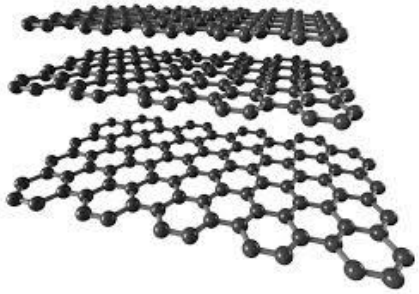
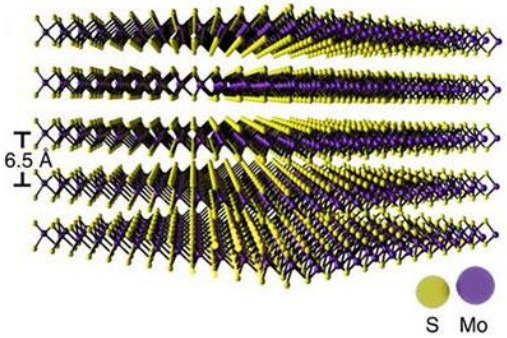
Sliding Friction of Graphene/*h*-BN Heterojunctions: Towards Robust Solid Nano-Lubrication

Davide Mandelli, Itai Leven, Oded Hod, Michael Urbakh

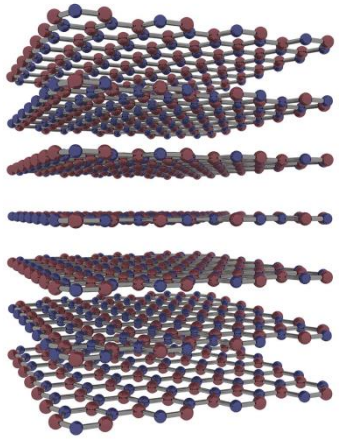
Layered Materials as Solid Lubricants



Graphite



MoS_2



***h*-BN**

Strong covalent intra-layer bonds
Weak Van-der-Waals interlayer interaction

Easy, low-strength shearing between adjacent layers

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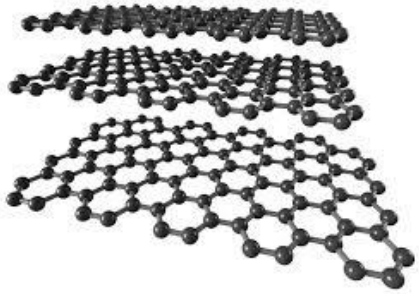

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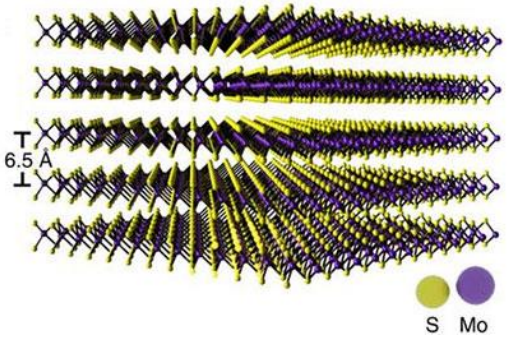

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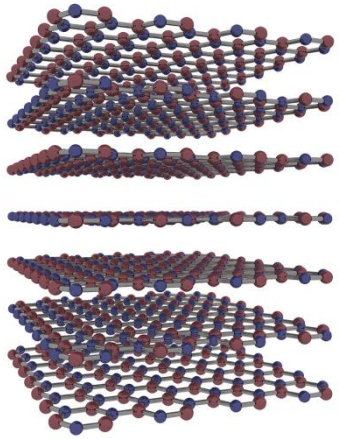

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ALREADY IN USE AS LUBRICANT ADDITIVES

Lubricants **2014**, *2*, 44-65; doi:10.3390/lubricants2020044

Graphite and Hybrid Nanomaterials as Lubricant Additives

Zhenyu J. Zhang, Dorin Simionesie and Carl Schaschke *

Wear 302 (2013) 981–986

Evaluation of hexagonal boron nitride nano-sheets as a lubricant additive in water

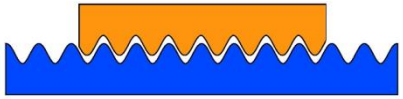
Dae-Hyun Cho [a], Jin-Seon Kim [a], Sang-Hyuk Kwon [a], Changgu Lee [**,a,b], Young-Ze Lee [*,a]

POTENTIAL APPLICATIONS IN NANO- AND MICRO-MECHANICAL DEVICES

NEMS, data storage, ...

