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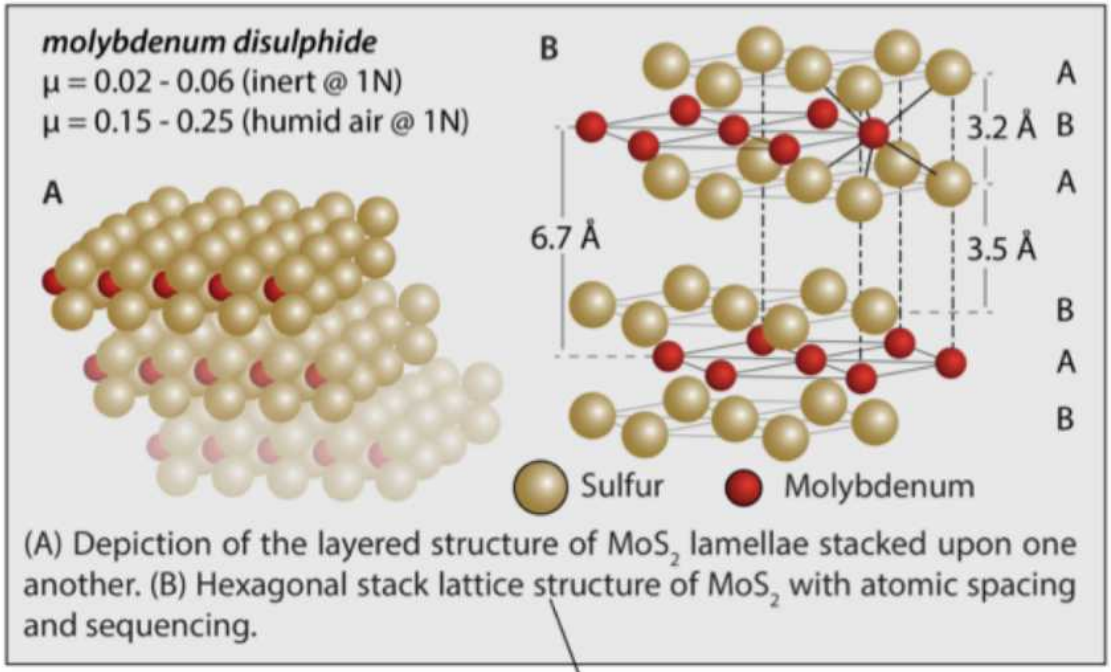
Atomistic Origins of Temperature-dependent Shear Strength in 2D Materials

Adam R. Hinkle, John F. Curry, Tomas F. Babuska, Michael T. Dugger, Mark A. Wilson, Brandon A. Krick, Nicolas Argibay, and Michael Chandross

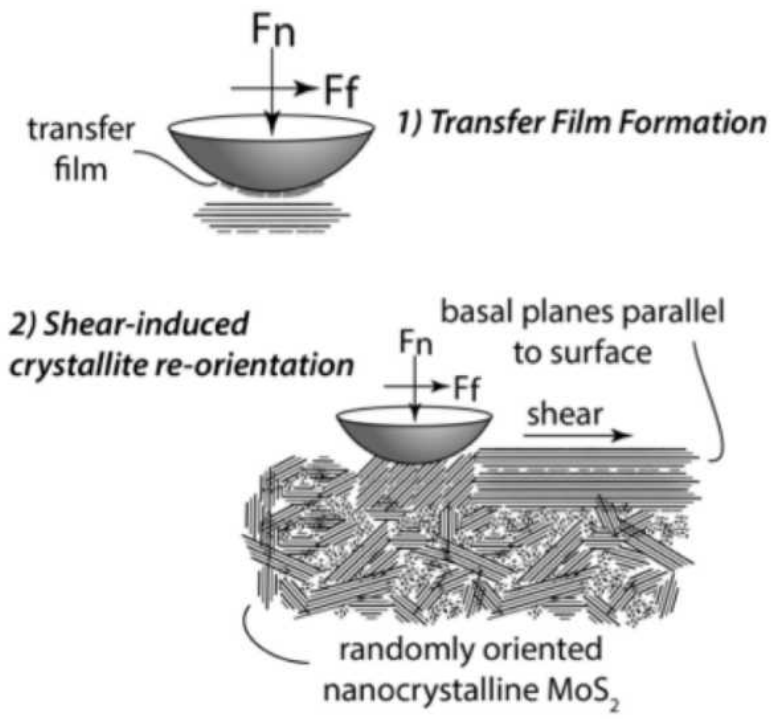
Sandia National Laboratories, Albuquerque, NM, USA

