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A Model of Interfacial Shear Strength in 2D Materials

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

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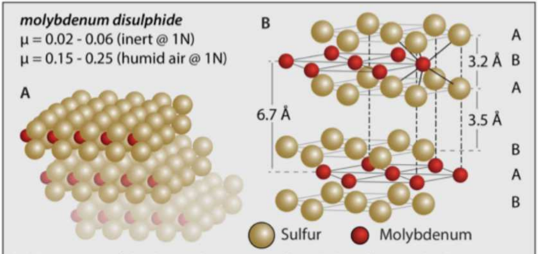
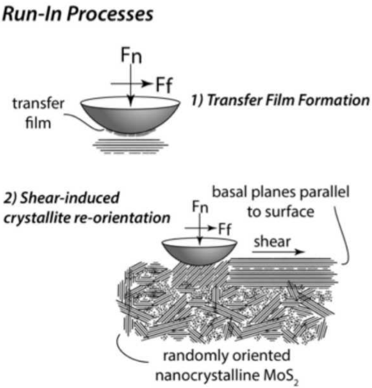
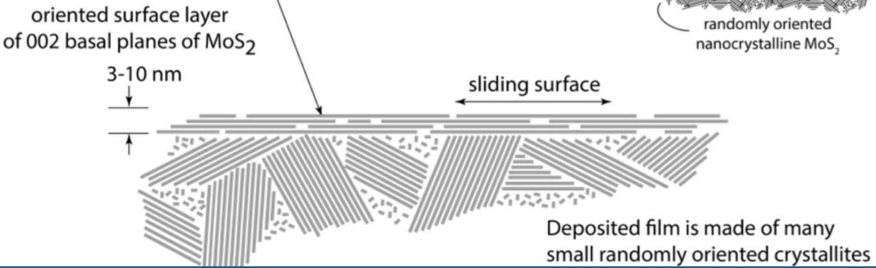
Molybdenum disulphide (MoS_2): Chemistry & sliding friction



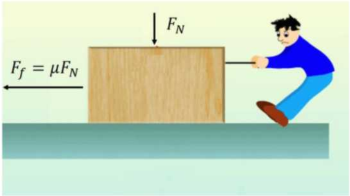
(A) Depiction of the layered structure of MoS_2 lamellae stacked upon one another. (B) Hexagonal stack lattice structure of MoS_2 with atomic spacing and sequencing.





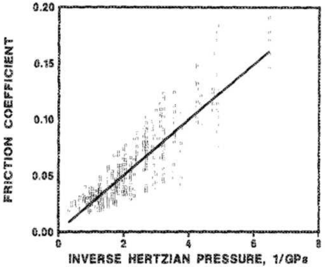
Friction: Amontonian v. Non-Amontonian

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)



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

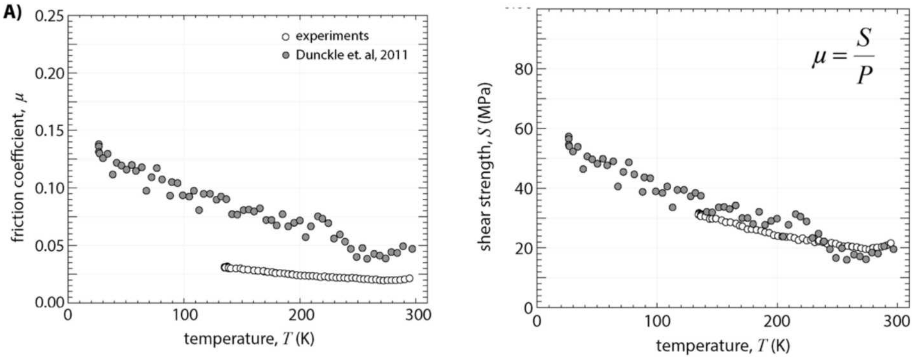
$$F_f = S_o A_{\text{real}} + \alpha F_N$$

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

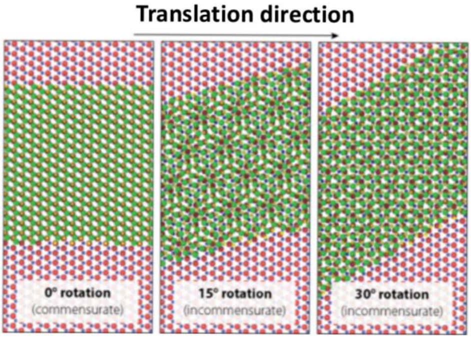
$$\approx \frac{S_o}{P} = S_o(T)\pi \left(\frac{3R}{4E}\right)^{\frac{2}{3}} F_N^{-\frac{1}{3}}$$

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

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



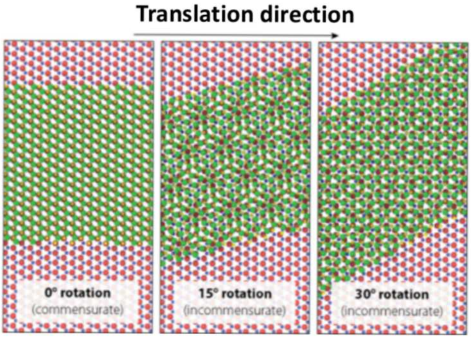
Nudged Elastic Band Calculations and Commensurate Sliding

