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A Model of Interfacial Shear Strength in 2D Materials

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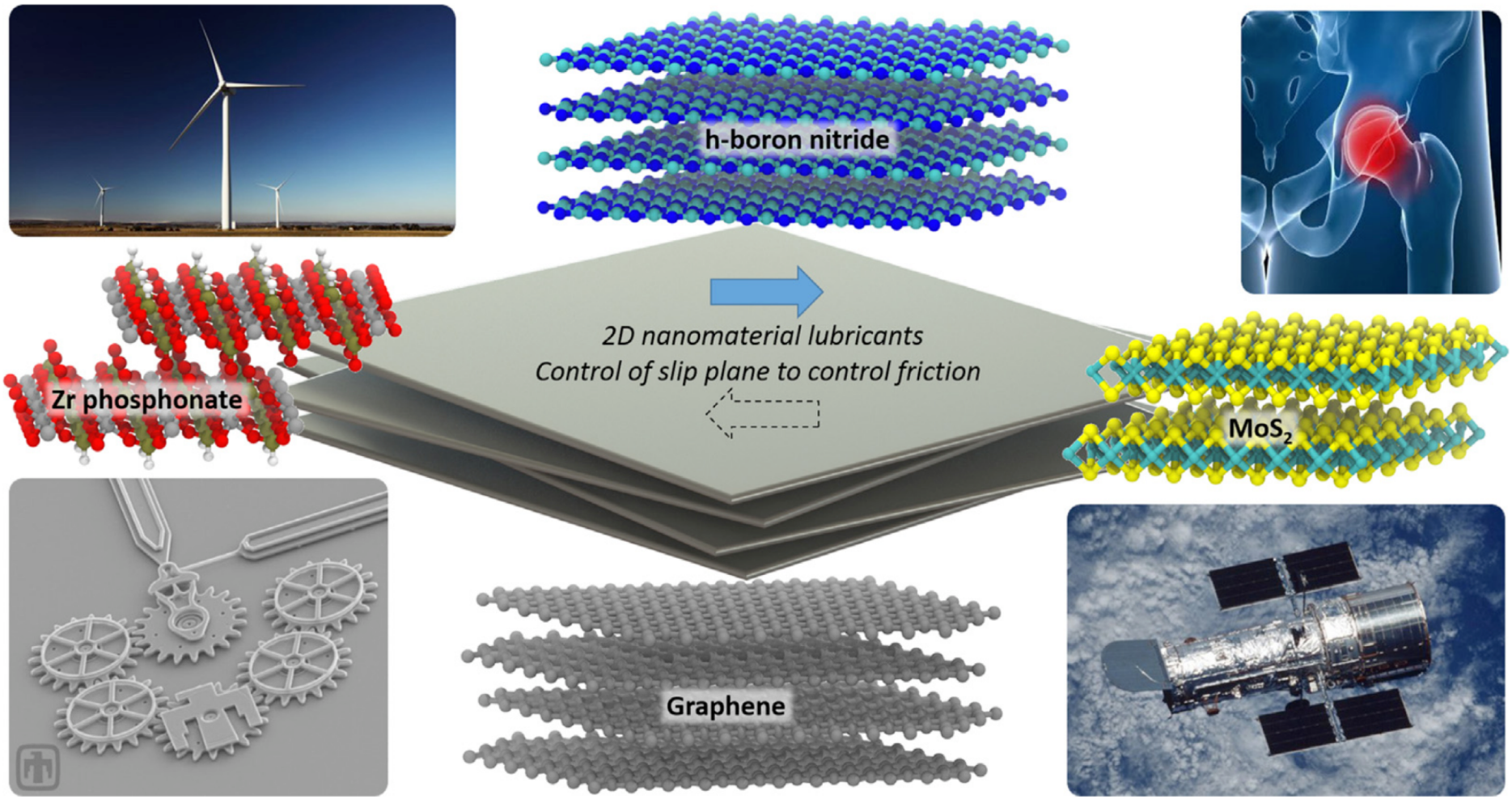
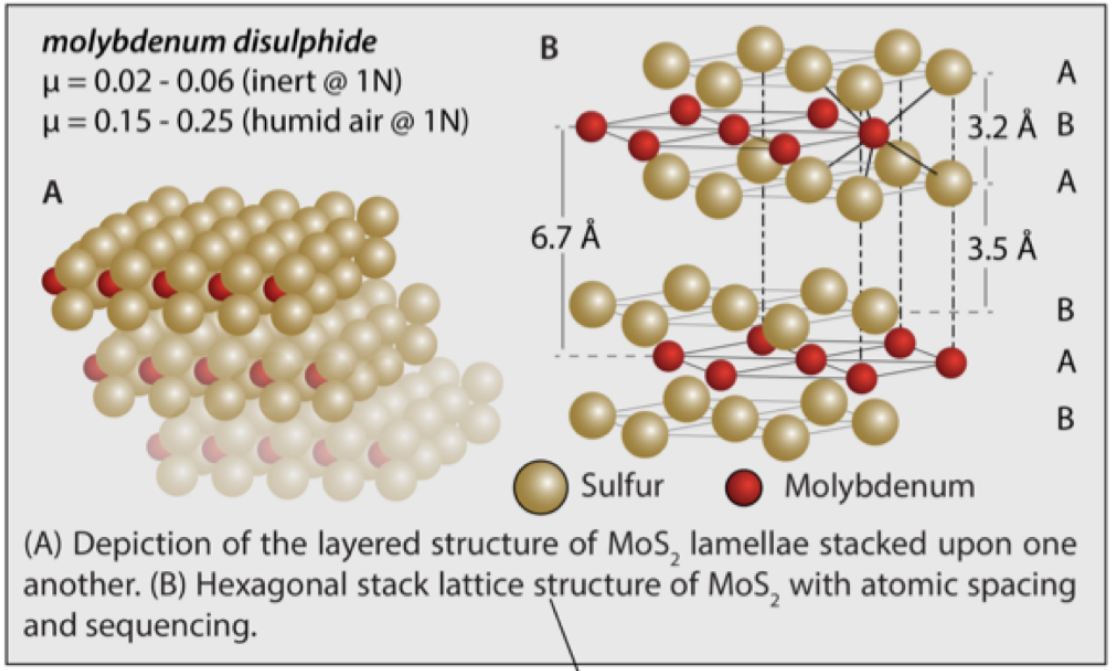
Tribology of 2D Materials

