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Thermally Activated Friction in MoS_2

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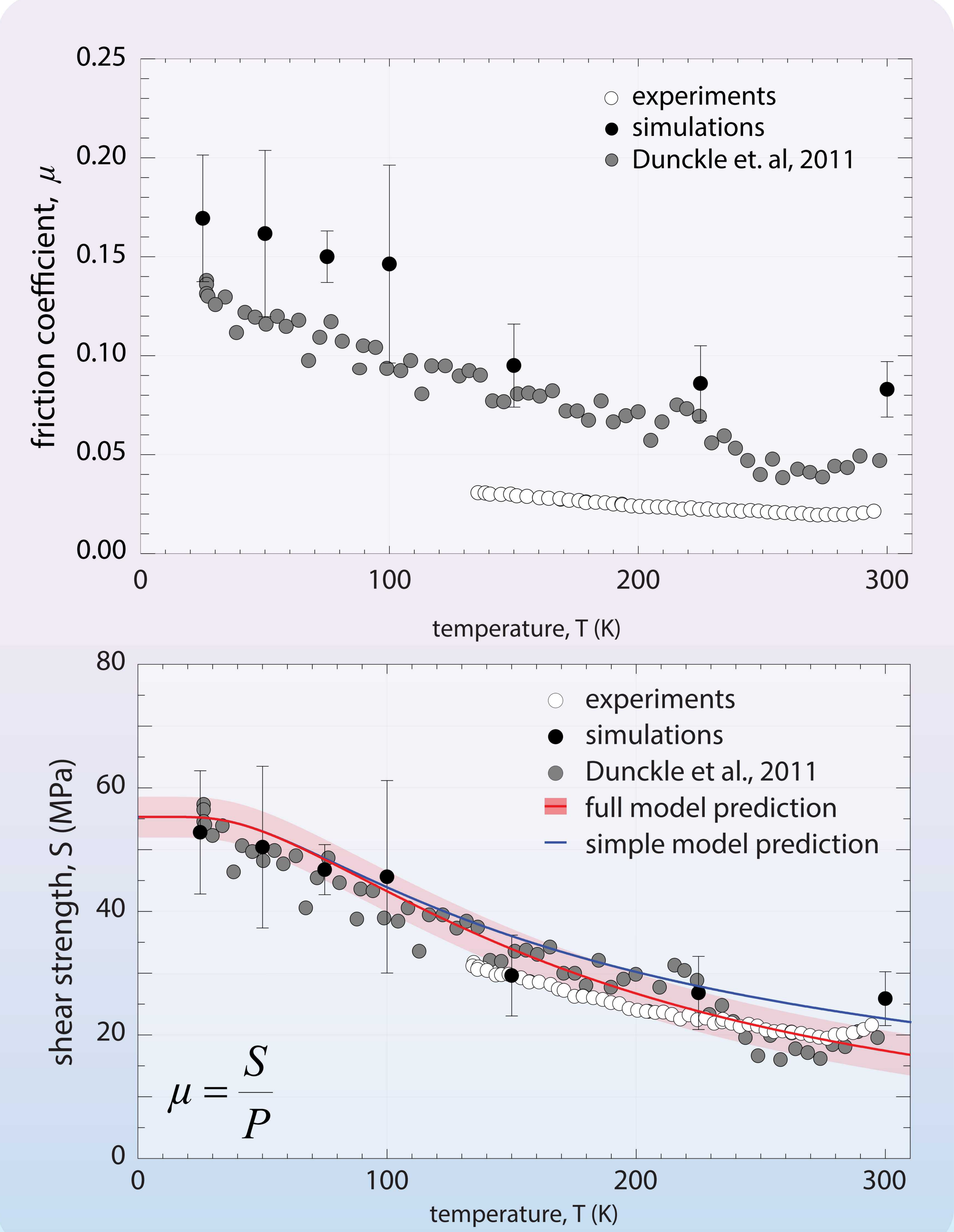
Abstract