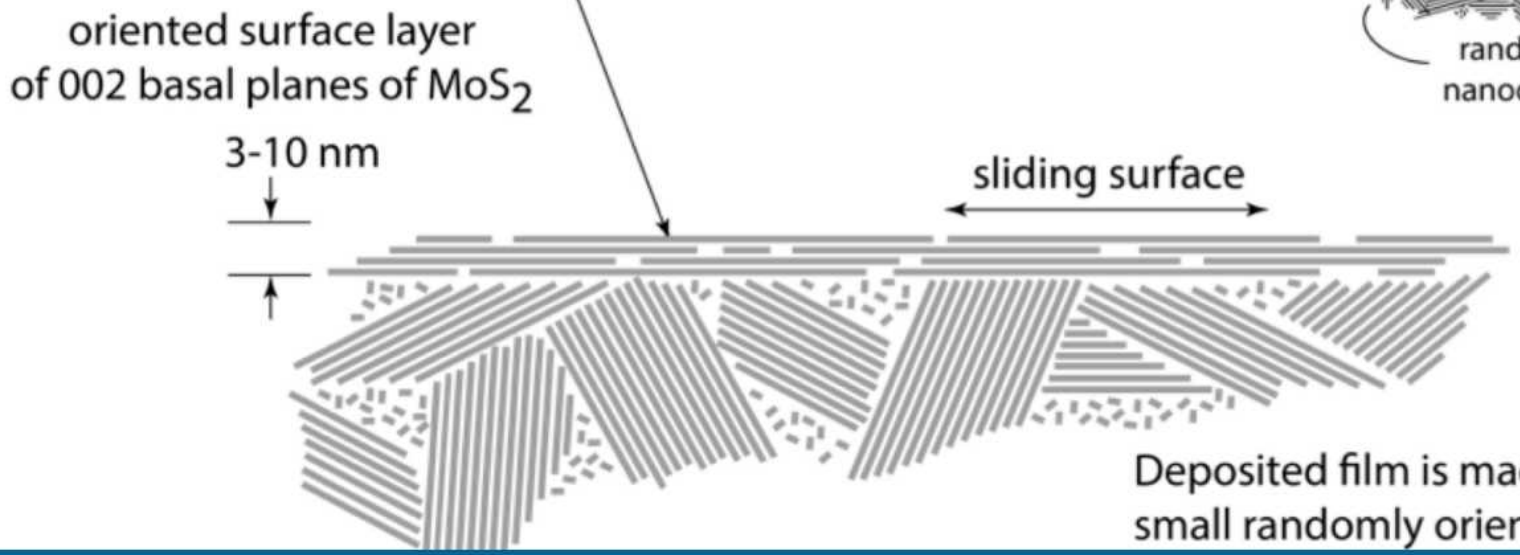
STLE Frontiers, Chicago, October 2018

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.

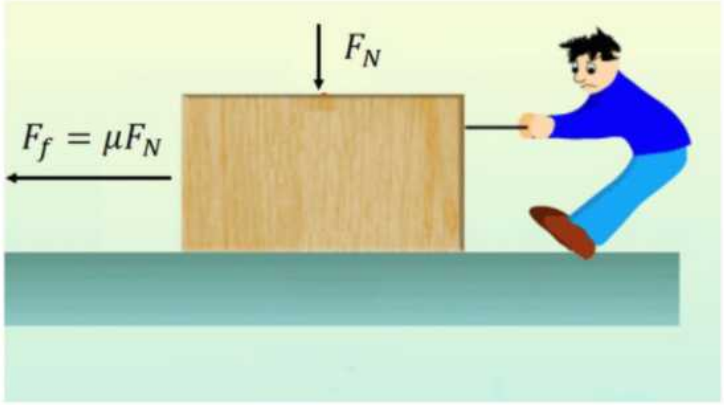




Deposited film is made of many small randomly oriented crystallites

Friction: Amontonian v. Non-Amontonian

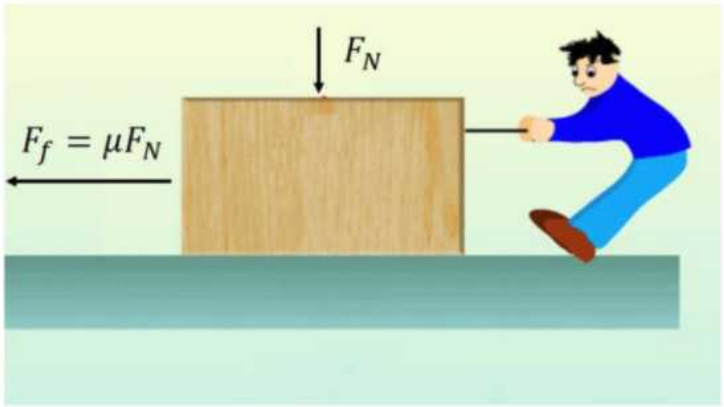
Amontonian Friction



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



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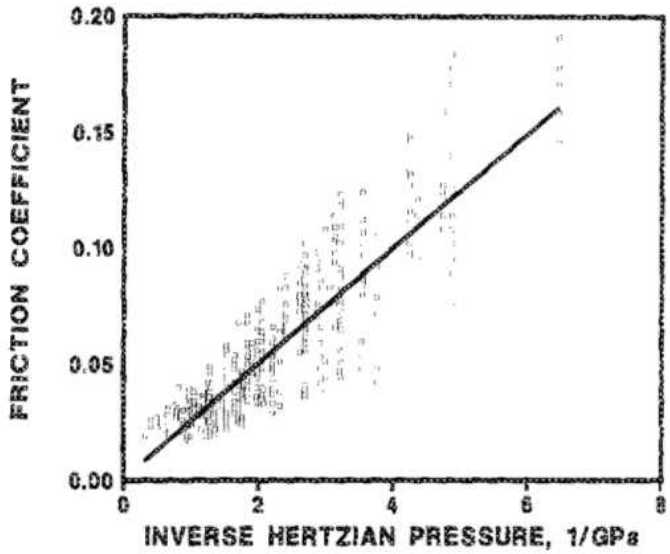
I.L. Singer et al., Appl. Phys. Lett. **50**, 995 (1990)