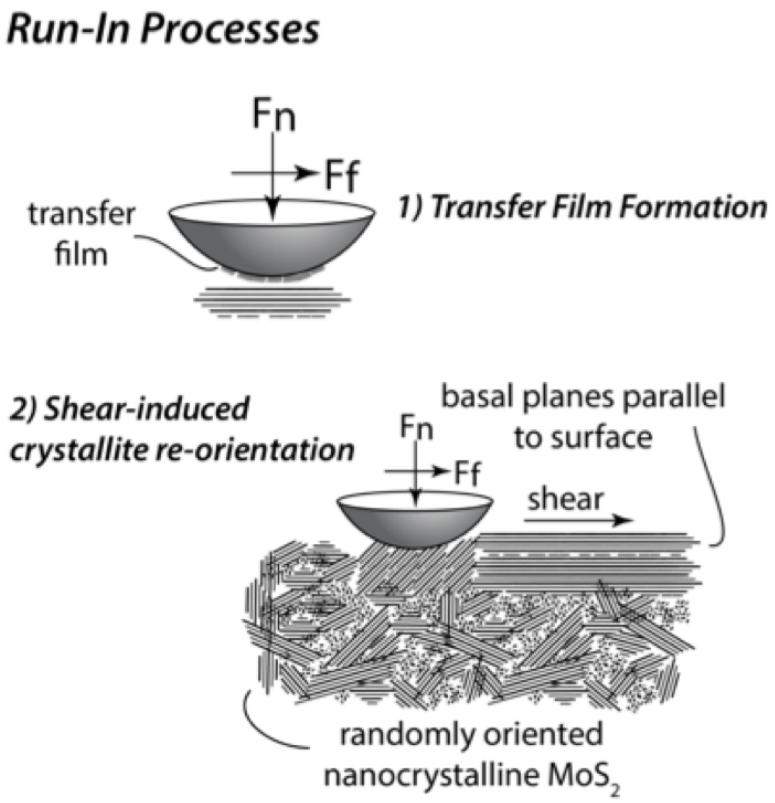


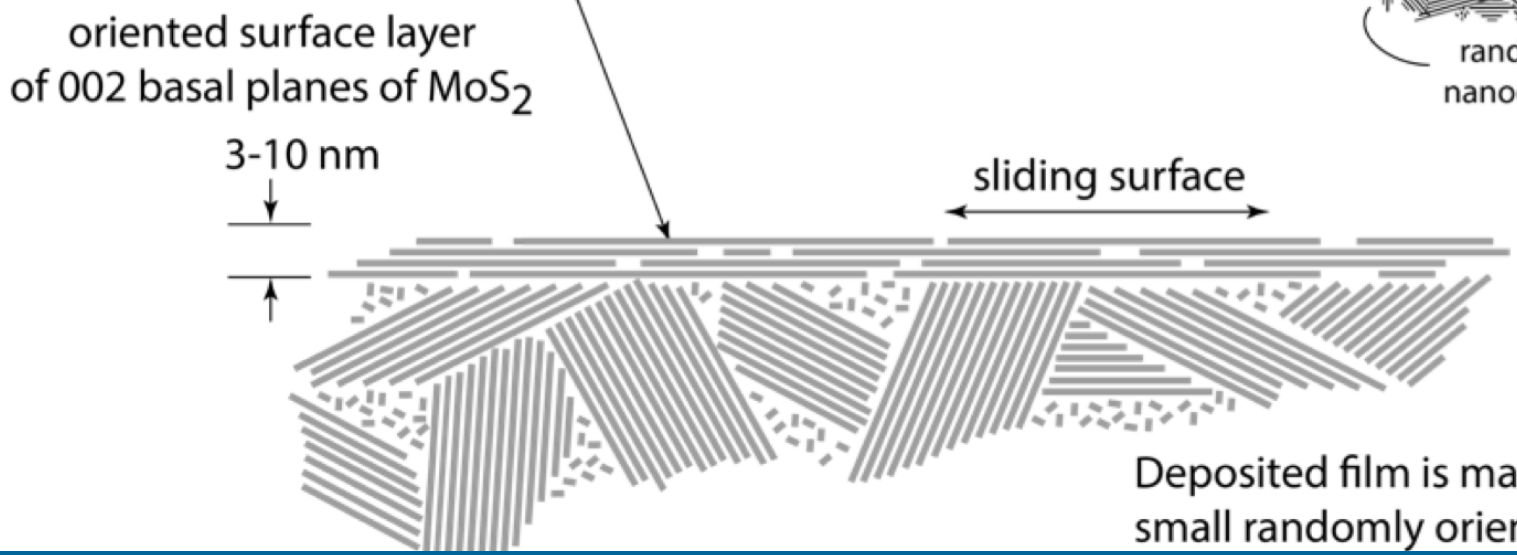
Figures: J.C. Spear et al., *2D-nanomaterials for controlling friction and wear at interfaces* Nano Today **10** 301-314 (2015)

Molybdenum disulphide (MoS_2): Chemistry & sliding friction



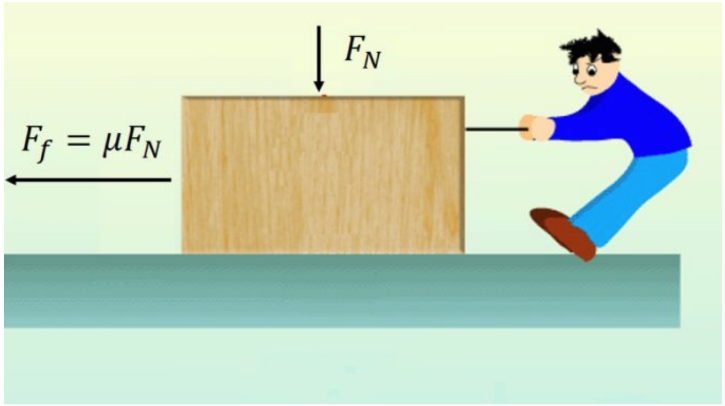
(A) Depiction of the layered structure of MoS_2 lamellae stacked upon one another. (B) Hexagonal stack lattice structure of MoS_2 with atomic spacing and sequencing.