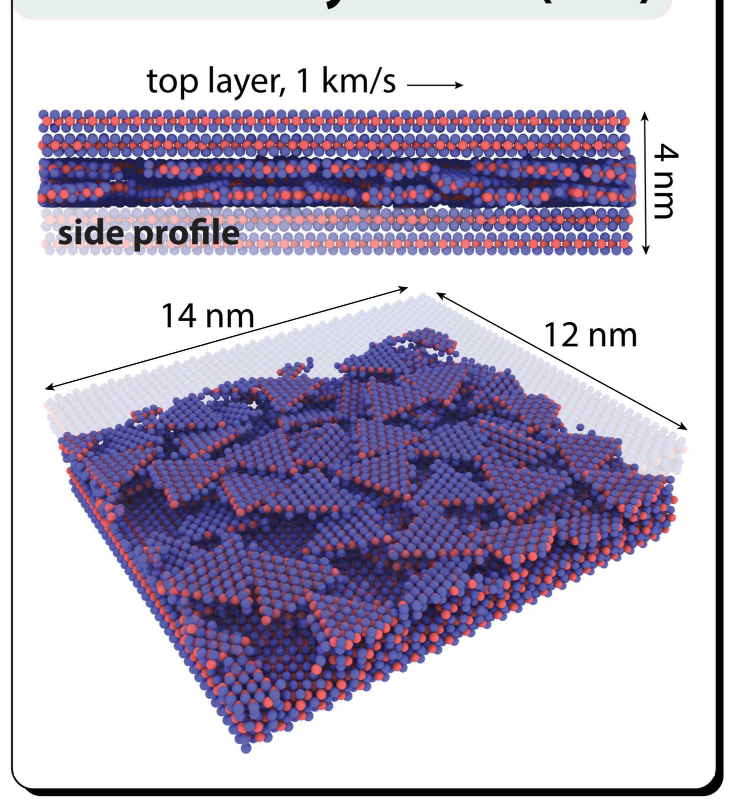
We present a model that predicts the macro-scale temperature-dependent interfacial shear strength of 2D materials like MoS_2 based on atomistic mechanisms and energetic barriers to sliding. Atomistic simulations were used to systematically determine the lamellar size-dependent rotation and translation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

Temperature Dependent Shear Strength

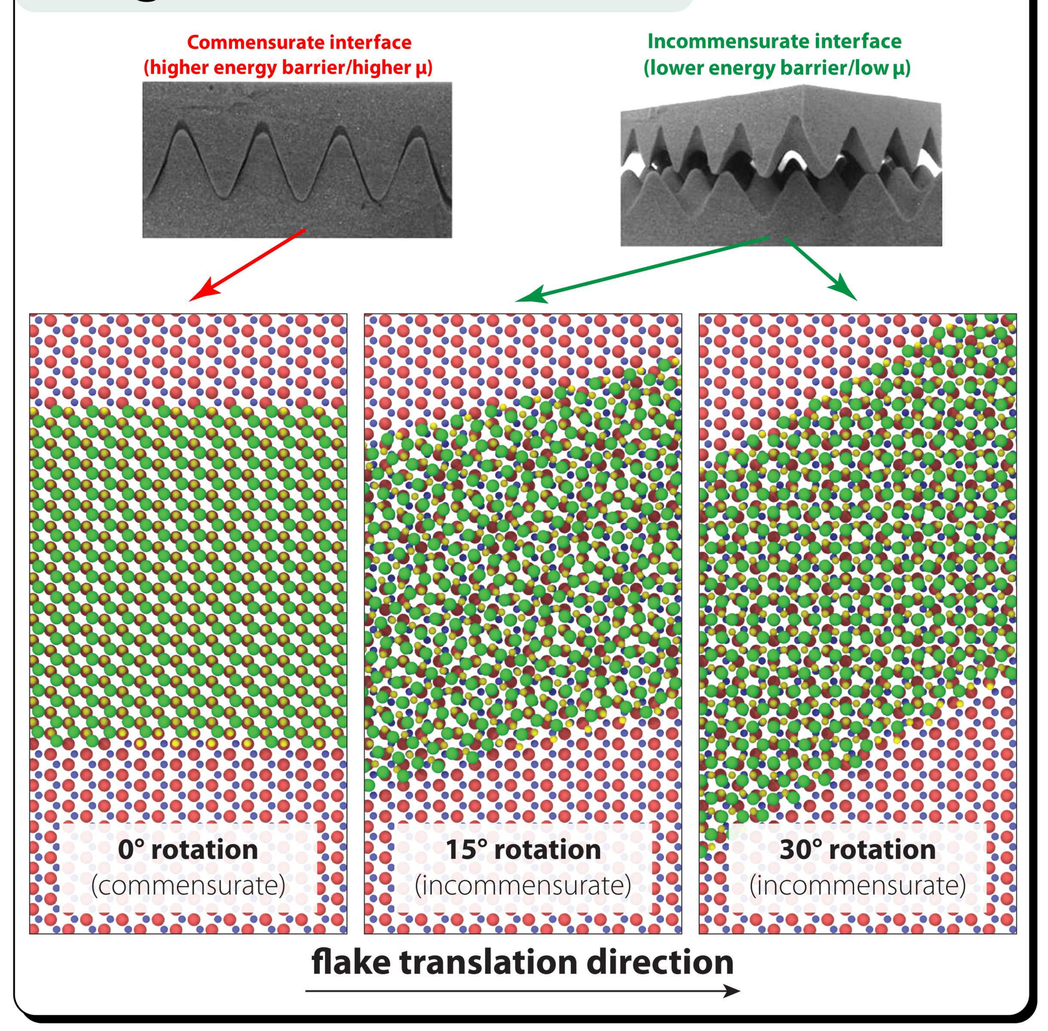


Simulation Methods MD & NEB

Molecular Dynamics (MD)