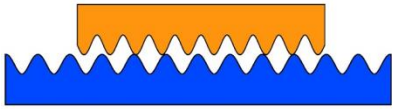
Structural lubricity: graphitic junctions

Commensurate
High barriers: large static friction
Stick-slip: large kinetic friction



Identical lattices

Incommensurate
Small barriers: small static friction
Smooth-sliding: small kinetic friction



Mismatched lattices

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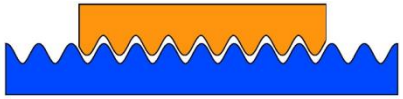

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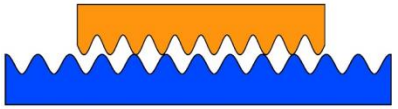

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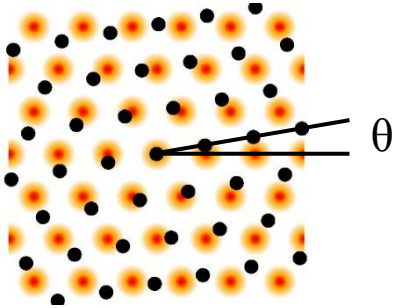
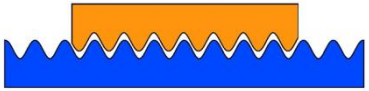
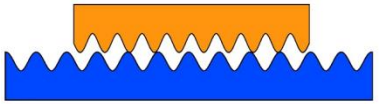
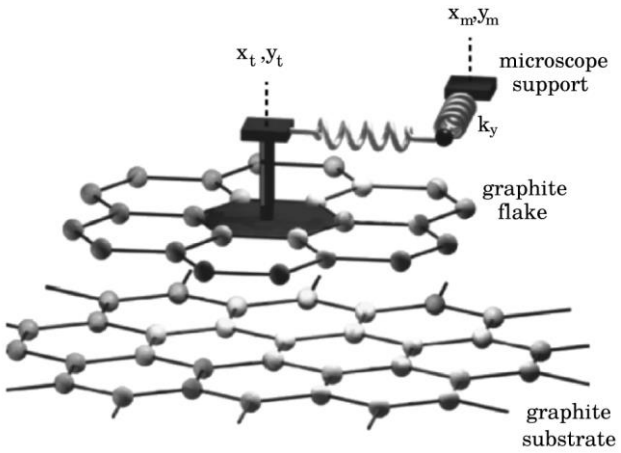


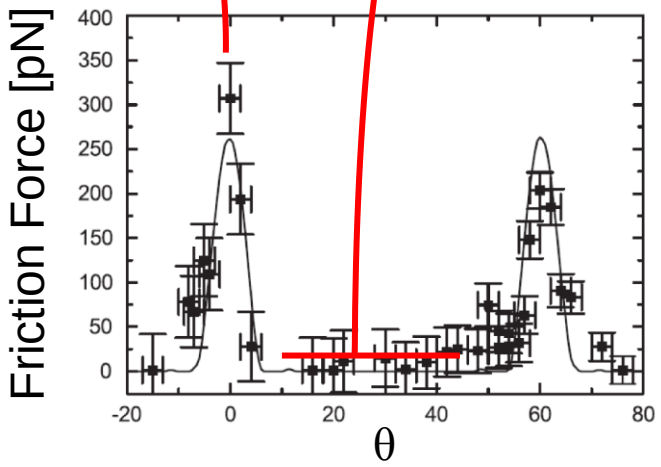
Aligned θ=k*60



Misaligned: 0<θ<60







Dienwiebel et al., Phys. Rev. Lett. 92, 126101 (2004)

Structural lubricity: graphitic junctions

Drawbacks of homogeneous junctions

PRL **100,** 046102 (2008) PHYSICAL REVIEW LETTERS week ending 1 FEBRUARY 2008

Torque and Twist against Superlubricity

Alexander E. Filippov,[1] Martin Dienwiebel,[2,3] Joost W. M. Frenken,[2] Joseph Klafter,[4] and Michael Urbakh[4]

Superlubricity in nano-sliders is only temporary as they tend to realign with the substrate.