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

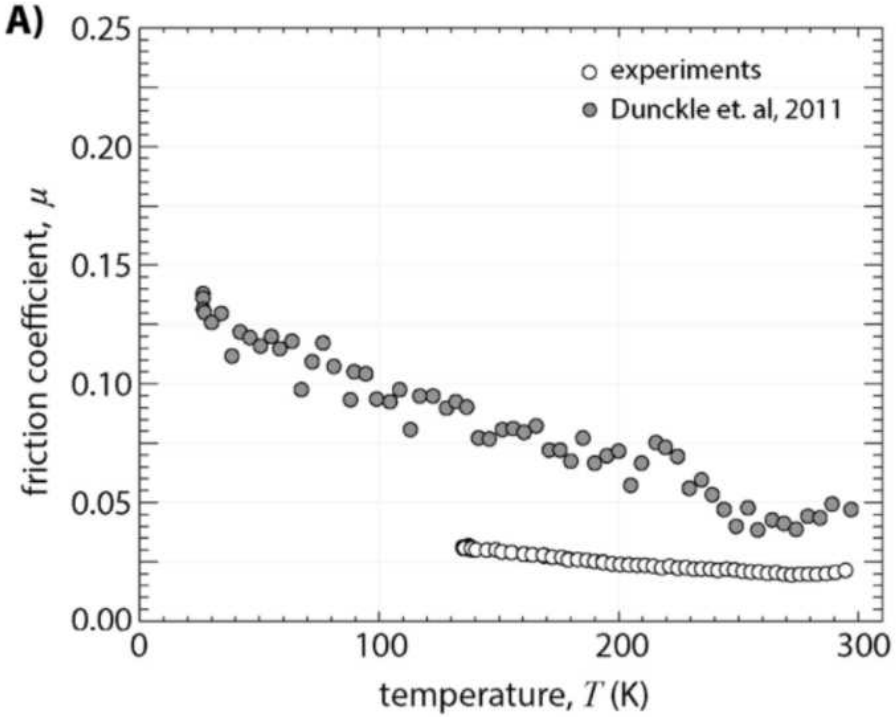
$$F_f = S_o A_{\text{real}} + \alpha F_N$$

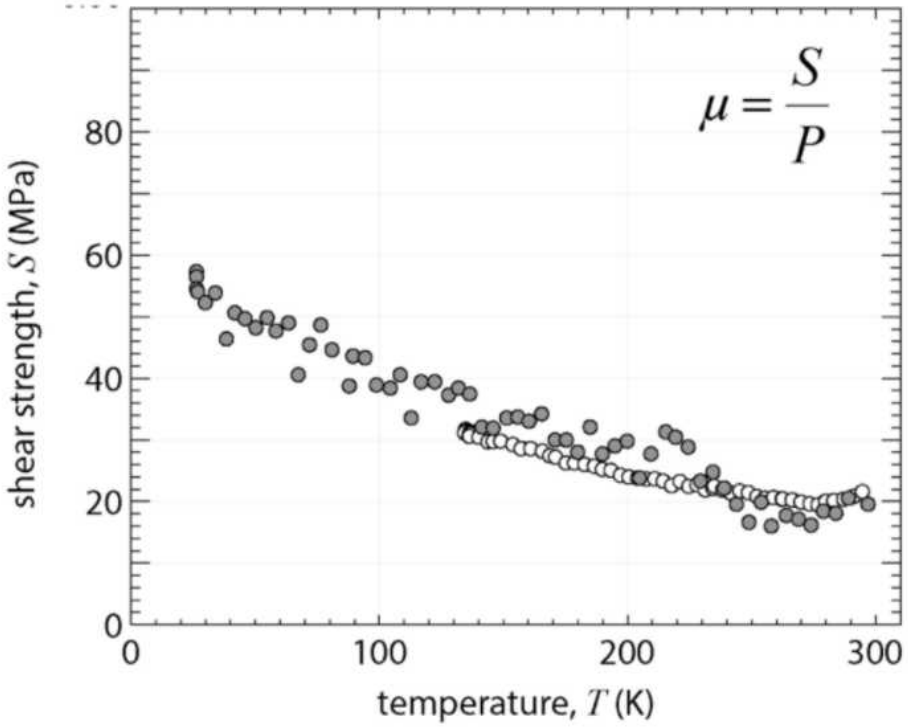
$$\mu = \alpha + S_o / P$$

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

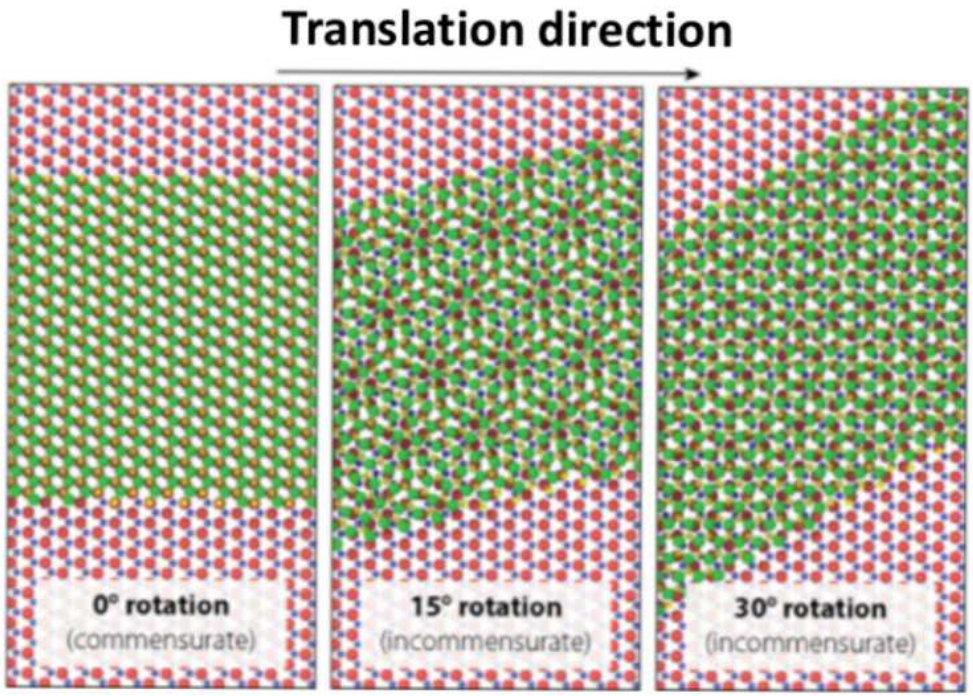
$$S_o = 25 \text{ MPa at } 300 \text{ K}$$