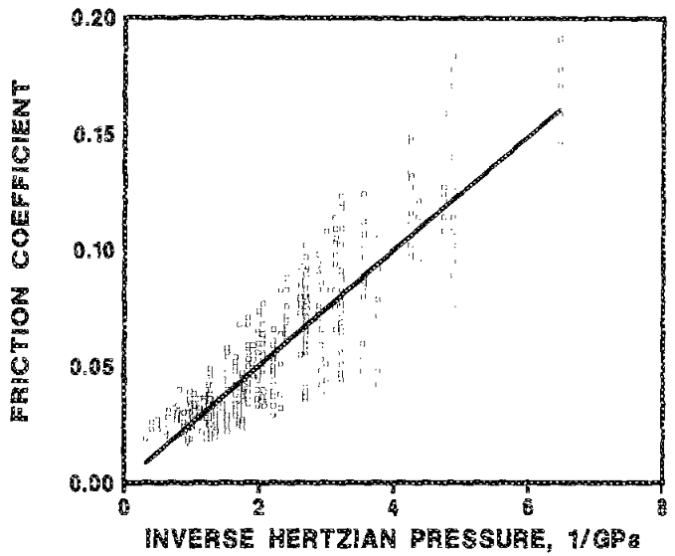
Friction: Amontonian v. Non-Amontonian

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

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



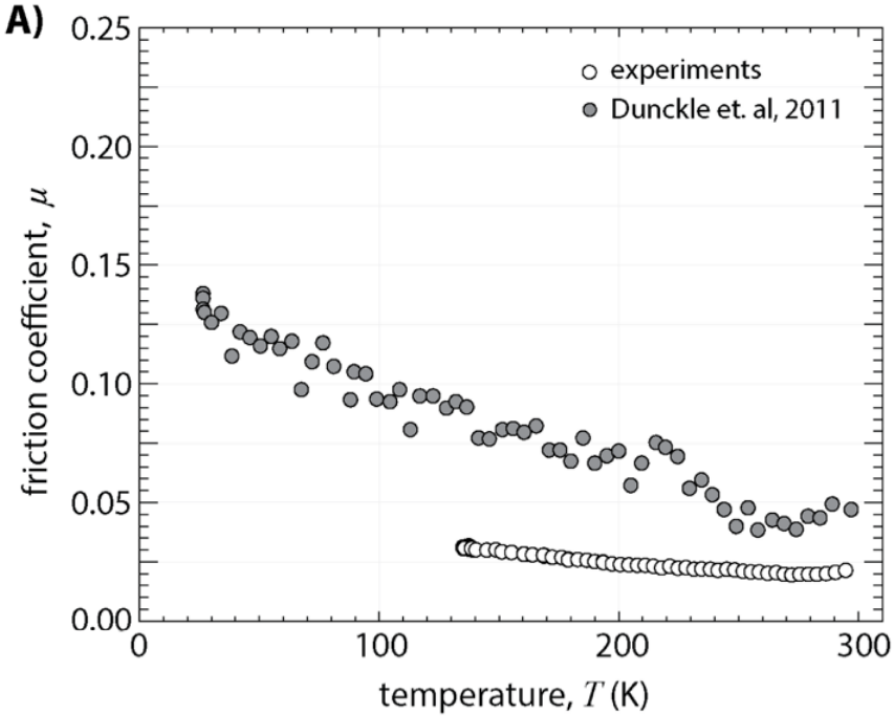
$$\mu(P,T) = \frac{S(P,T)}{P}, \text{ where } S = S_o(T) + \alpha P$$

