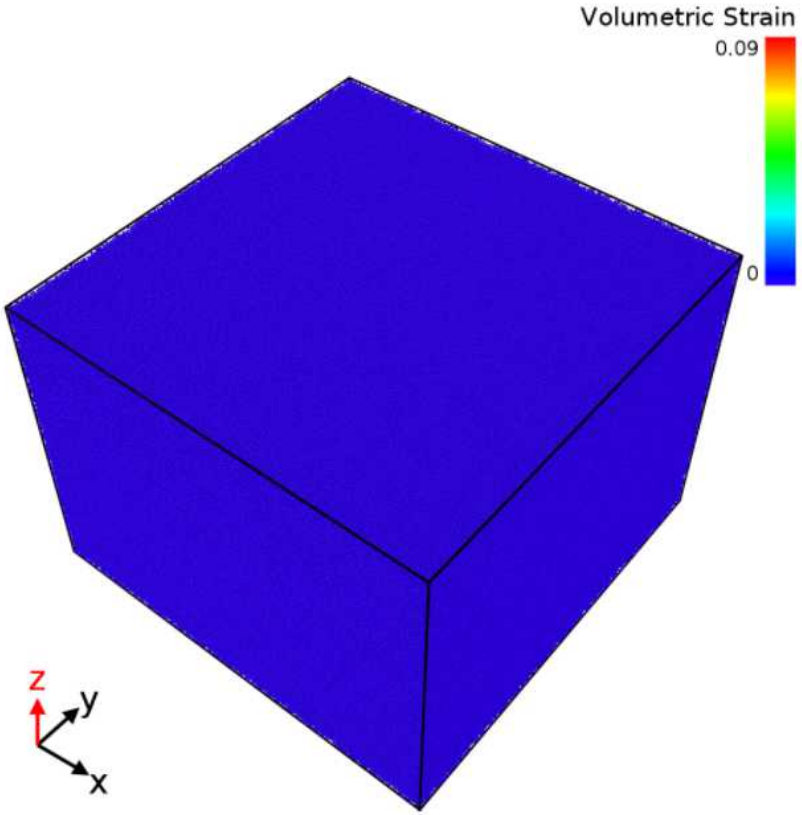
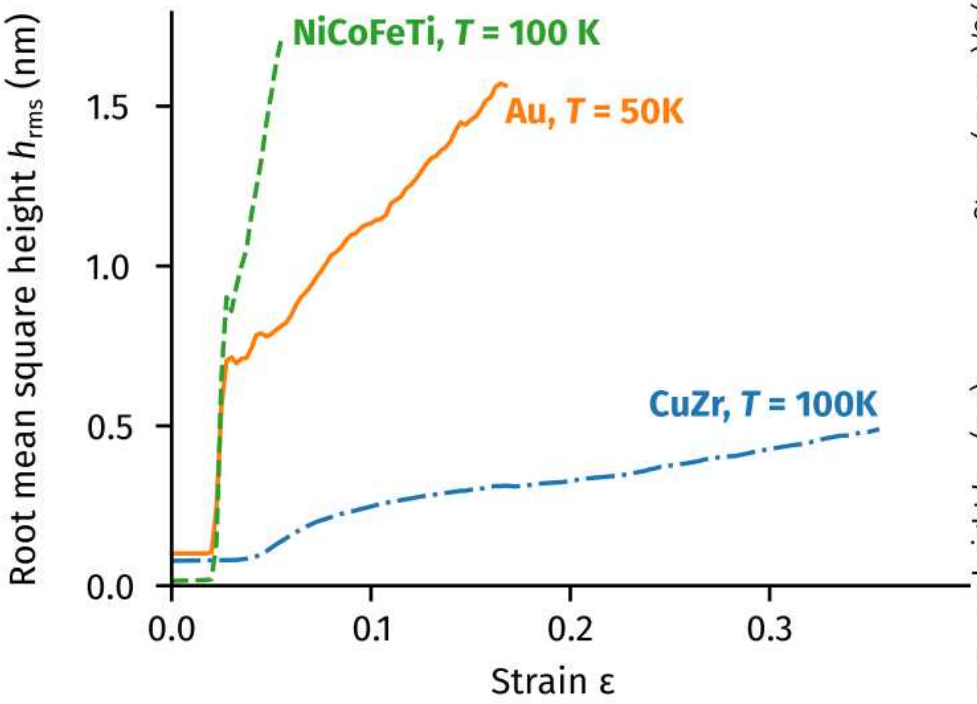