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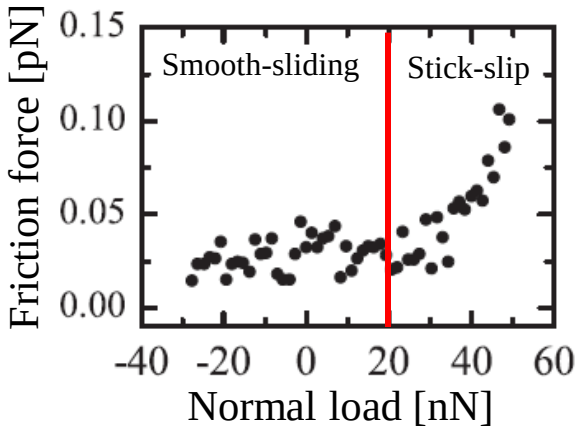
PHYSICAL REVIEW B **88**, 235423 (2013)

Superlubric to stick-slip sliding of incommensurate graphene flakes on graphite

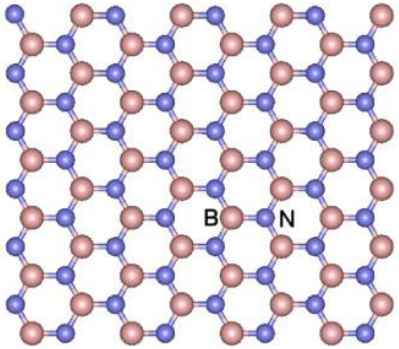
M. M. van Wijk,[1] M. Dienwiebel,[2,3] J. W. M. Frenken,[4] and A. Fasolino[1]



Even in misaligned, incommensurate conditions superlubricity may break at sufficiently high normal loads.

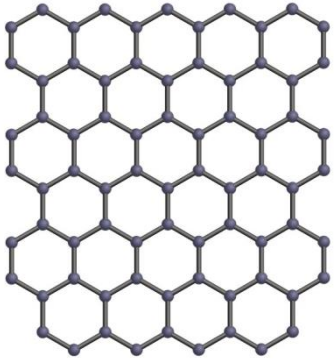
Heterogeneous graphene/*h*-BN junctions

h-BN



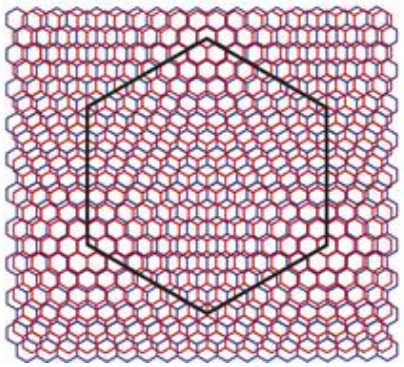
$a_{h\text{-BN}}$ = 2.50 Å

Graphene



a_g = 2.46 Å

Graphene/*h*-BN



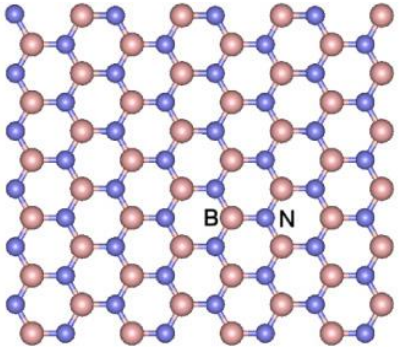
$a_{Moiré}$ ~ 14 nm

The natural intra-layer mismatch envisages the possibility to achieve superlubricity even in aligned configurations, when the size of the contact exceeds the Moiré periodicity. [1]

1. Leven, I.; Krepel, D.; Shemesh, O.; Hod, O. *Journal of Physical Chemistry Letters 2013, **4**, 115-120*

Heterogeneous graphene/*h*-BN junctions

h-BN



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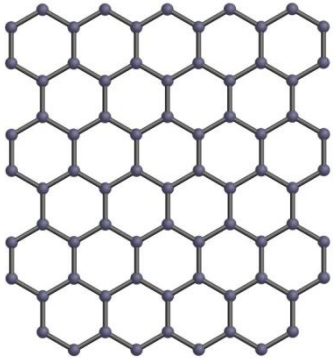

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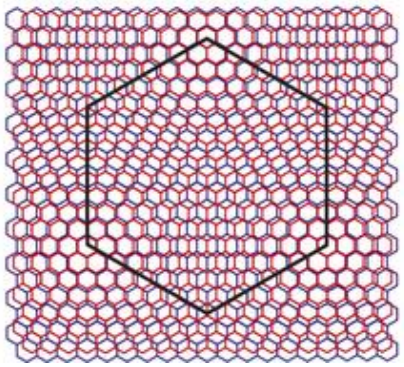