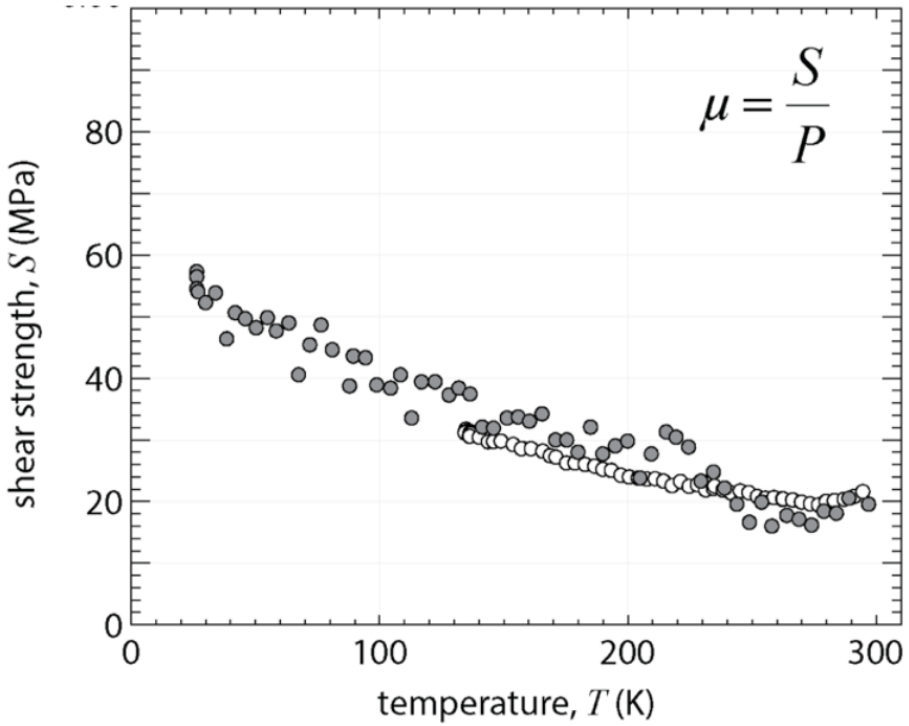
$$= \frac{S_o(T)}{P} + \alpha$$

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

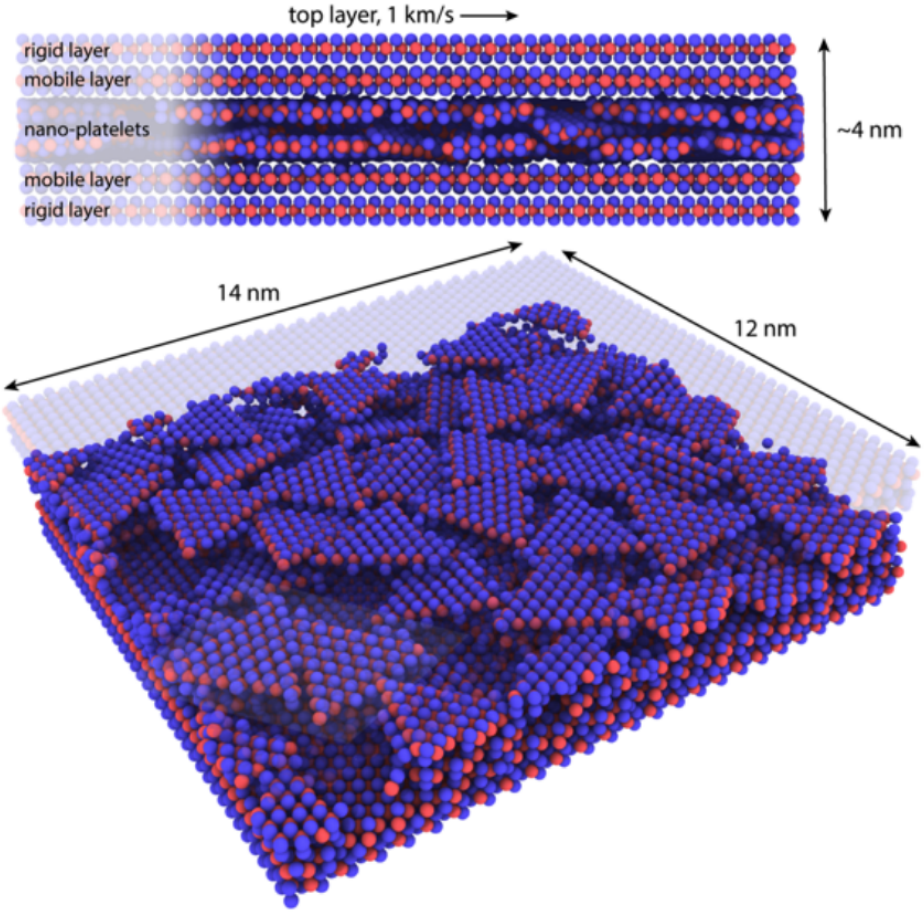
$$S_o = 25 \text{ MPa at } 300 \text{ K}$$

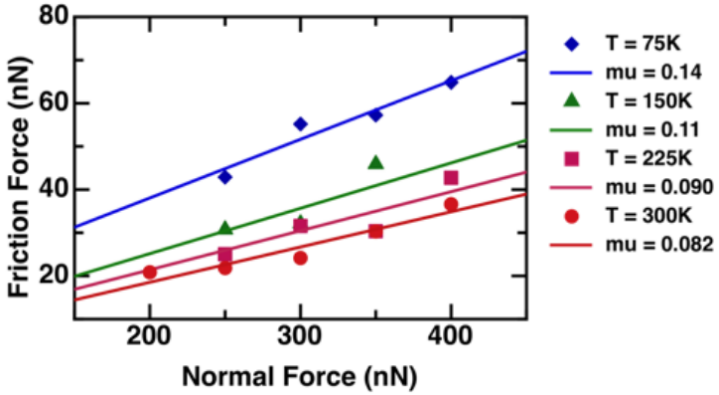
T-dependence $\mu = \mu(T, P)$ and $S = S(T)$ via MoS_2 Friction Experiments