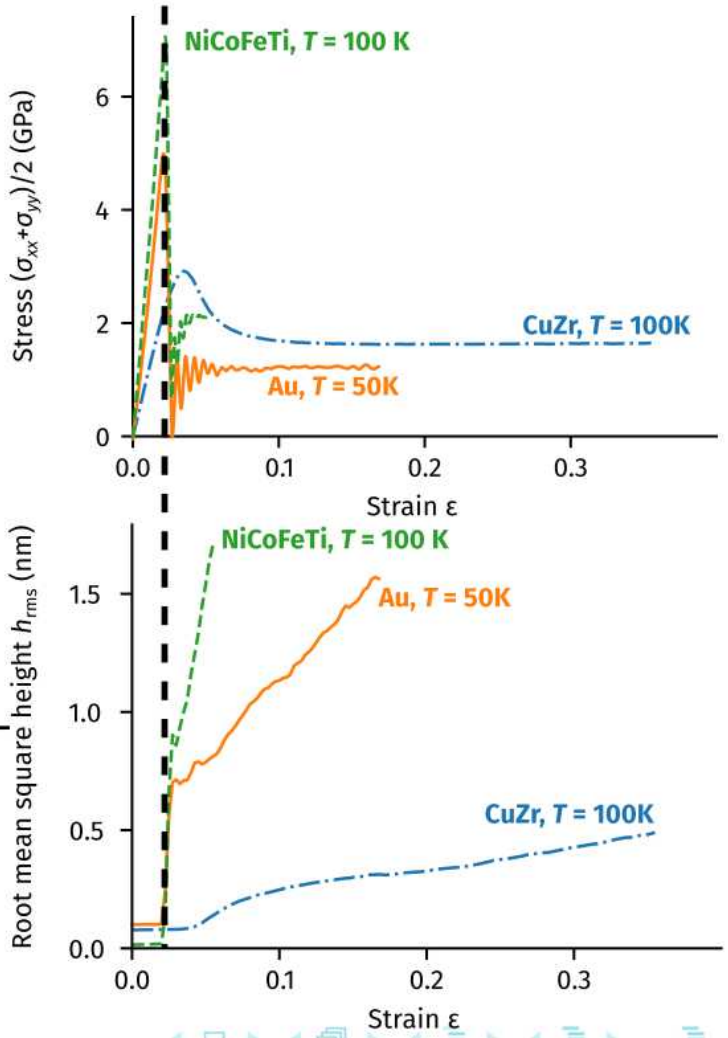
CuZr

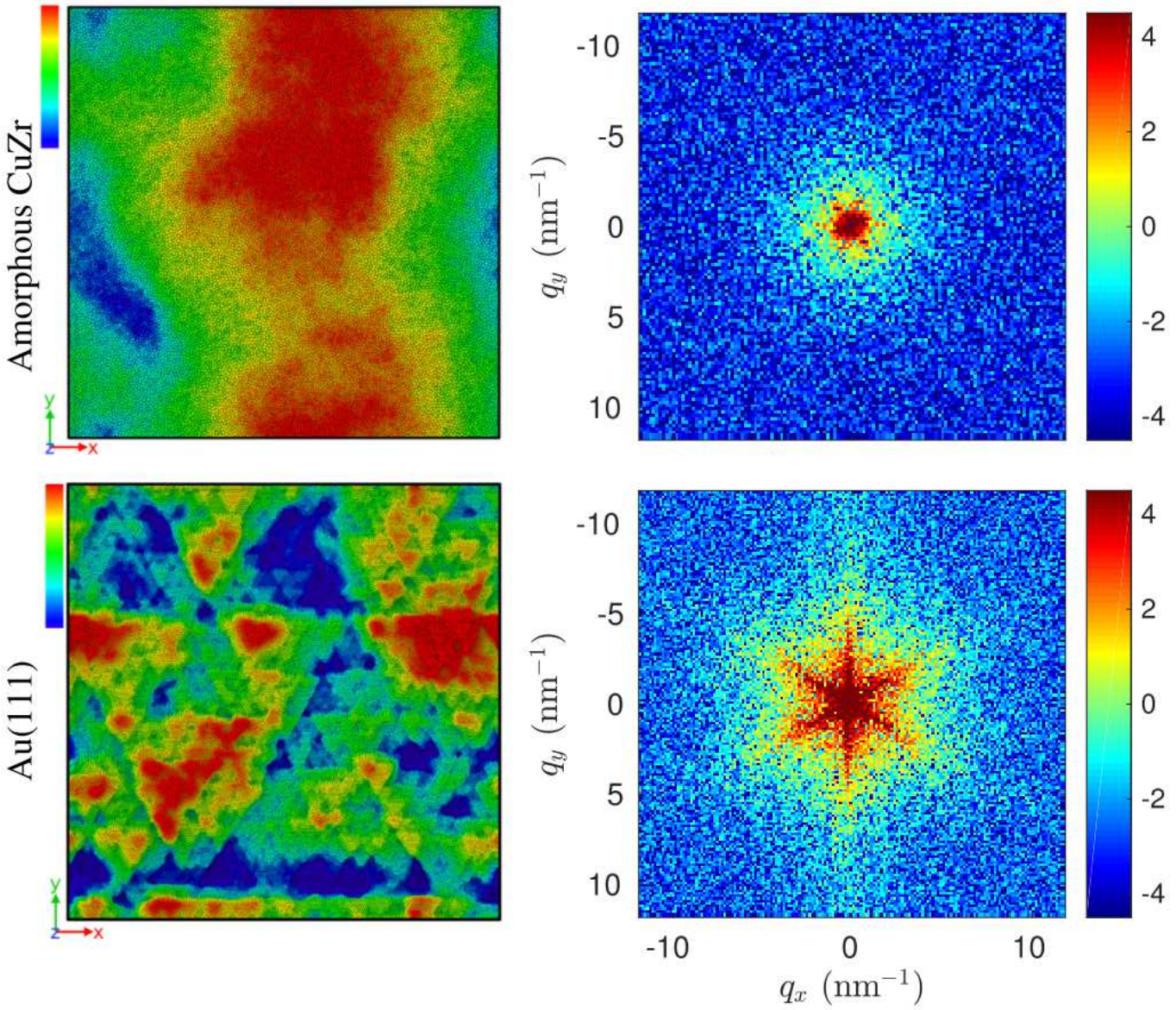


Root-mean square height

$$h_{\mathrm{rms}} = \sqrt{\frac{1}{mn}\sum_{i=1}^{n}\sum_{j=1}^{m}\left(z(x_i, y_i) - \mu\right)^2}$$