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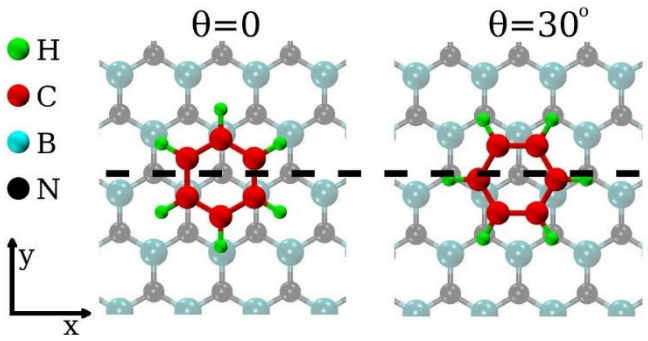
We performed fully atomistic molecular dynamics simulations of the sliding friction at **graphene/graphene** and **graphene/*h*-BN** interfaces

1. Leven, I.; Krepel, D.; Shemesh, O.; Hod, O. *Journal of Physical Chemistry Letters 2013, **4**, 115-120*

Model and simulation protocol



Hexagonal graphene flakes of increasing size N_C .

Edge carbons are saturated with Hydrogen atoms.

Sliding along high symmetry *'x'* direction.

Substrate: *rigid* monolayer.

$$H = V_{inter} + V_{intra}^{flake} \left(+V_{intra}^{substrate}\right)$$

h-BN/graphene-ILP for the heterojunction.[1]
Kolmogorov-Crespi + CH-ILP for the homojunction.[2]

REBO-potential.[3]

1. Leven, I.; Maaravi, T.; Azuri, I.; Kronik, L.; Hod, O. *Journal of Chemical Theory and Computation* 2016, ***12***, 2896-2905.
2. Kolmogorov, A. N.; Crespi, V. H. *Physical Review B* 2005, ***71***, 235415.
3. Brenner, D. W.; Shenderova, O. A.; Harrison, J. A.; Stuart, S. J.; Ni, B.; Sinnott, S. B. *Journal of Physics: Condensed Matter* 2002, ***14***, 783-802.

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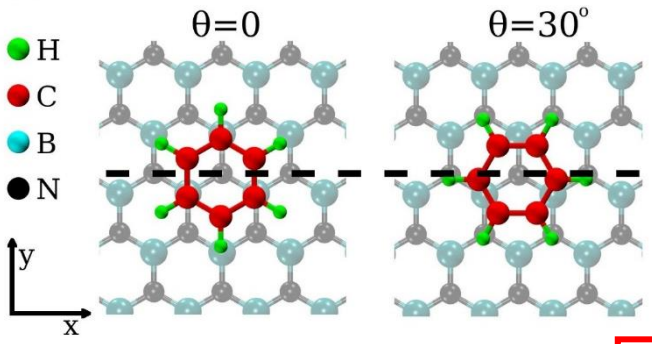

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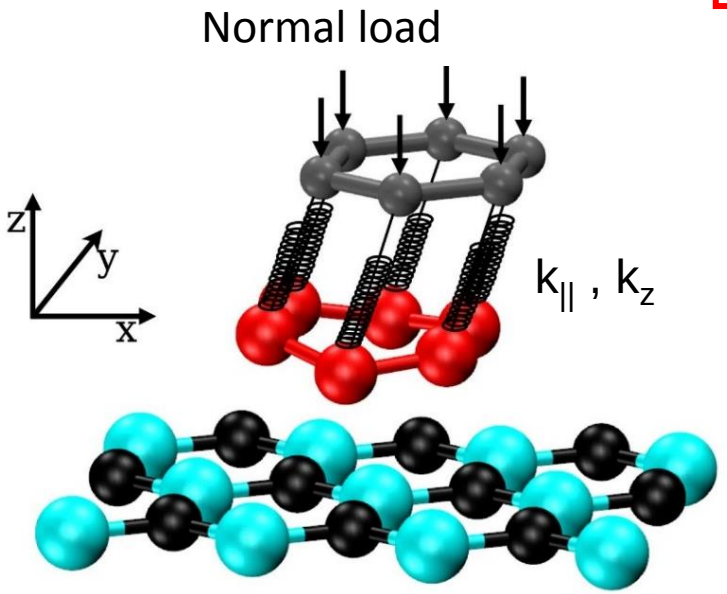
Sliding along high symmetry *'x'* direction.
Substrate: *rigid* monolayer.