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





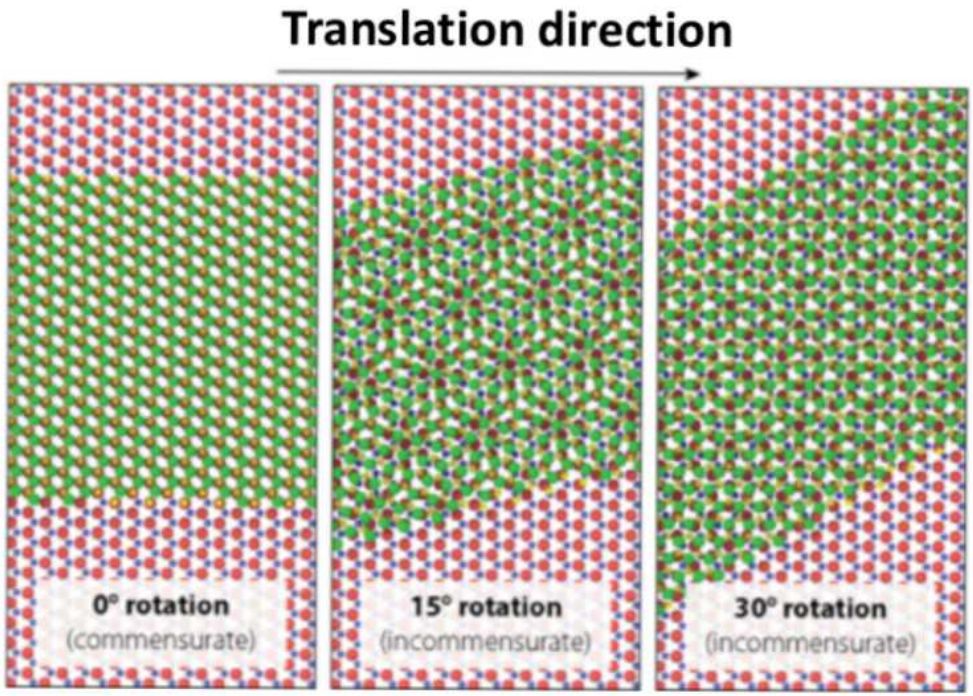
Nudged Elastic Band Calculations and Commensurate Sliding