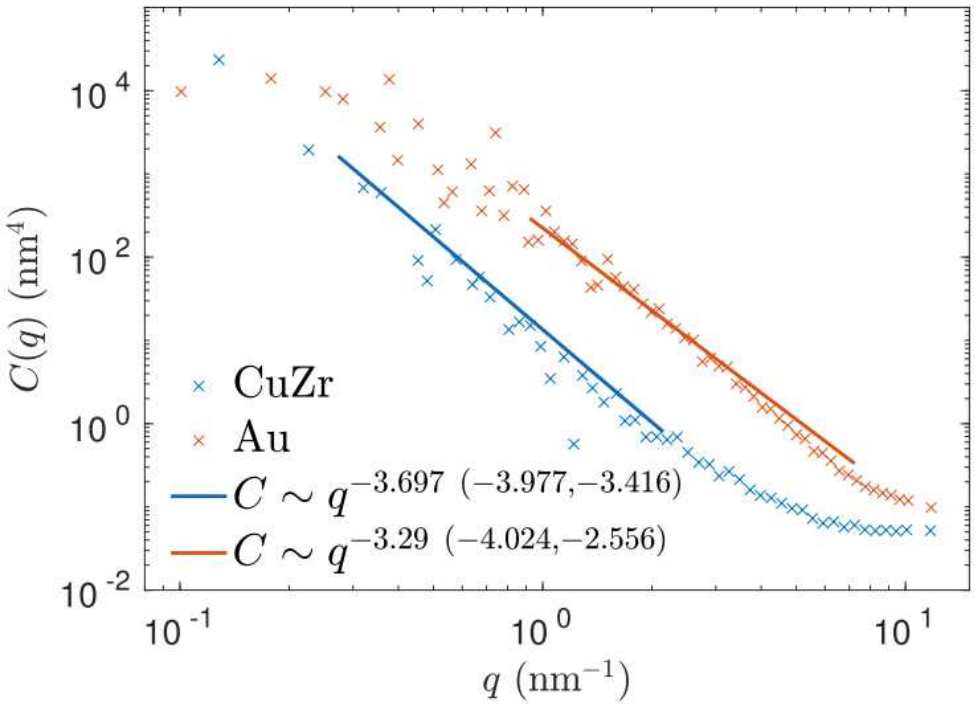


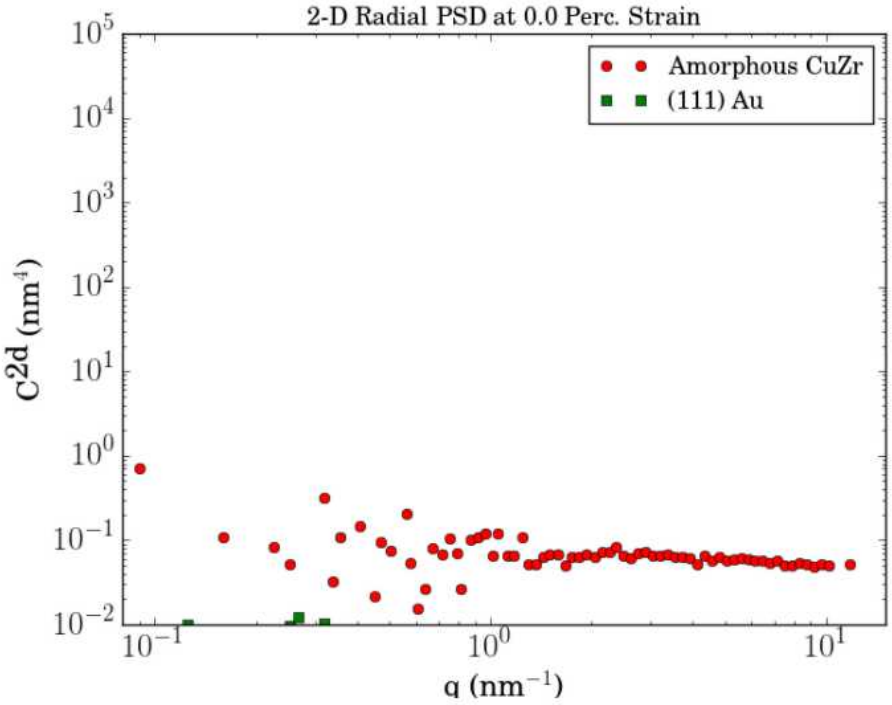



Amorphous CuZr
Au(111)
y
z
x
-10
-5
0
5
10