$$H = V_{inter} + V_{intra}^{flake} + 1/2 \sum_{i=1}^{N_{tot}} \{k_{\|} |\boldsymbol{r}_{i\|}^{f} - \boldsymbol{r}_{i\|}^{tip}|^2 + k_z^i (z_i^f - z^{tip})^2\}$$

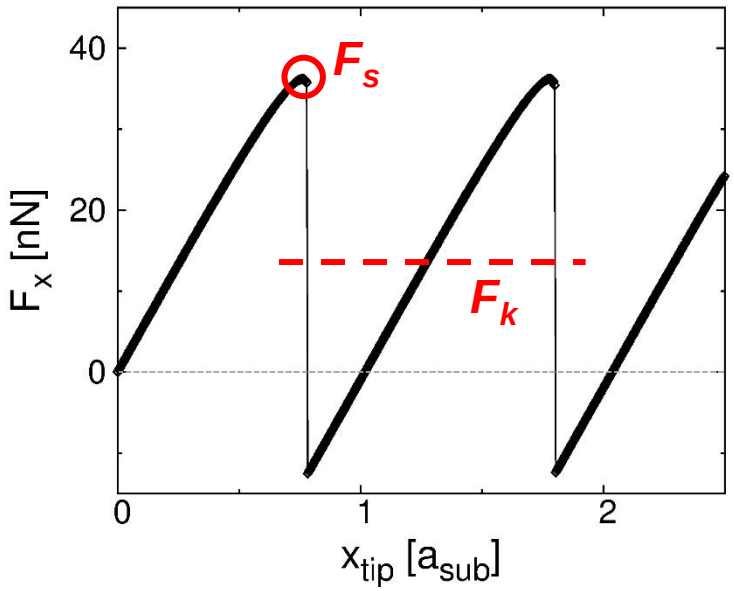
DRIVING



Quasi-static protocol

Rigid tip displaced in step Δx=0.012 Å.
Load applied along *'z'* to the tip center-of-mass.
Geometry optimized until $Max_i(F_i)<3.14\times10^{-4}$eV/ Å.
$k_{||}$ =16 meV/Å^2
$k_{z,C}$ =150 meV/Å^2
$k_{z,H}$ =43 meV/Å^2
Load/atom= 0.05 – 0.2 nN = 2 – 8 GPa.