commensurate
egg shell

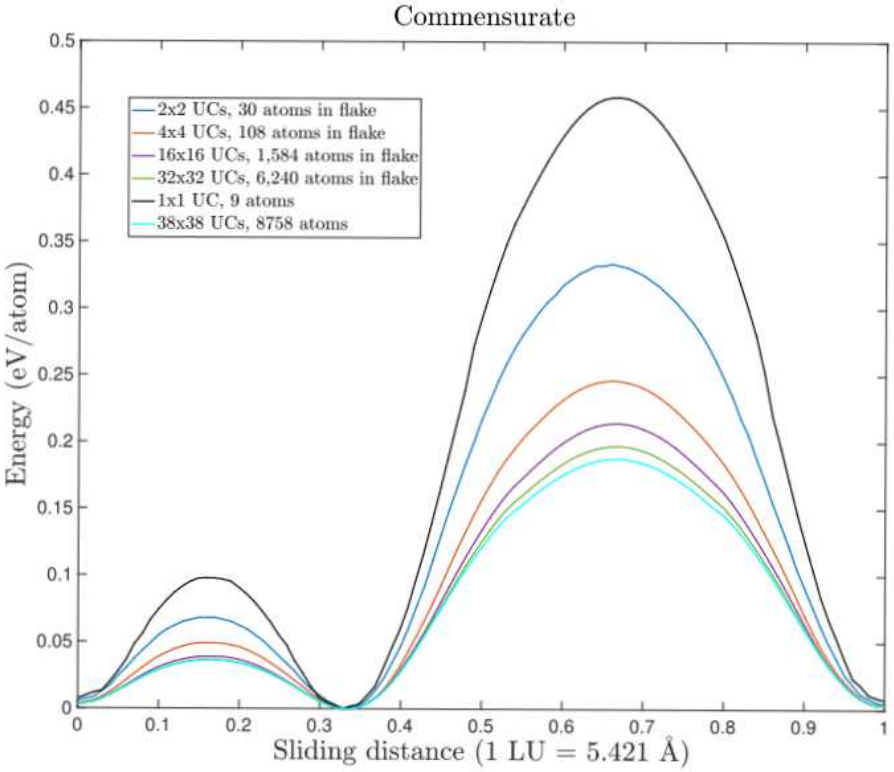
incommensurate
egg shell

Nudged Elastic Band Calculations and Commensurate Sliding

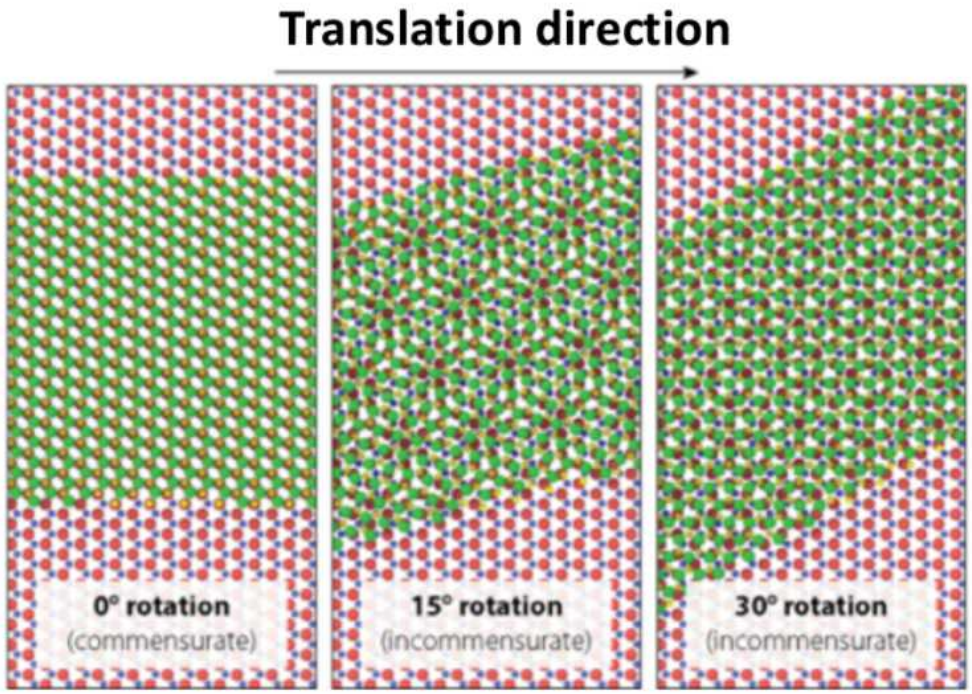


commensurate
egg shell

incommensurate
egg shell

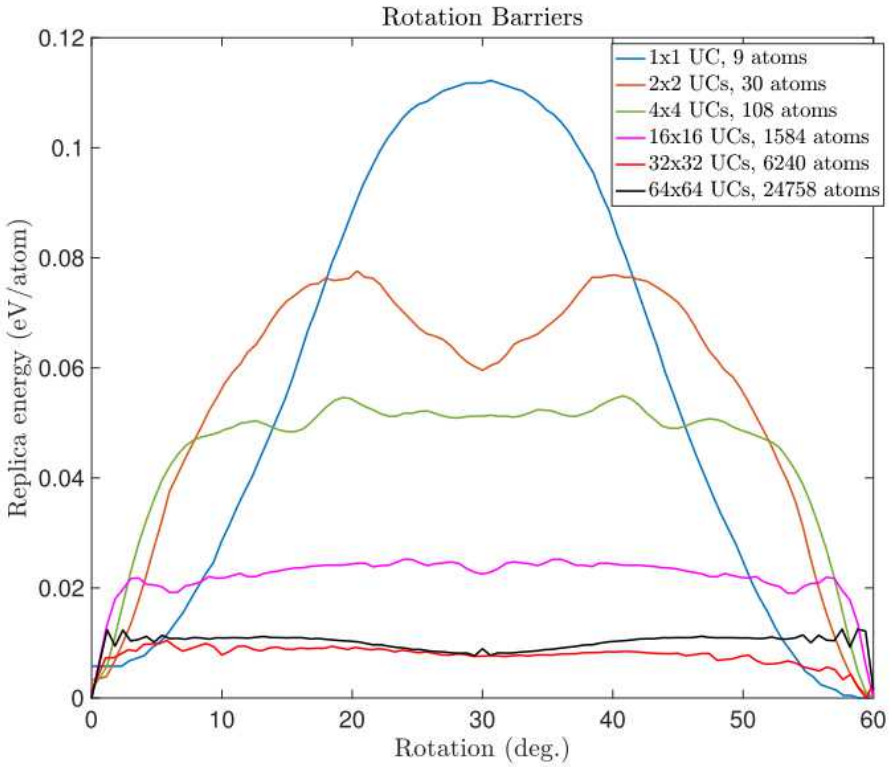


Rotation Barrier

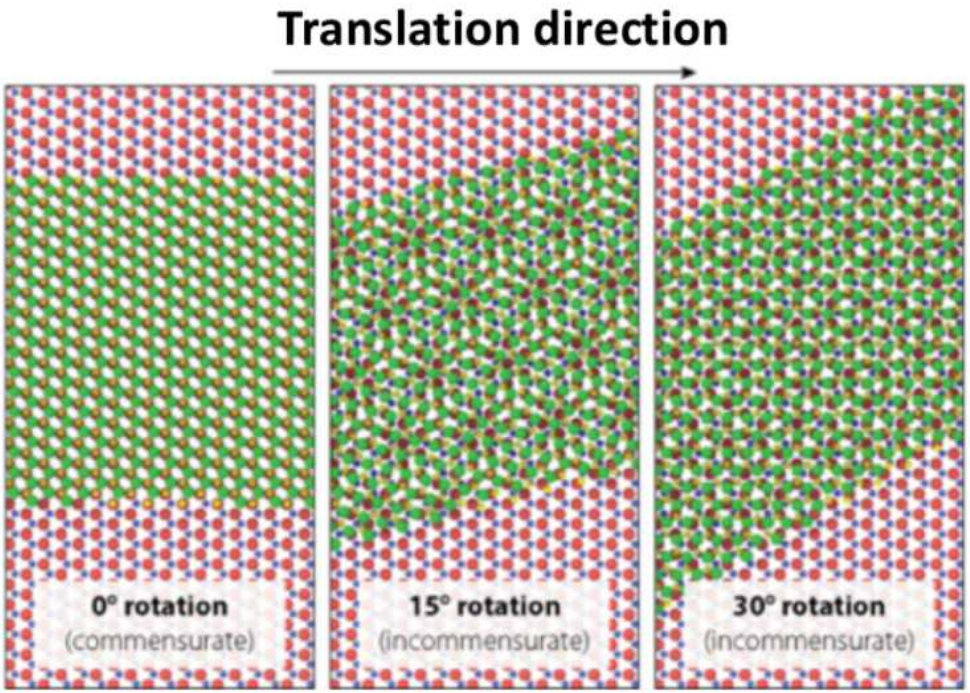