q_y (nm^{-1})
q_x (nm^{-1})
4
2
0
-2
-4

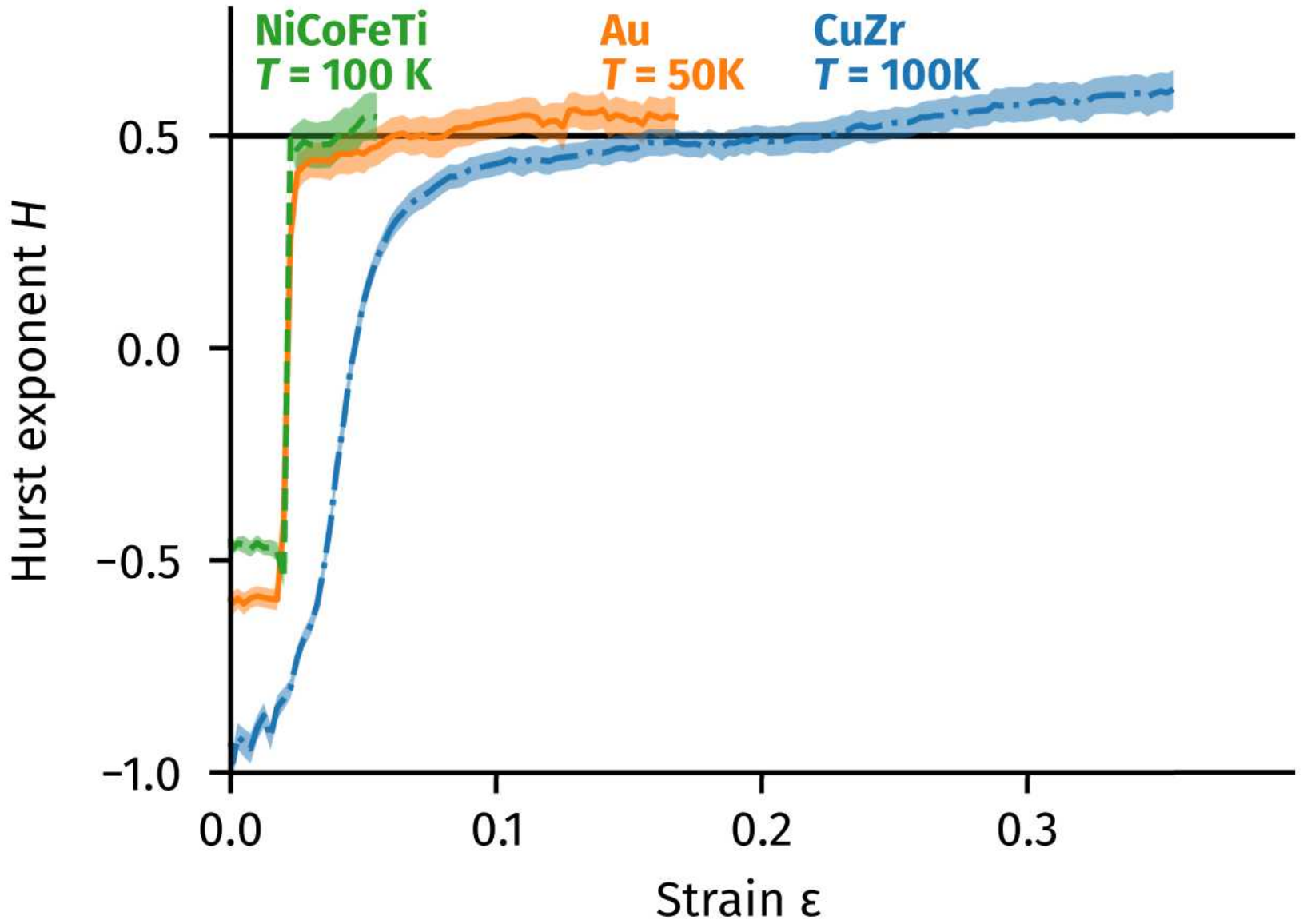
The radially averaged PSD for amorphous CuZr and Au(111)