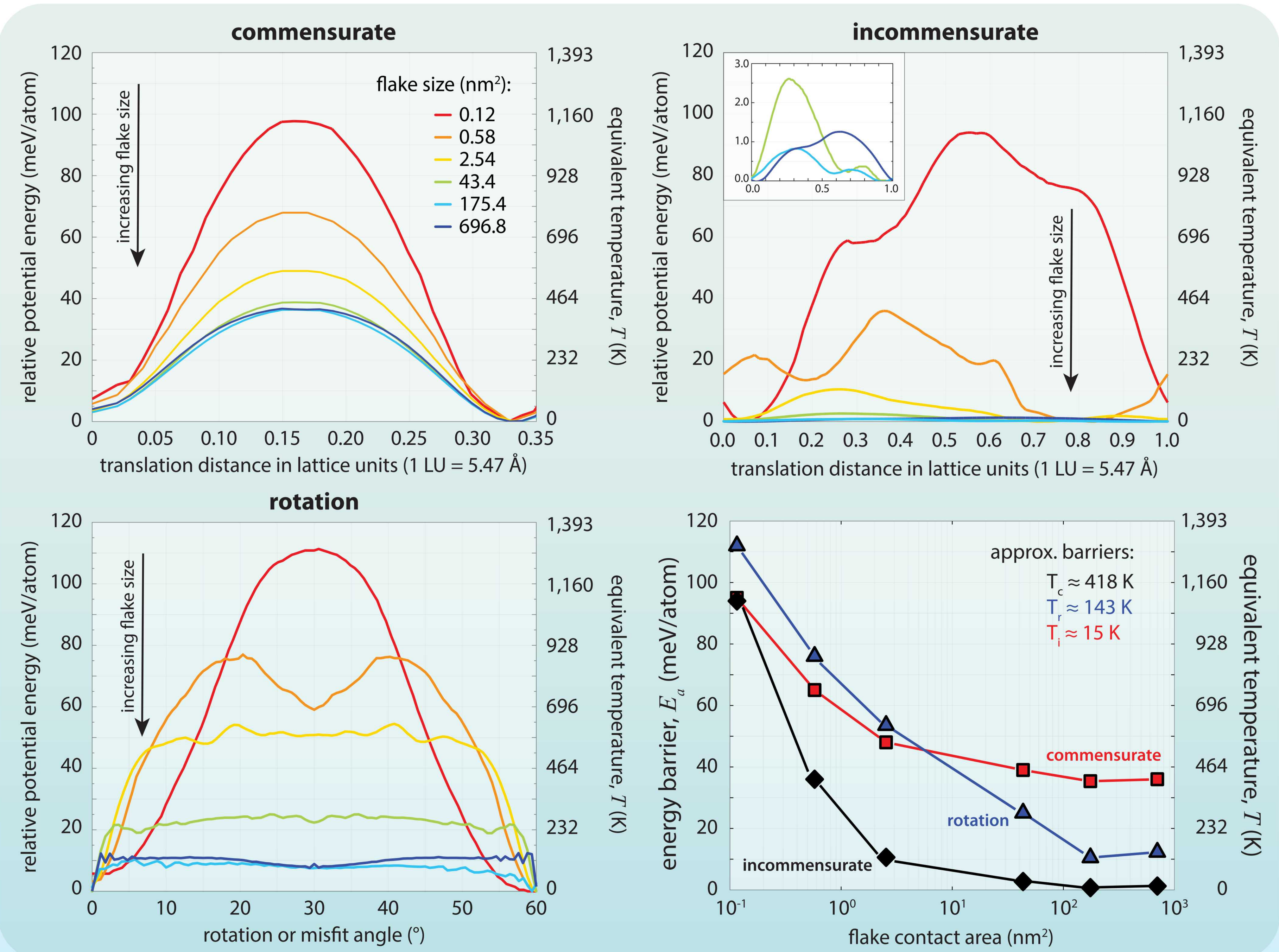


Nudged Elastic Band (NEB)



Barriers to Translation & Rotation

Run-in processes form large flakes of MoS_2 from initially amorphous states, as such it is useful to understand dependence of these barriers on flake size.