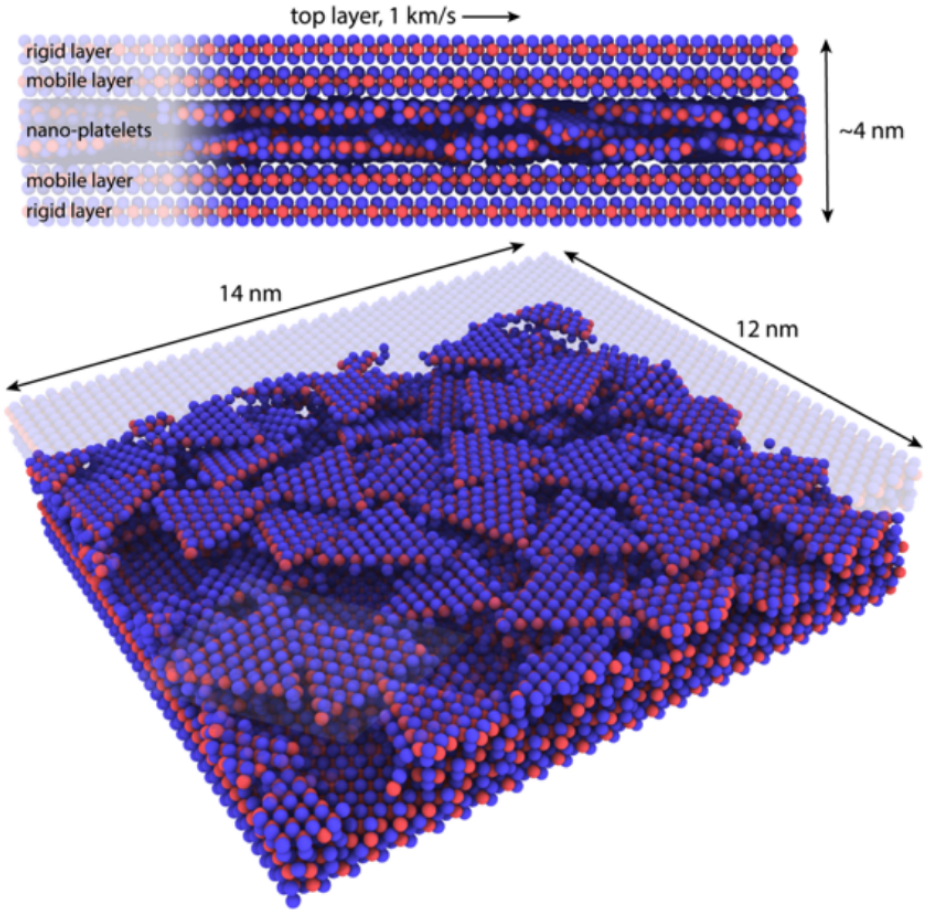
MD ReaxFF Simulations

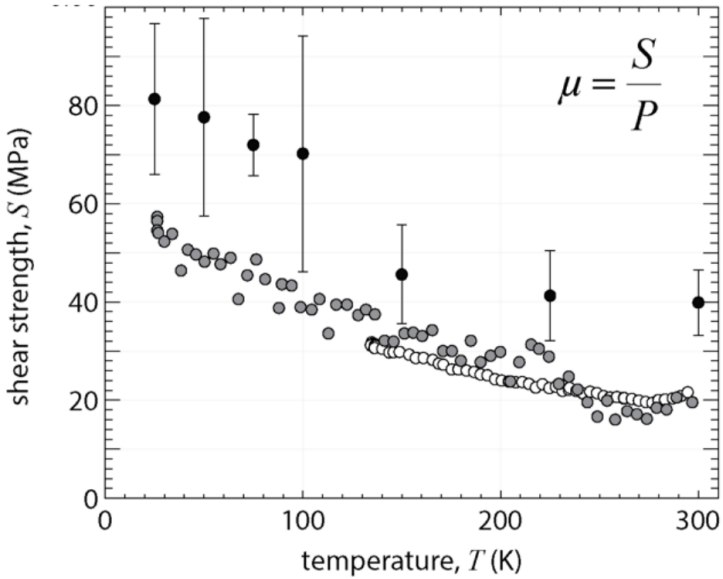




- Six normal forces used at each temperature
- $\mu = \frac{\mathrm{d}F_f}{\mathrm{d}F_N}$

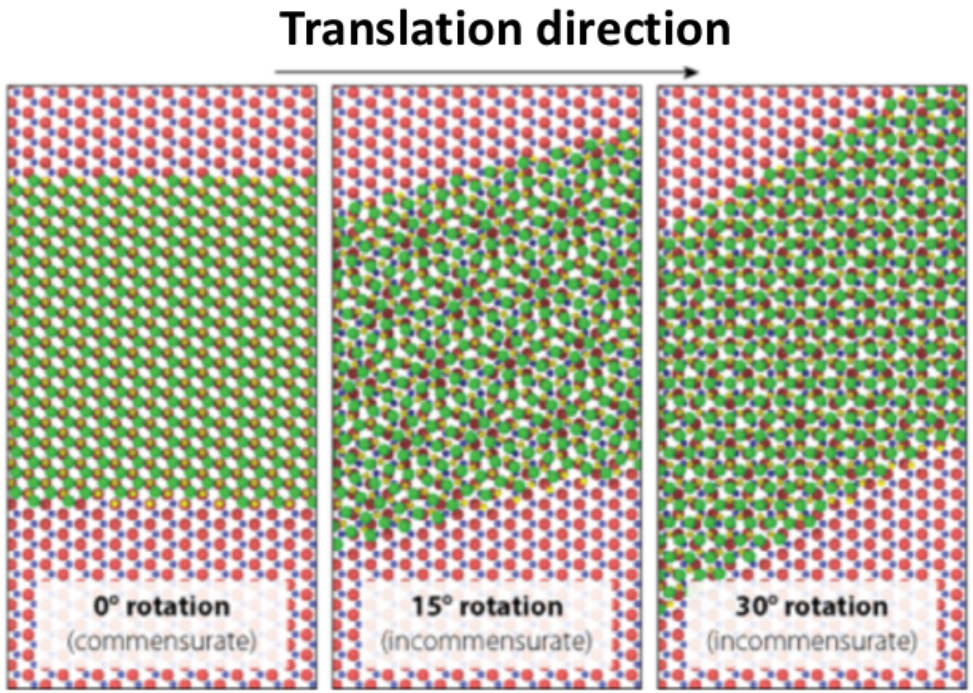
MD ReaxFF Simulations

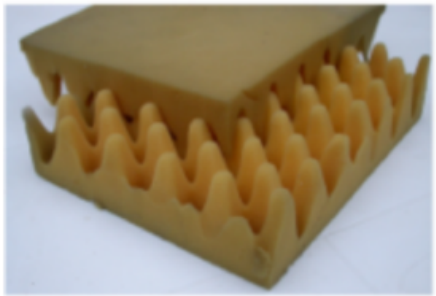




- MD has higher defect density, similar to $S_{T=0K}$ prior to shear-induced ordering
- Non-Arrhenius behavior, temperature transition, and elastic contact $\rightarrow$ activated processes and energy barriers?