commensurate
egg shell

incommensurate
egg shell

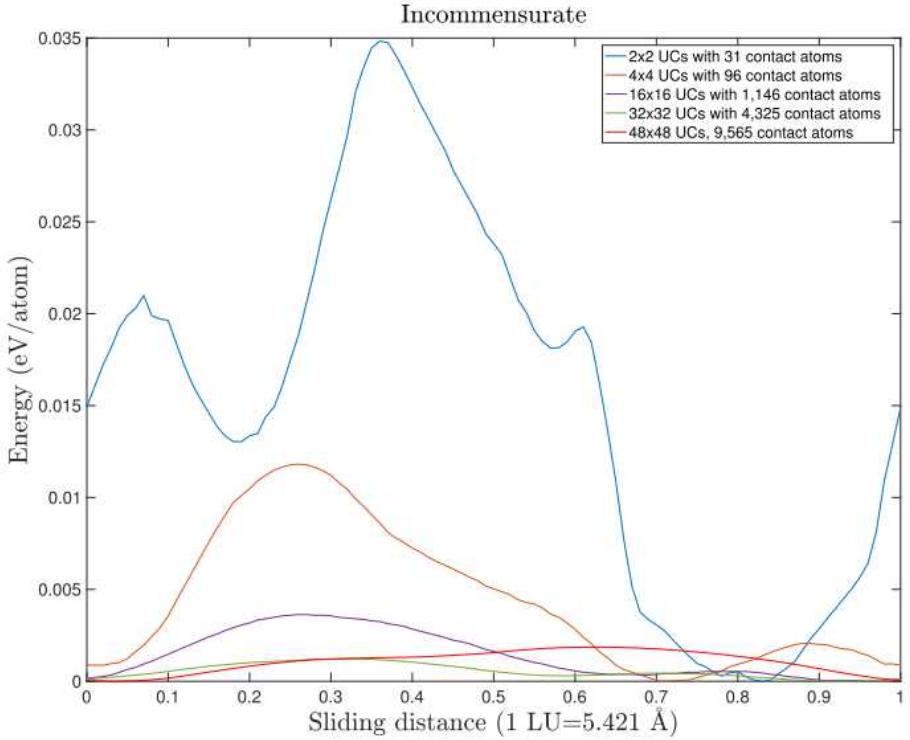


Incommensurate Barrier

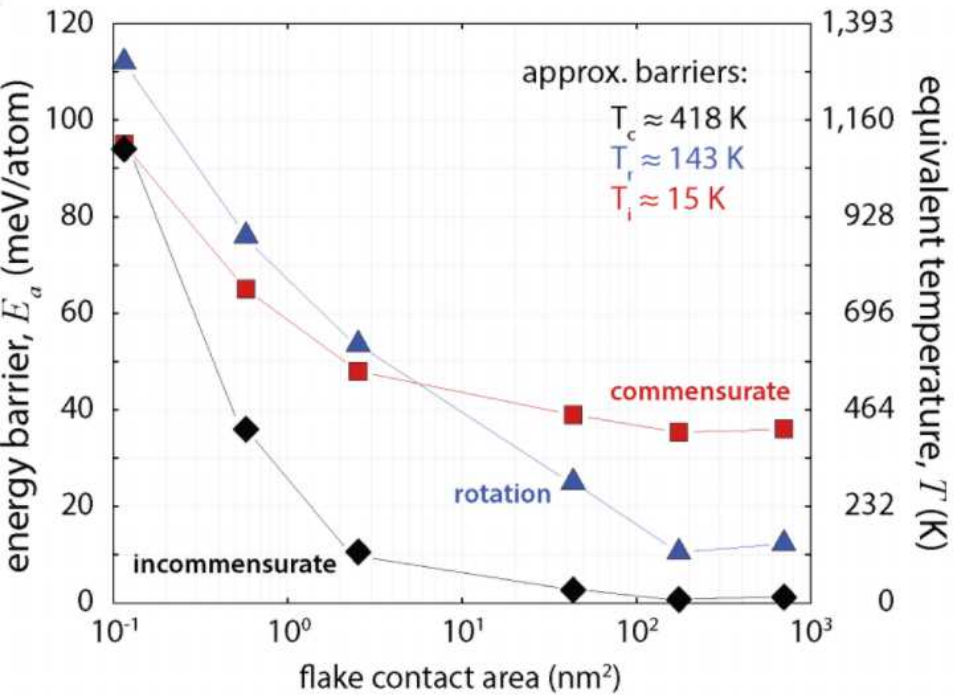


commensurate
egg shell

incommensurate
egg shell



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



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):