$$C(q) \sim q^{-2(1+H)}$$





$C(q) \sim q^{-2(1+H)}$: H as a function of strain



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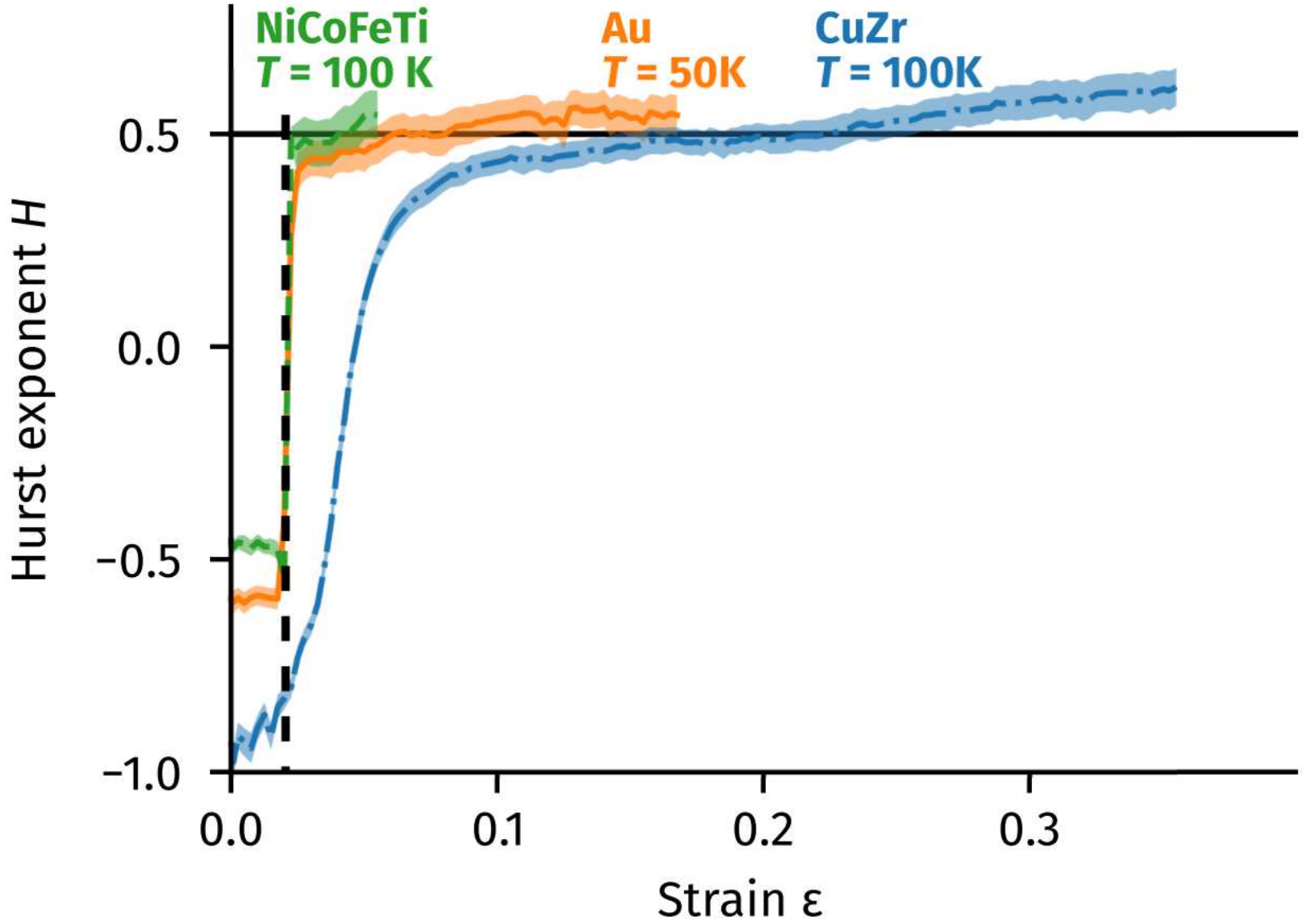
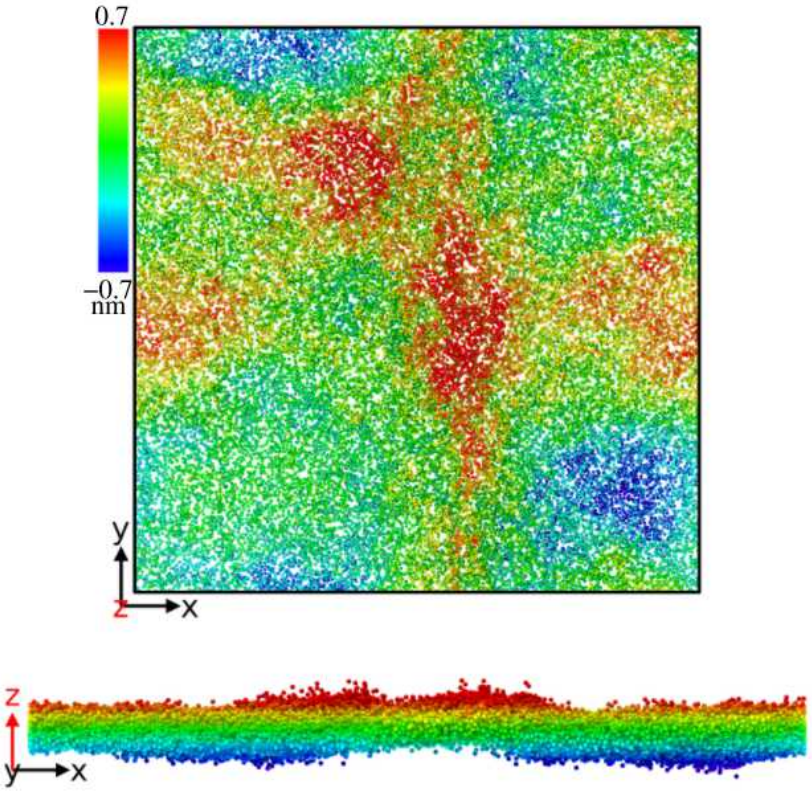
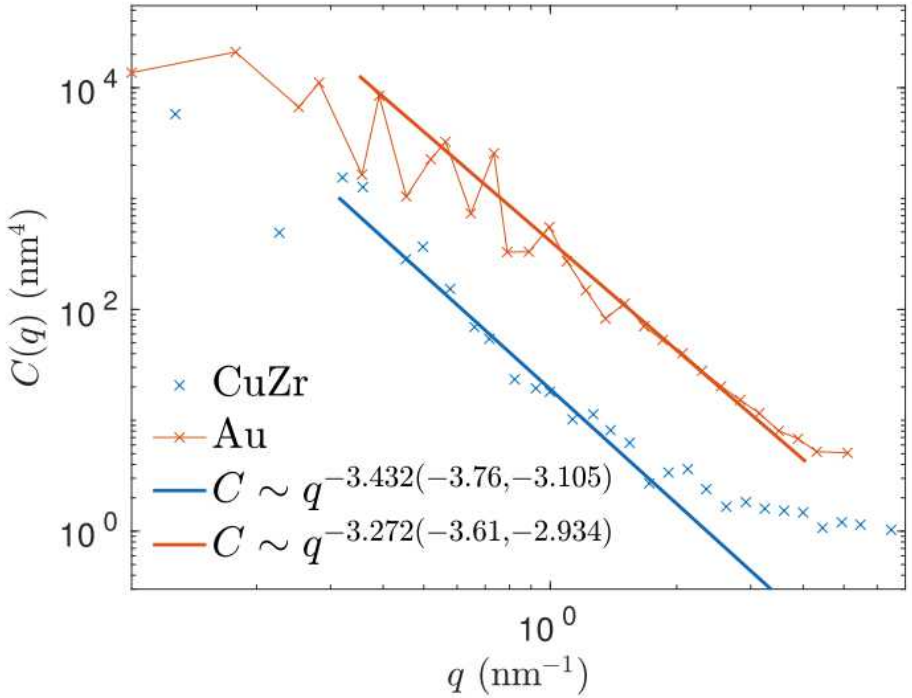