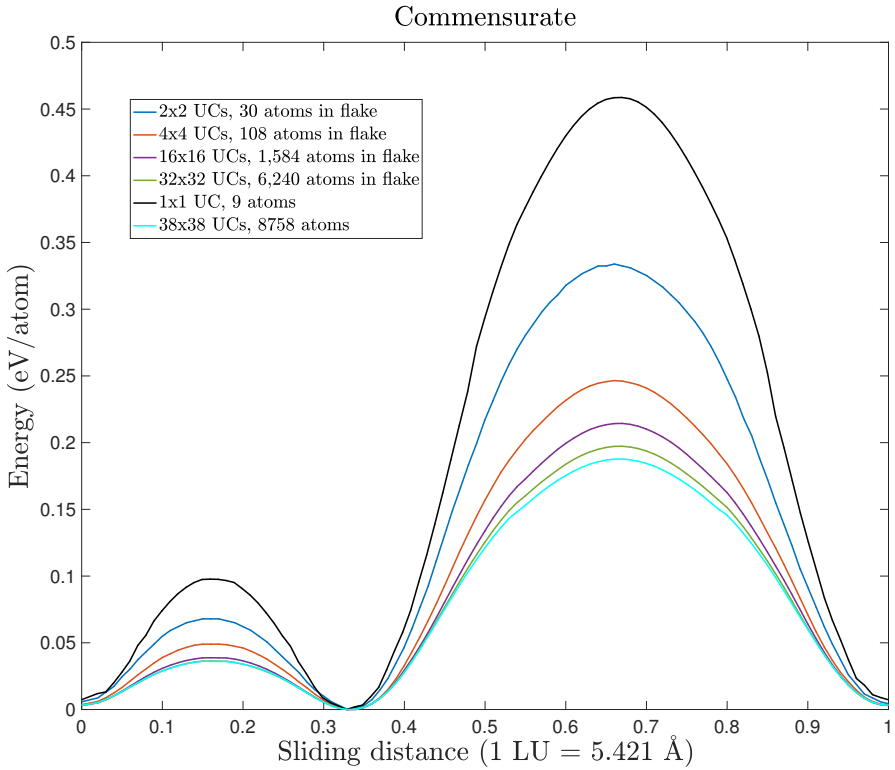
Nudged Elastic Band Calculations and Commensurate Sliding