Predicting S(T) with Energy Barriers

The probability (p_n) and failure (f_n) to overcome a barrier:

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

$$f_n = 1 - p_n$$

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

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

$$f_{slide} = 1 - p_{slide} = 1 - \left(p_r p_i + f_r p_c\right)$$

T=0K shear strength; successfully rotate; slide incommensurately; failure to rotate; slide commensurately

$$S(T) = S_0\left(\left[1-\exp\left(-\frac{\Delta E_i + \Delta E_r}{k_B T}\right)\right] - \exp\left(\frac{-\Delta E_c}{k_B T}\right) + \exp\left(-\frac{\Delta E_c + \Delta E_r}{k_B T}\right)\right)$$

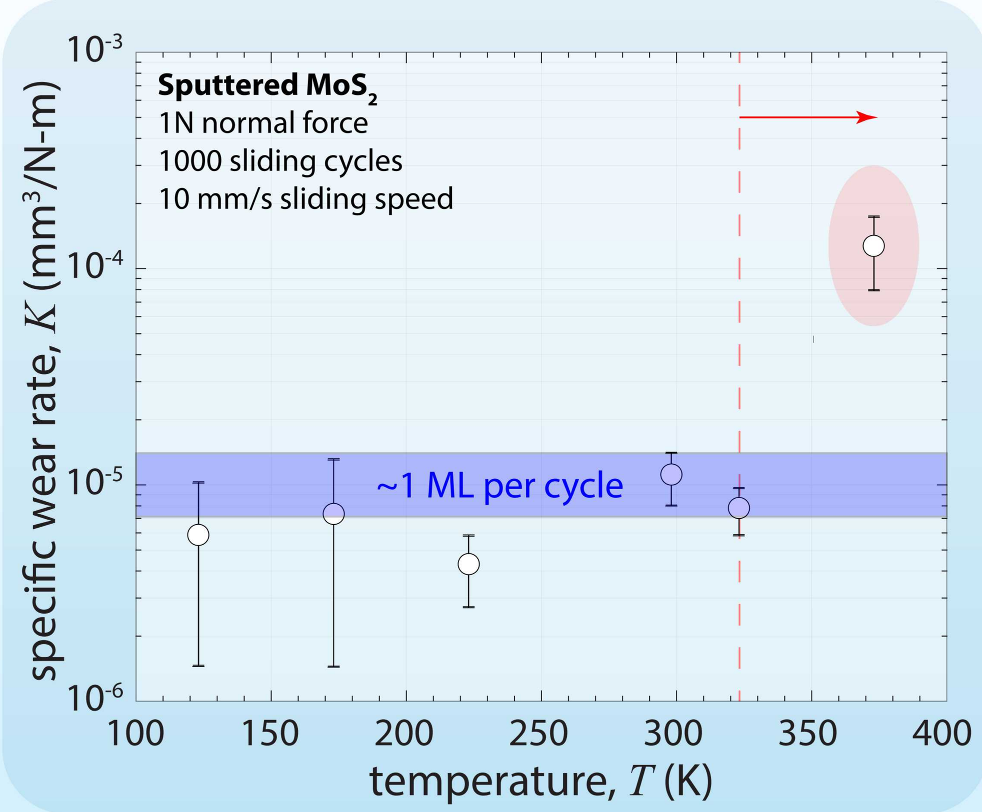
simple model prediction

full model prediction

Converged barriers (**Fig. 4**) infer model based on two routes of accomodating shear: incommensurate and commensurate translation. Typical Arrhenius describes probability of lamella sliding diffusively - friction, however, is associated with application of stress to induce sliding, so we consider failure to slide thermally (1-exp). Fit of simplified model (**Fig. 1**) also suggest incommensurate translation is most important factor.

Wear & Thermally Activated Processes

Wear rates measured in the temperature range 100-300 K **[3]** were low, with specific wear rates in the range K = 1×10^{-6} to 1×10^{-5} mm^3/Nm, indicating monolayer removal rates. Above room temp, wear increases, representing an upper bound of our model.



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[2] I. L. Singer, R. N. Bolster, J. Wegand, S. Fayeulle, and B. C. Stupp, Appl. Phys. Lett. 57, 995 (1990).
[3] T. F. Babuska, A. A. Pitenis, M. R. Jones, B. L. Nation, W. G. Sawyer, and N. Argibay, Tribol. Lett. 63, 1 (2016).

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