PSD of plane of atoms within the bulk





Bulk zz-displacement correlation

3D displacement correlations

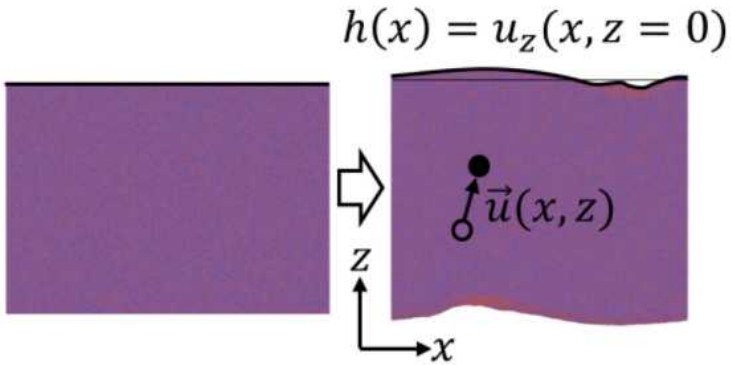
$$G_{zz}(\vec{r}) = \langle u_z(0) u_z(\vec{r}) \rangle$$

Fourier transform:

$$G_{zz}(\vec{q}) \sim q^{-3-2H}$$

2D in-plane correlations

$$C(q) \sim q G_{zz}(q)$$



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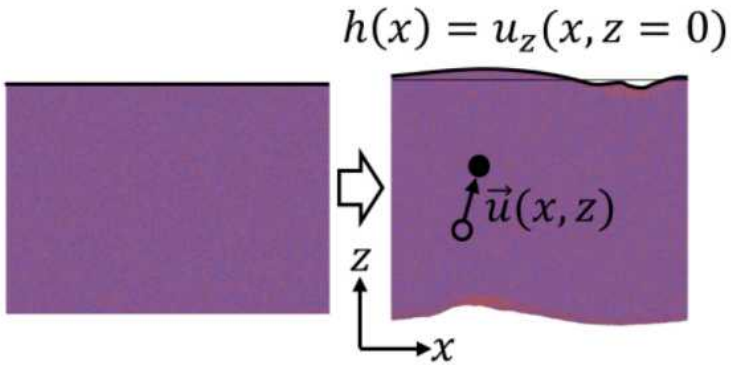
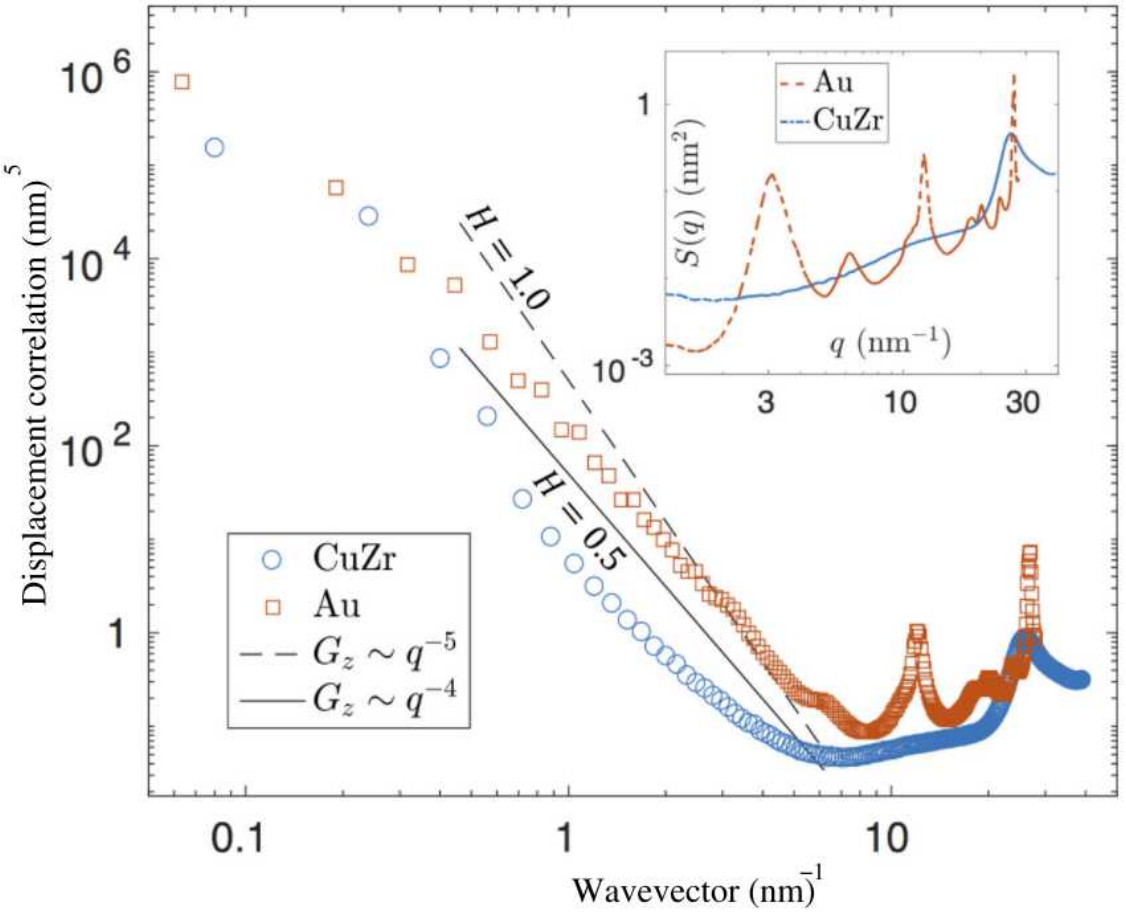




Elastic Limit in crystalline materials

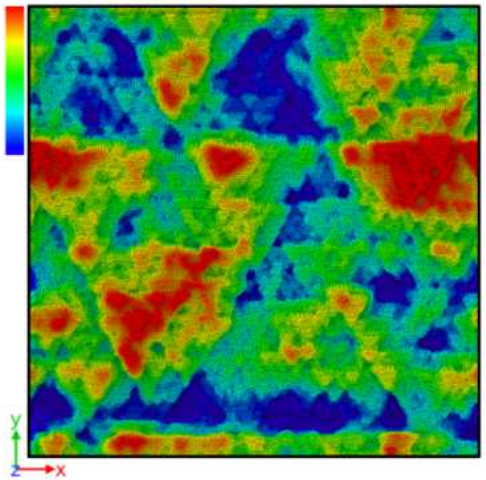
Thermal disorder and elastic constants

Campana, Müser, PRB 74, 075420

(2006)

$$H = -\frac{1}{2}$$

$$C(q) \sim q^{-2-2H} = q^{-1}$$



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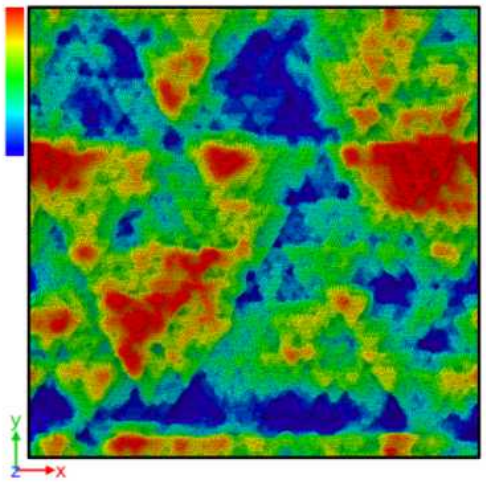