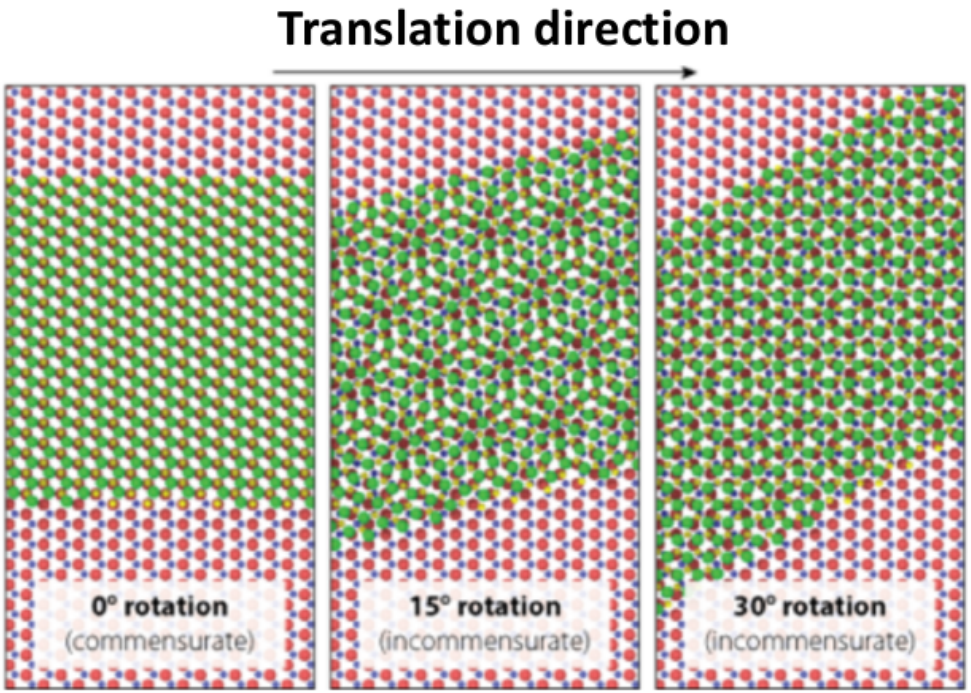


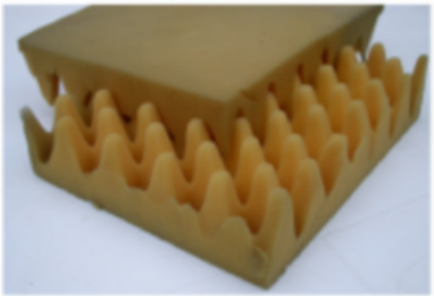
commensurate
egg shell

incommensurate
egg shell



Rotation Barrier





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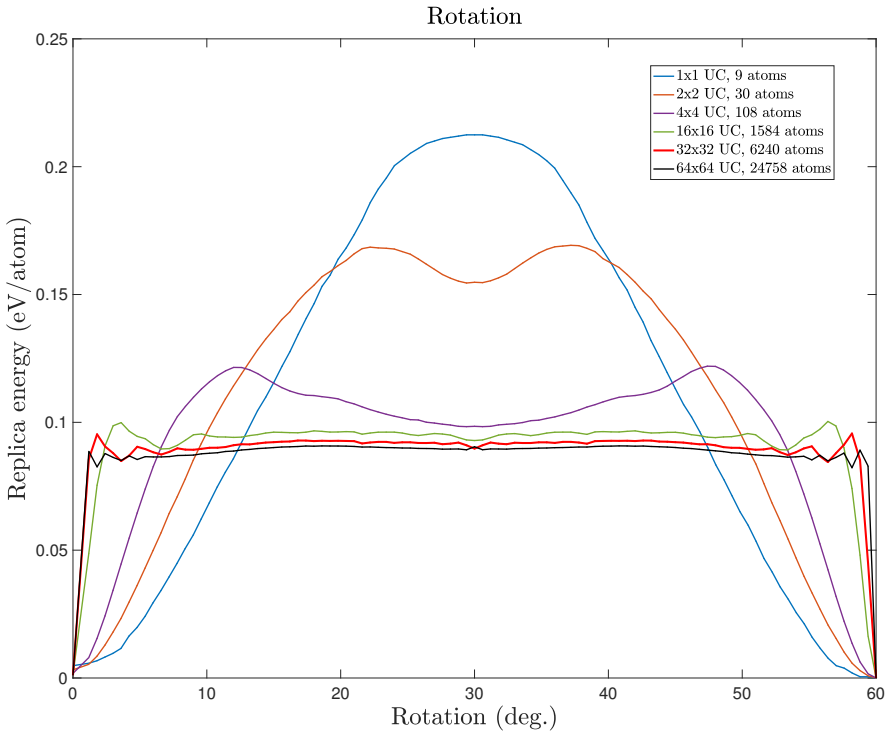
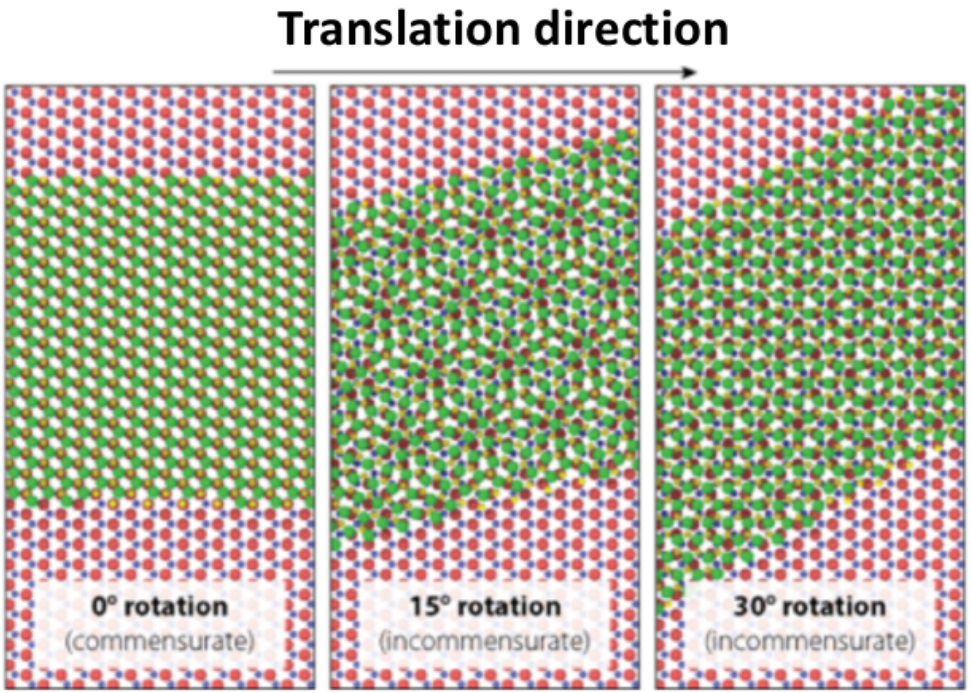
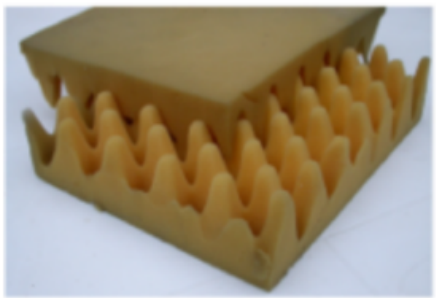


Incommensurate Barrier





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egg shell

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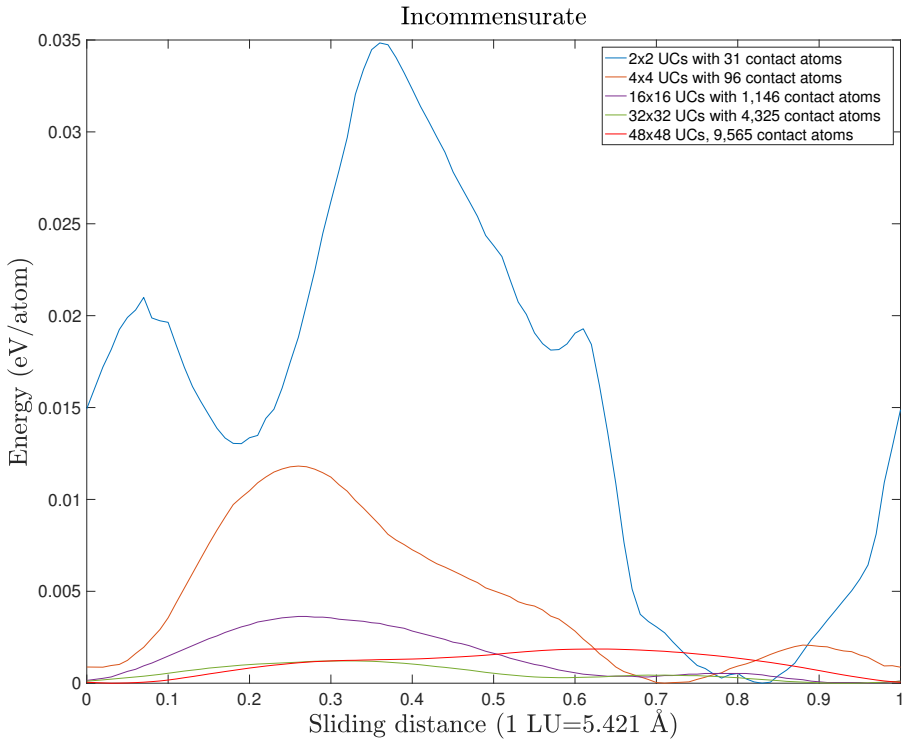
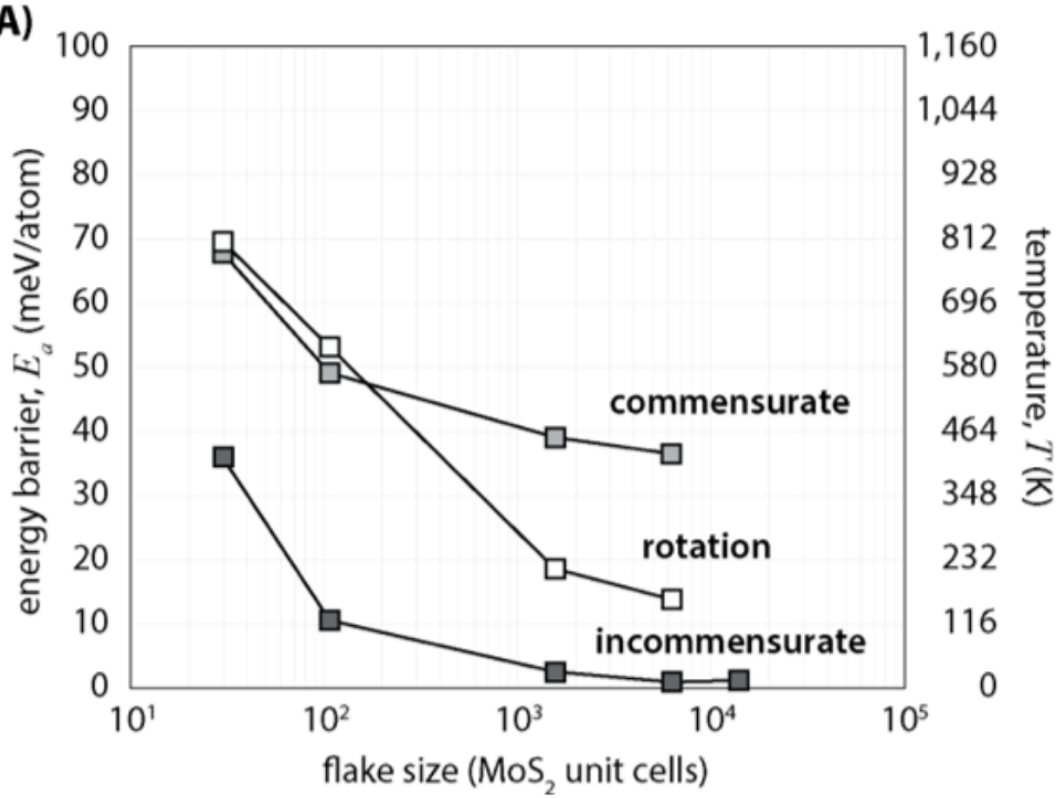