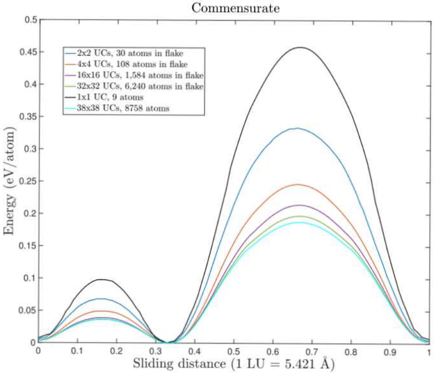


commensurate
egg shell

incommensurate
egg shell

Nudged Elastic Band Calculations and Commensurate Sliding

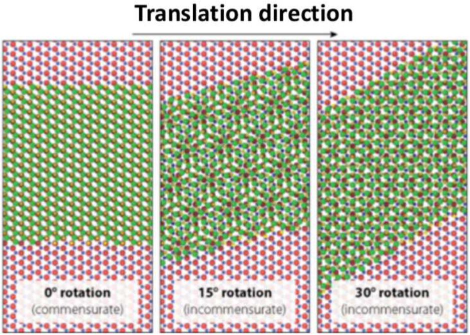




commensurate
egg shell

incommensurate
egg shell

Rotation Barrier



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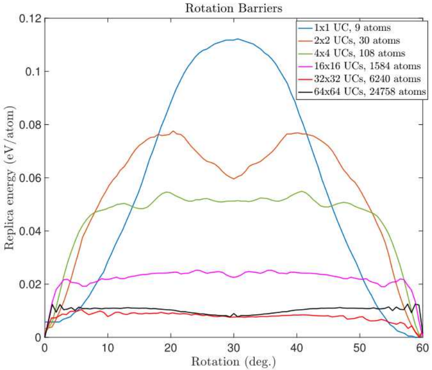
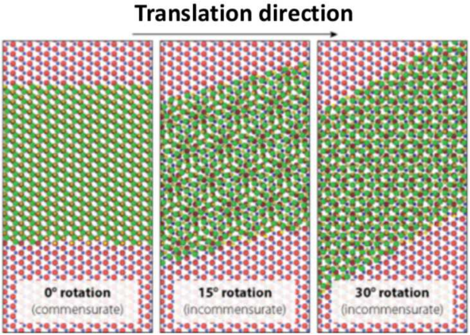


Incommensurate Barrier



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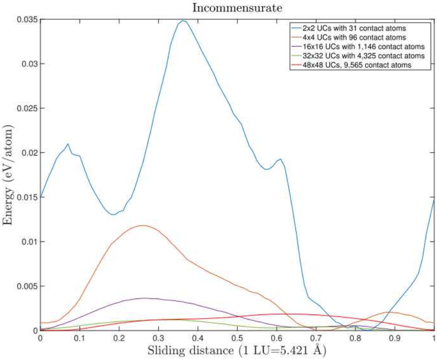
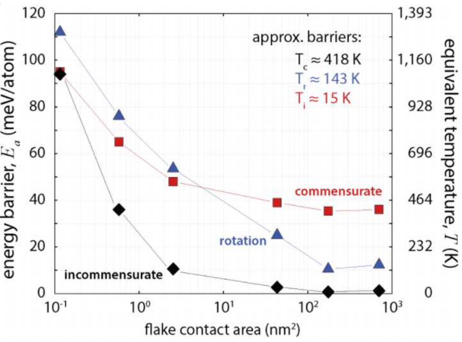


A Toy Model in terms of energy barriers (mechanisms to sliding)



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):

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

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

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

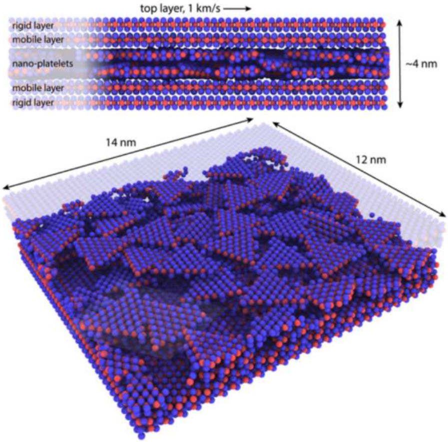
The model and scaled data from $S(T) = S_L f_{slide}(T)$

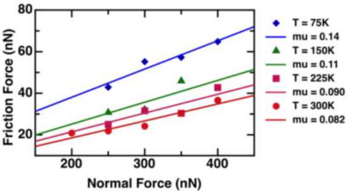
$$S(T) = S_L f_{slide}(T)$$

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

What is S_L?

MD ReaxFF Simulations

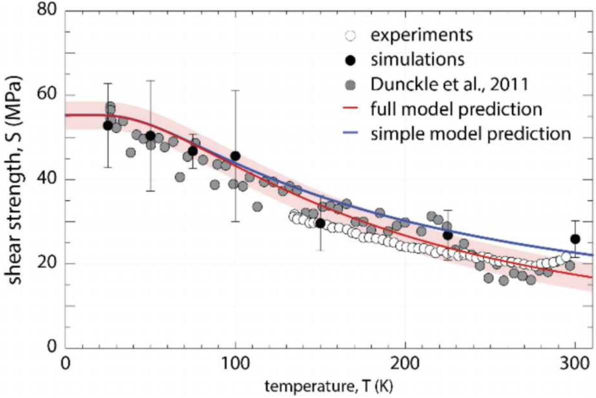




- Six normal forces used at each temperature
- $\mu = \frac{\mathrm{d}F_f}{\mathrm{d}F_N}$

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