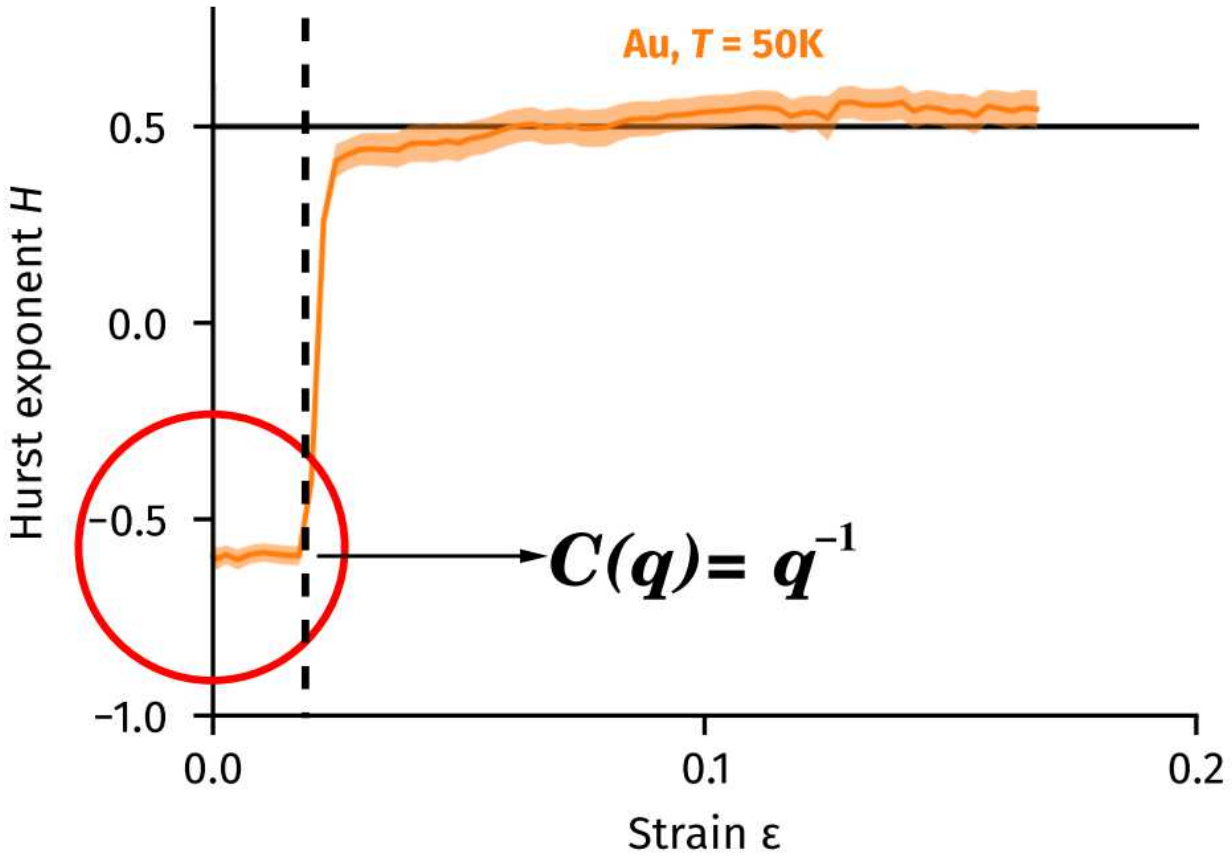

Elastic Limit in crystalline materials

Elastic regime of amorphous solid

DiDonna, Lubensky, PRE 72,

066619 (2005)

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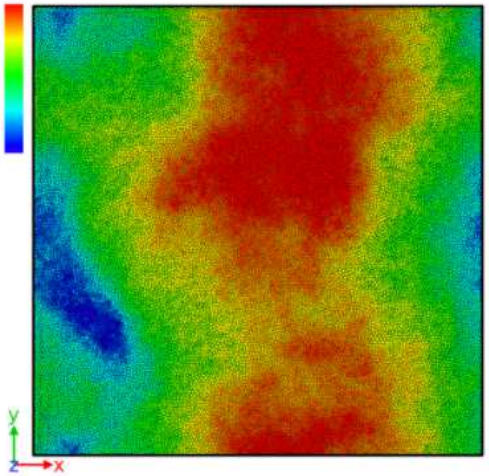