A Toy Model in terms of energy barriers (mechanisms to sliding)



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):

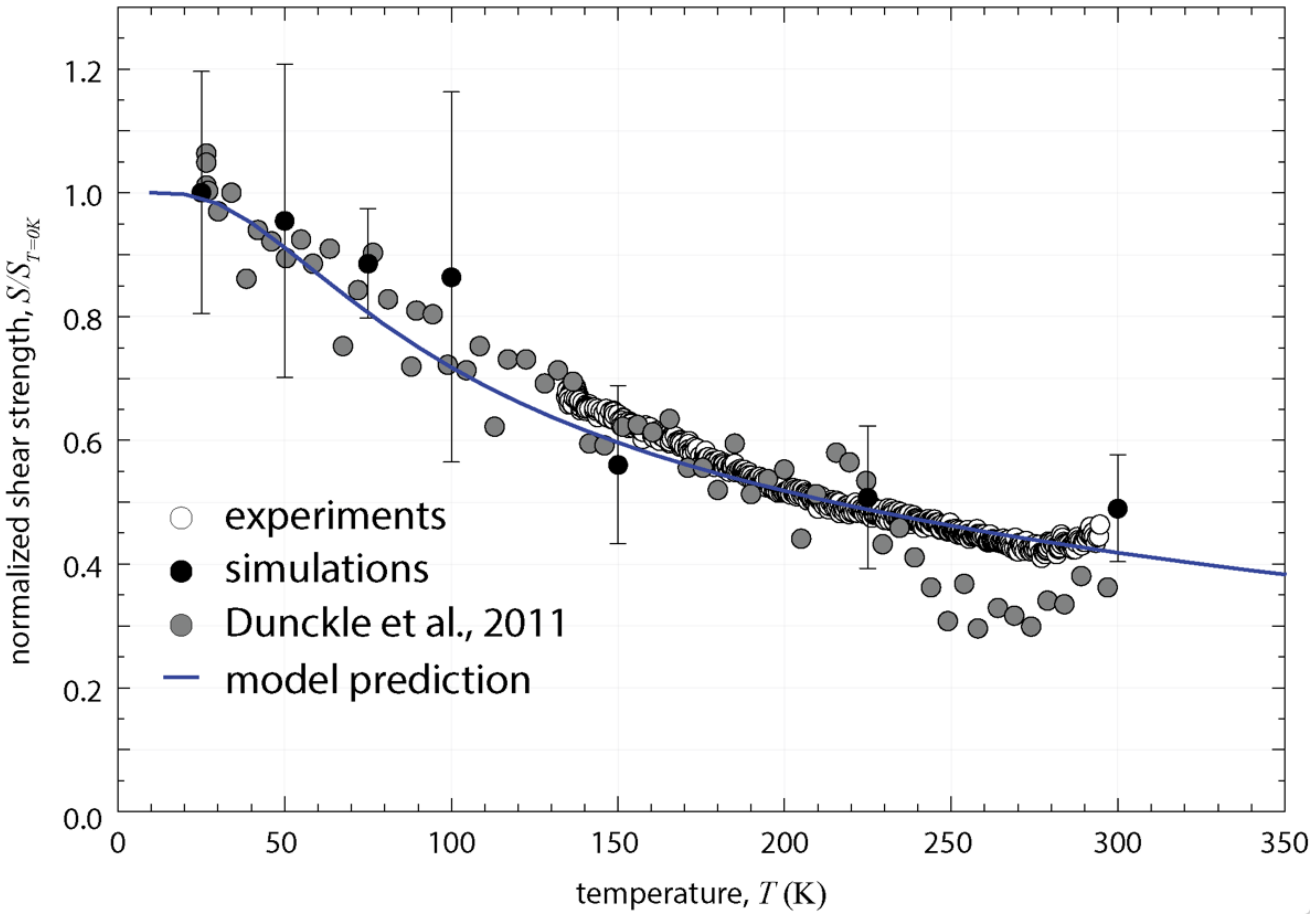
$$p_{slide} = p_r p_i + f_r p_c$$

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

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

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

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



Acknowledgements & Questions

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