Definitions



FRICTION FORCE

$$F_x = \sum_{i=1}^{N_{tot}} k_{\parallel}(x_i^{tip} - x_i^f)$$

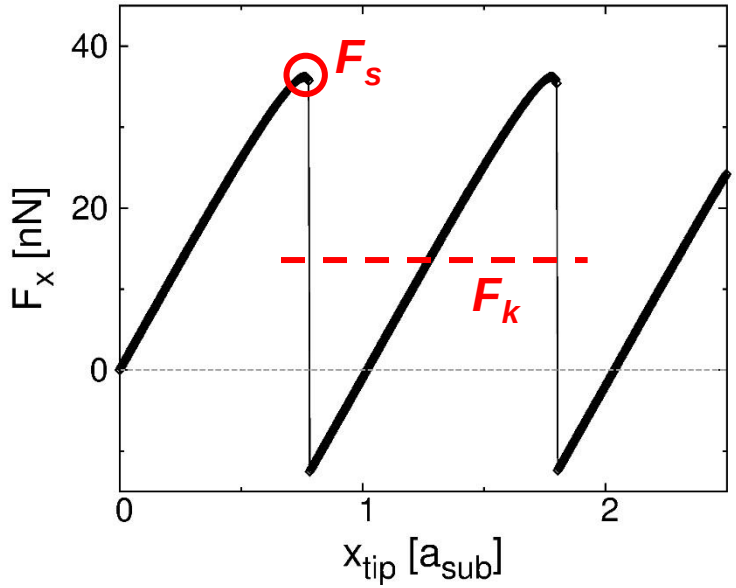
STATIC

$F_s = Max\ (F_x)$

KINETIC

$F_k =< F_x >$

Definitions



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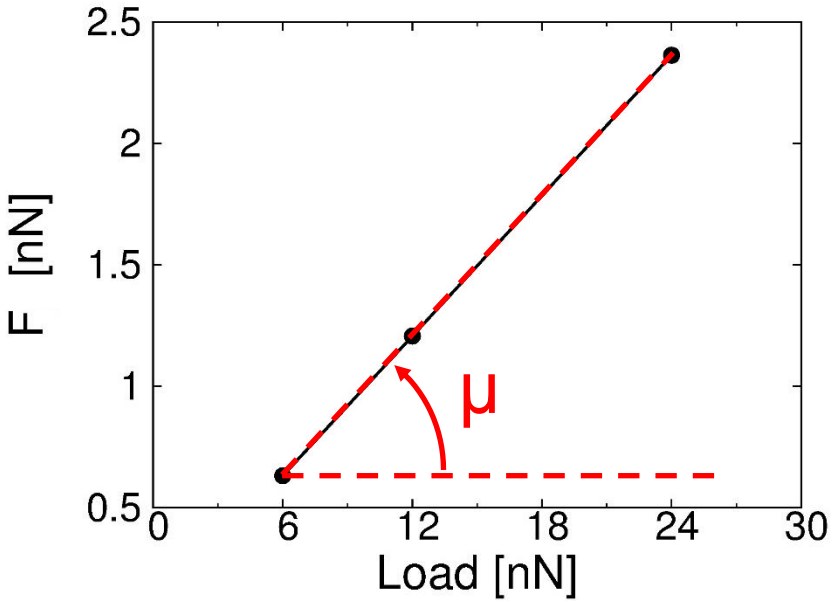

FRICTION COEFFICIENTS

$$F \approx \alpha + \mu \cdot Load$$

STATIC