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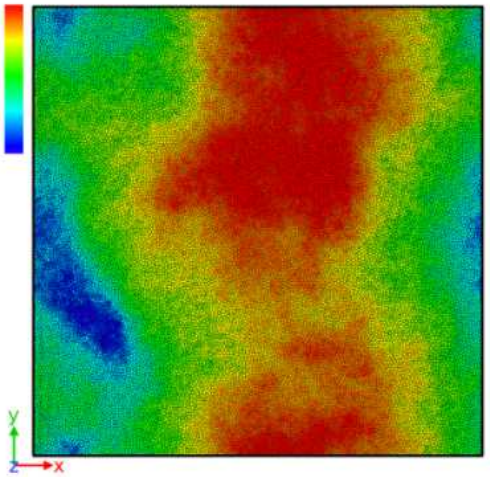
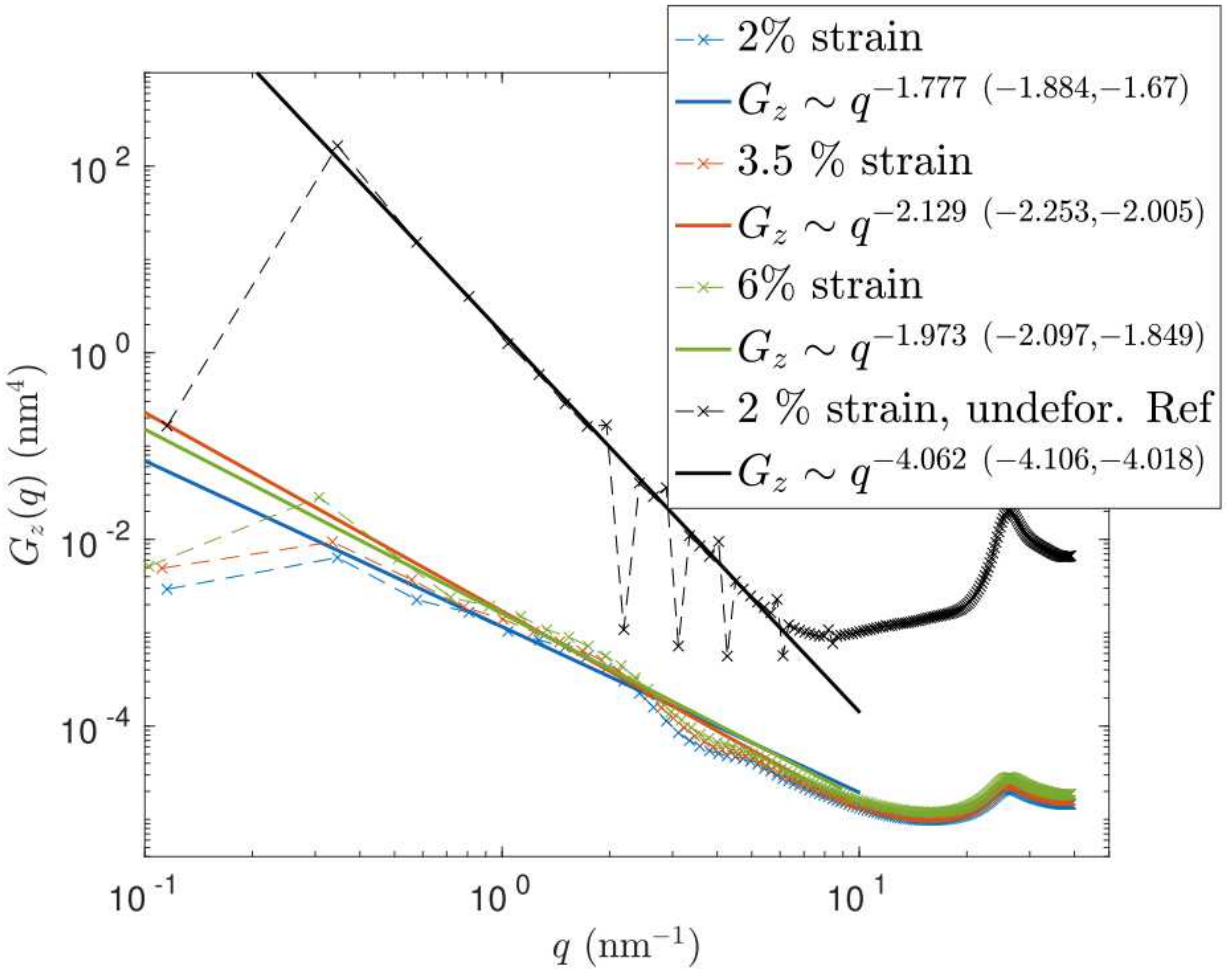
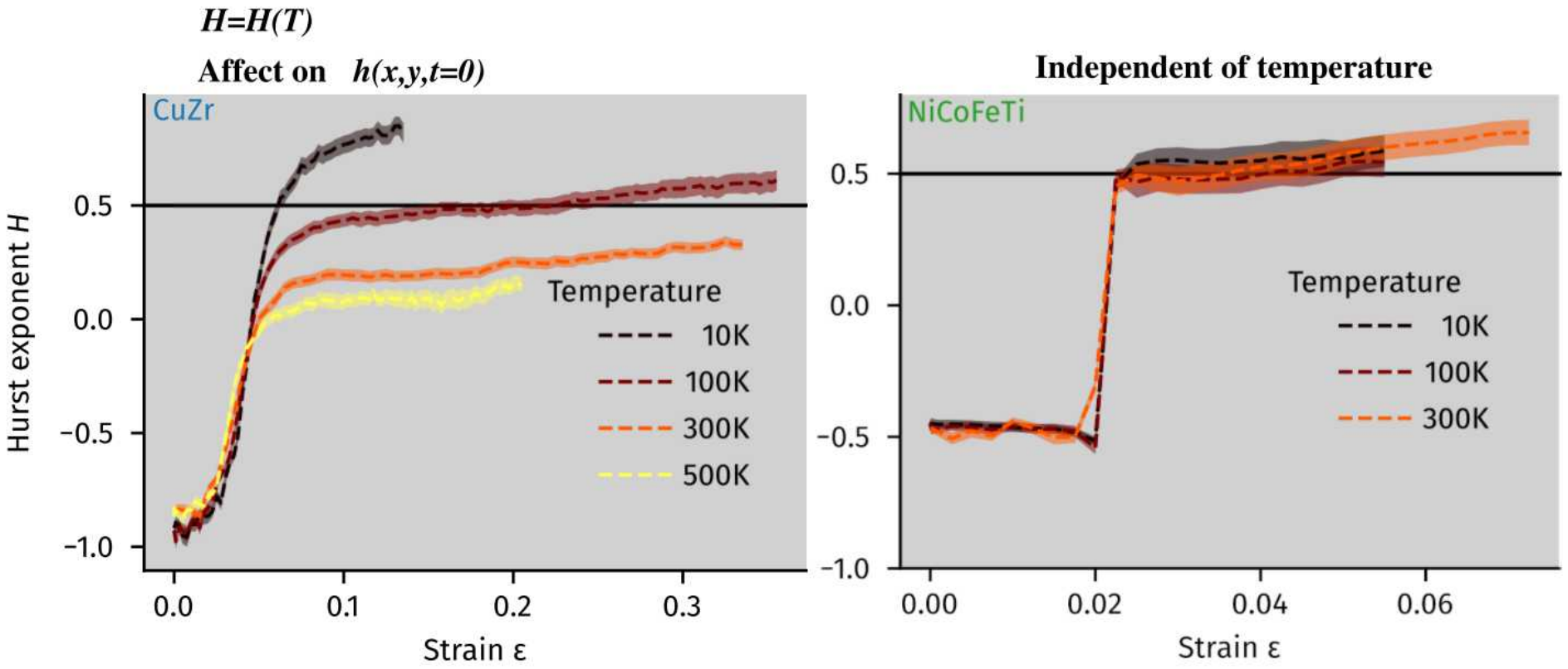




Temperature dependence on the self-affinity



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- DFG Emmy-Noether (grant PA 2023/2) and ERC Starting Grant (757343)
- Jülich Supercomputing Centers (JURECA and JUQEEN)