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

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

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

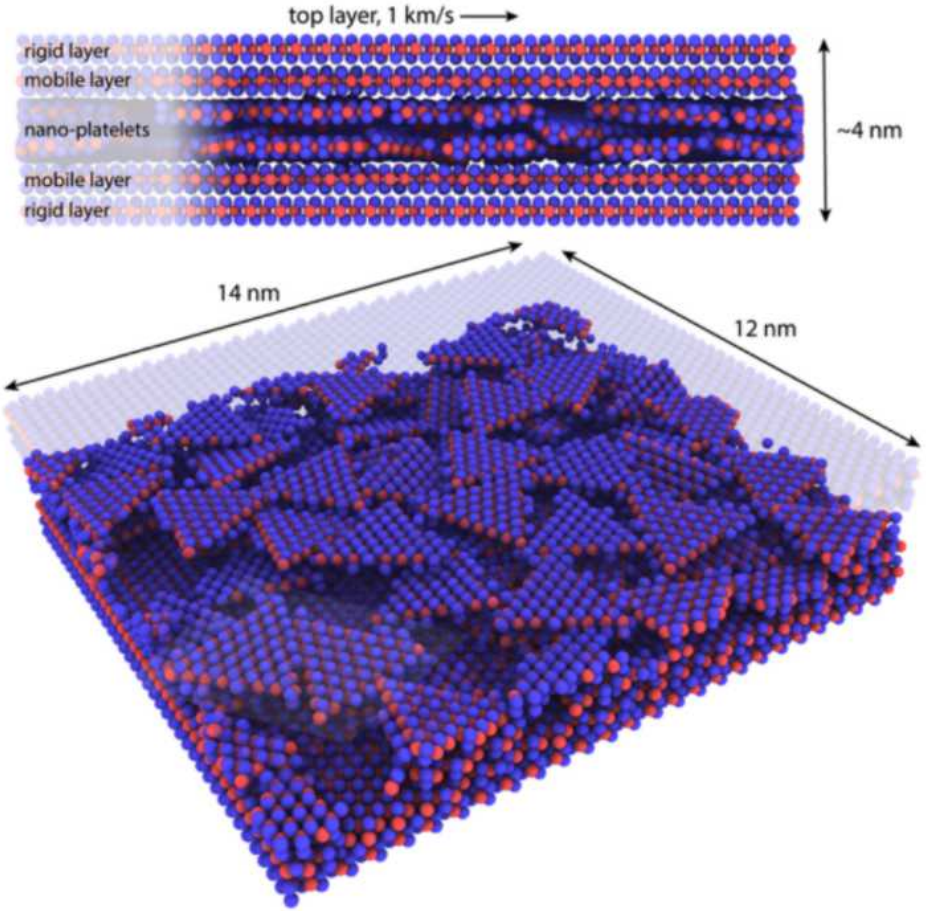
The model and scaled data from $S(T) = S_L f_{slide}(T)$

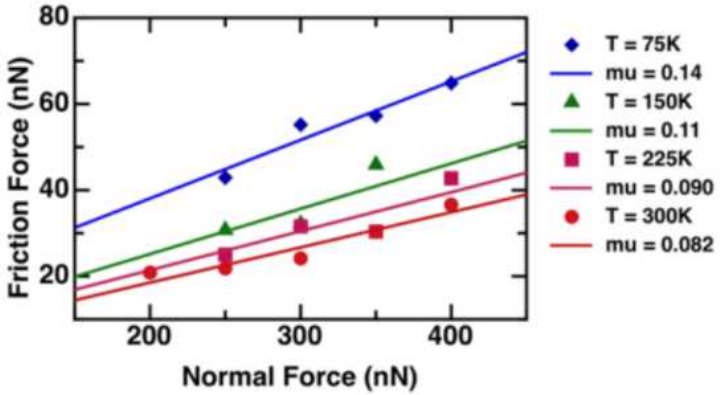
$$S(T) = S_L f_{slide}(T)$$

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

What is S_L?

MD ReaxFF Simulations





- Six normal forces used at each temperature
- $\mu = \frac{\mathrm{d}F_f}{\mathrm{d}F_N}$
- $S = \mu P$

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

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

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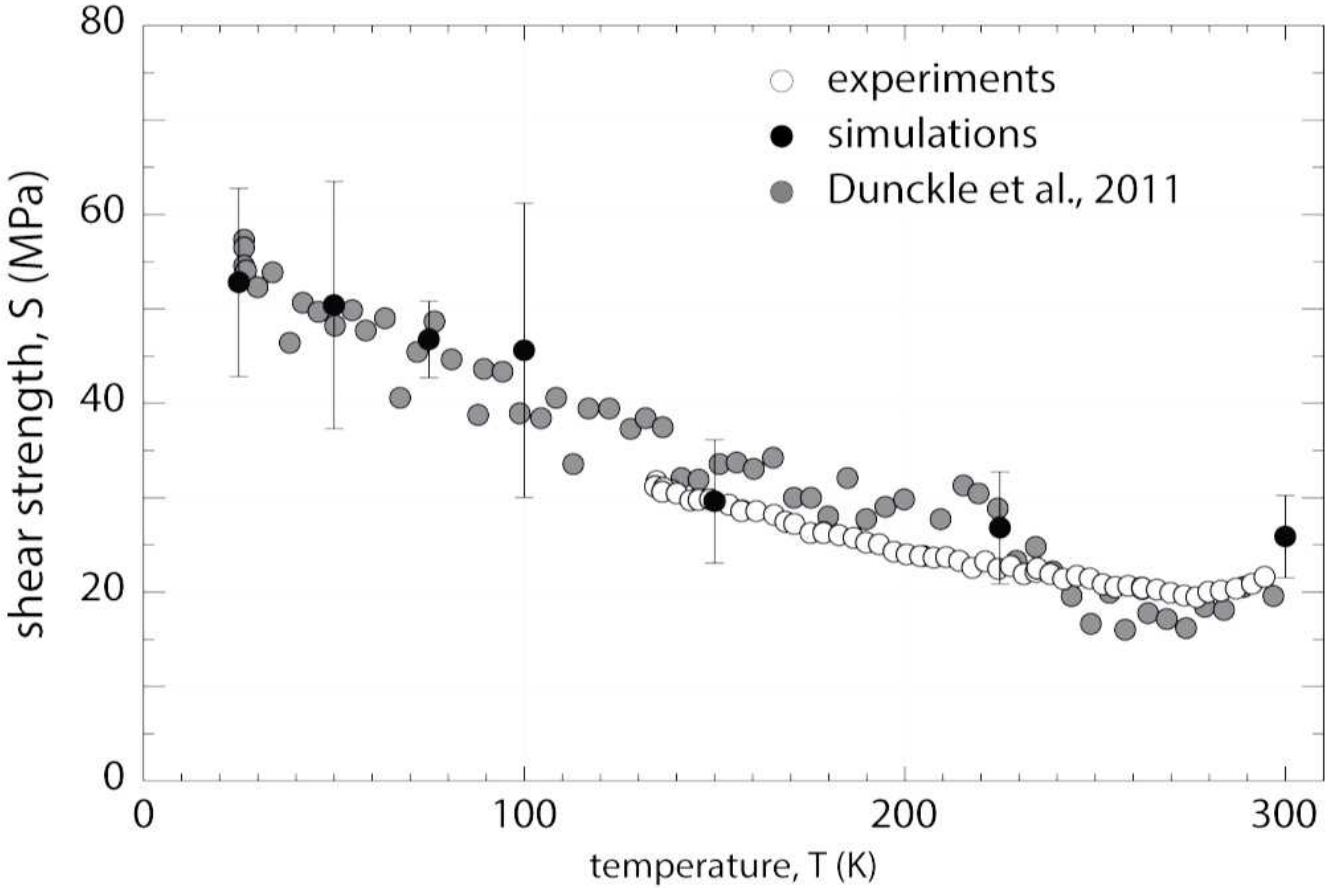