$$\mu_s =< \frac{\Delta F_s}{\Delta L} >$$

KINETIC

$$\mu_k =< \frac{\Delta F_k}{\Delta L} >$$

PHYSICAL REVIEW B 88, 235423 (2013)

Superlubric to stick-slip sliding of incommensurate graphene flakes on graphite

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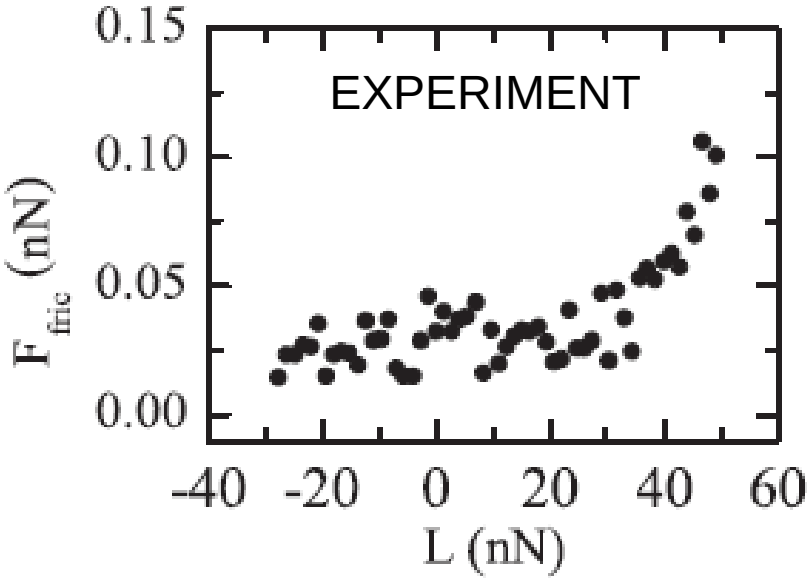
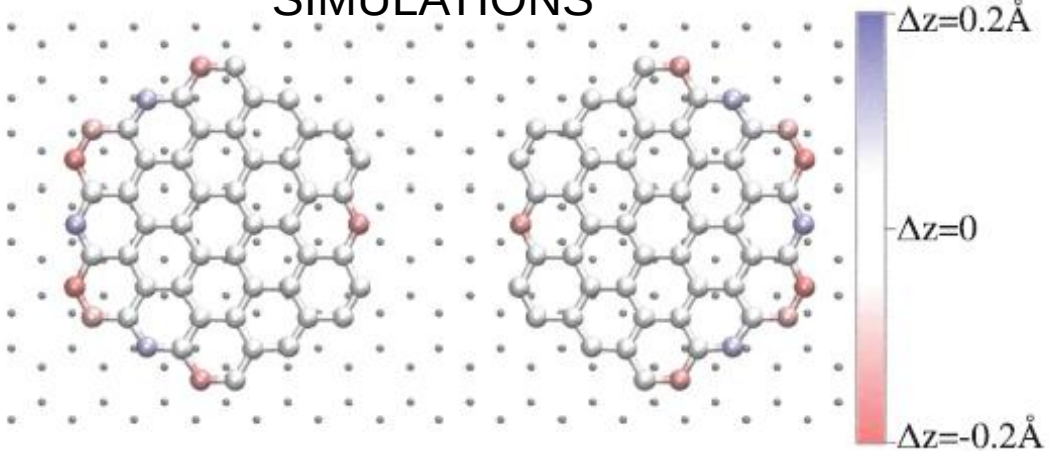
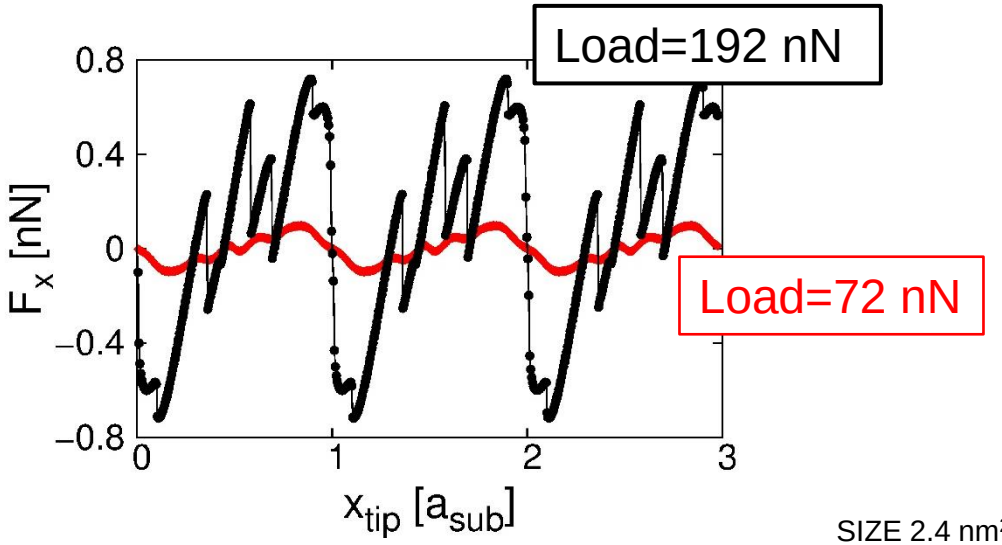