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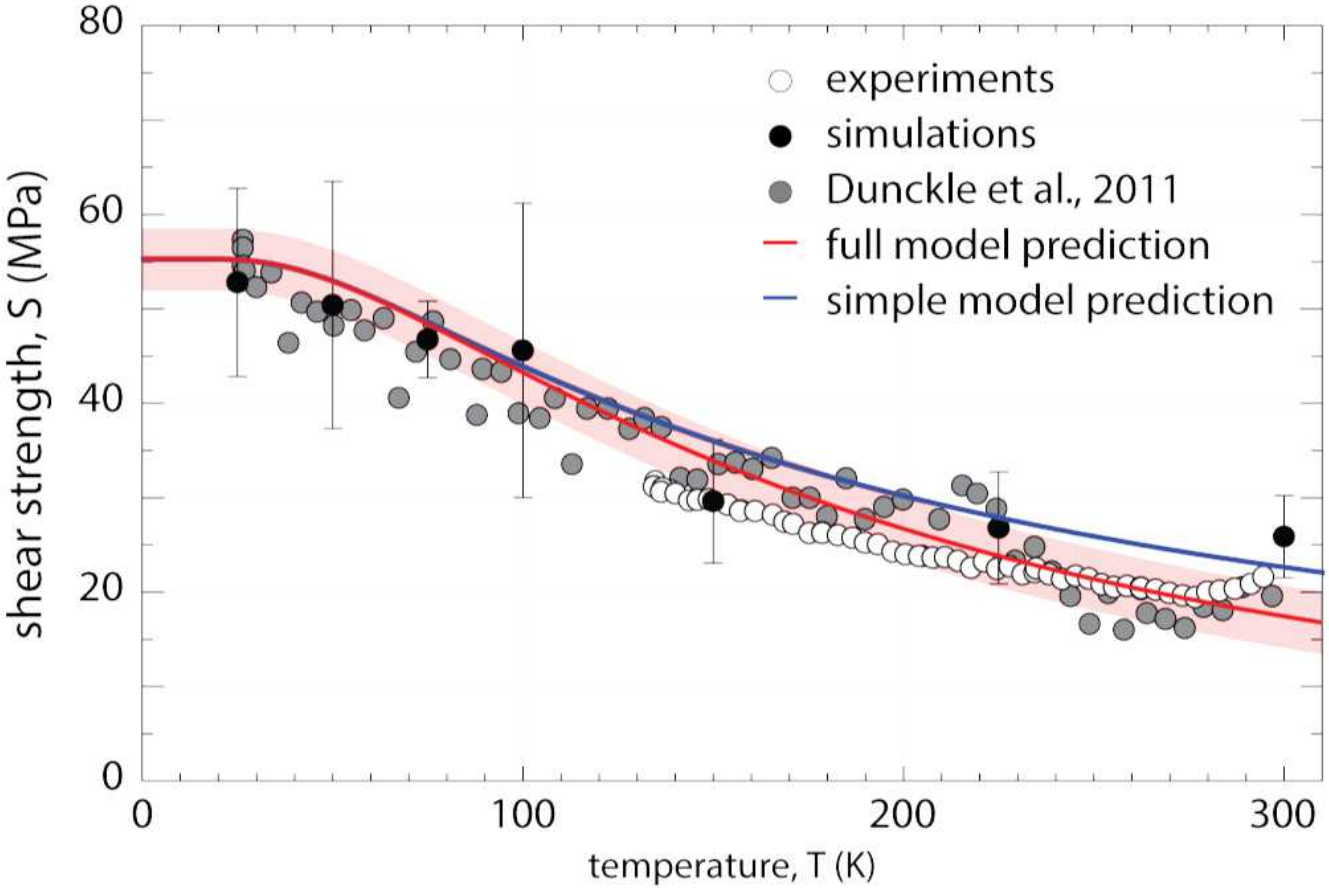

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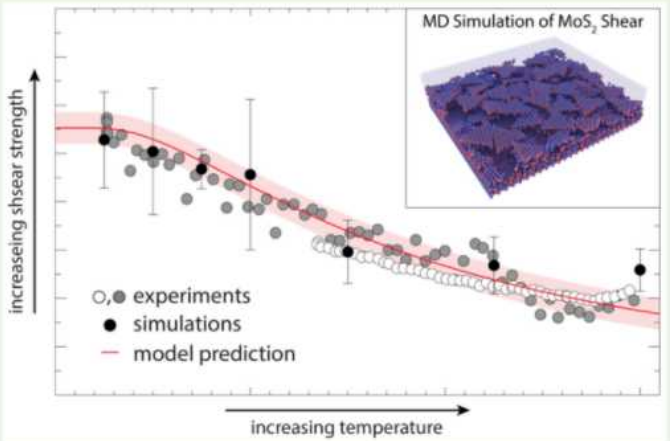
Atomistic Origins of Temperature-Dependent Shear Strength in 2D Materials

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 & Questions

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- James Batteas, Department of Chemistry, Texas A&M University, College Station