SIMULATIONS



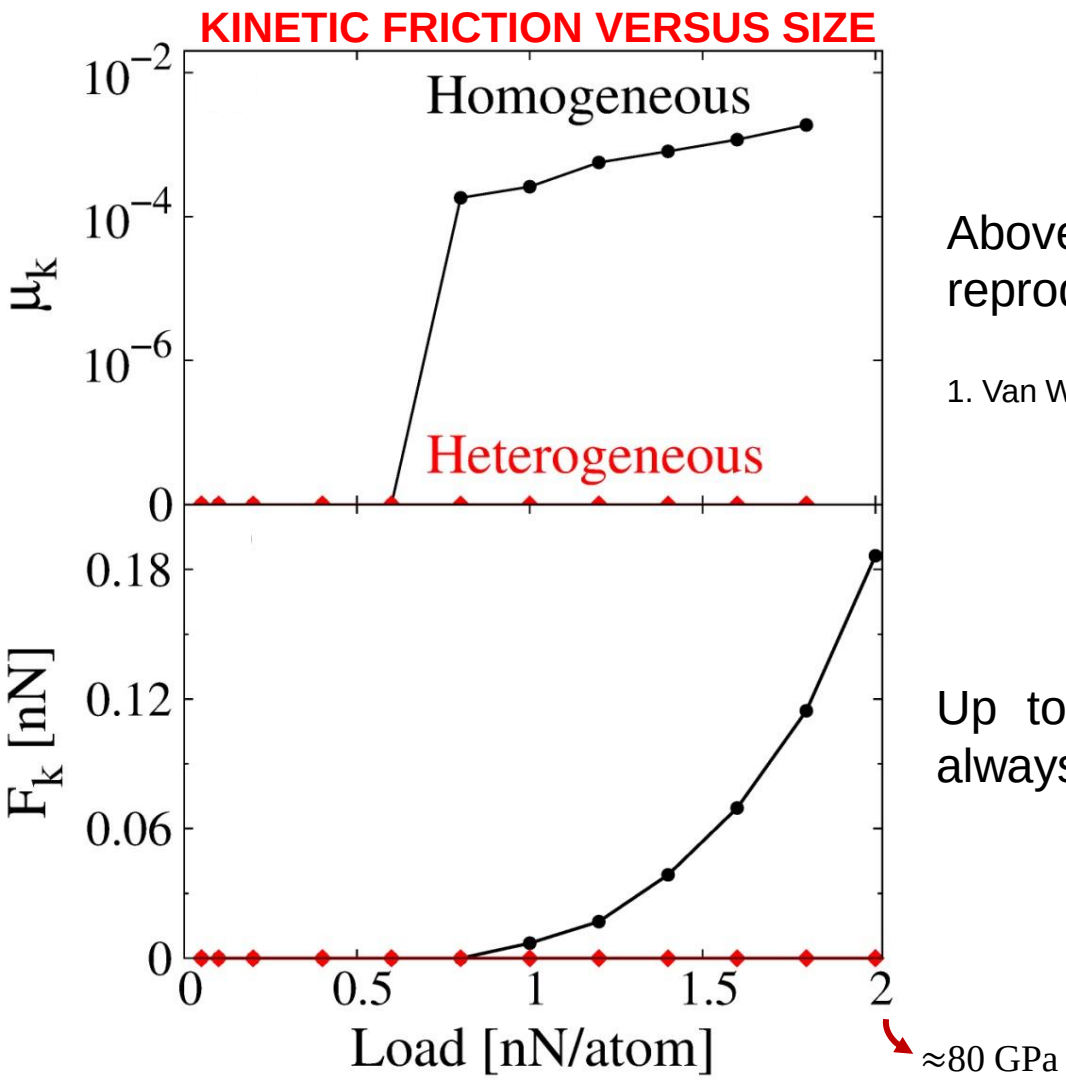
EDGE ATOMS ARE MORE MOBILE

At high loads they tend to lock the flake to the substrate.



SIZE 2.4 nm^2

Results: misaligned interfaces θ=30°



Homogeneous junction

Above L=0.8 nN/atom onset of stick-slip, reproducing the results of van Wijk *et al.*.[1]

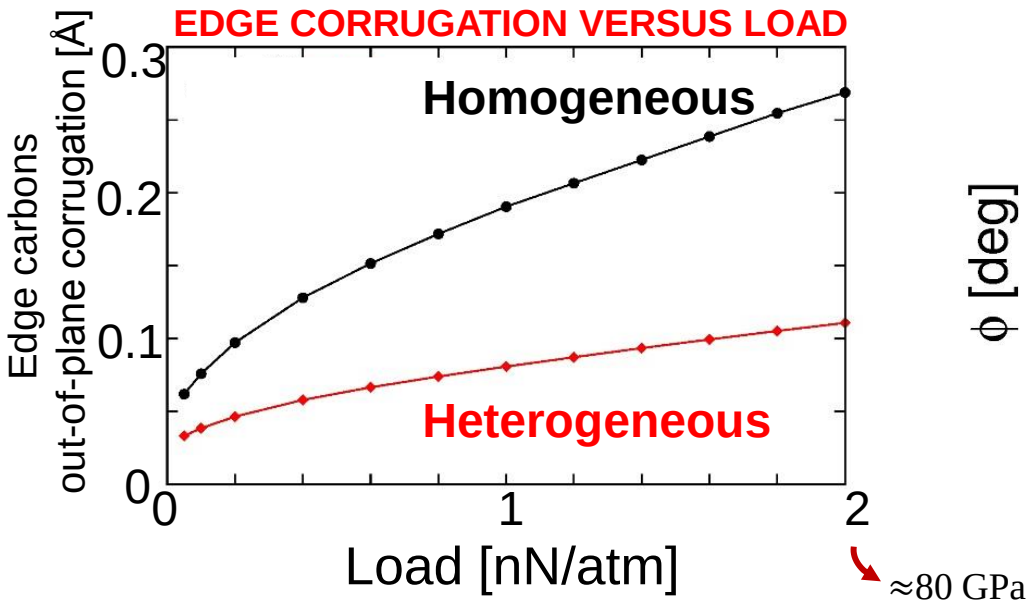
1. Van Wijk *et al.*, PRB **88**, 235423 (2013).

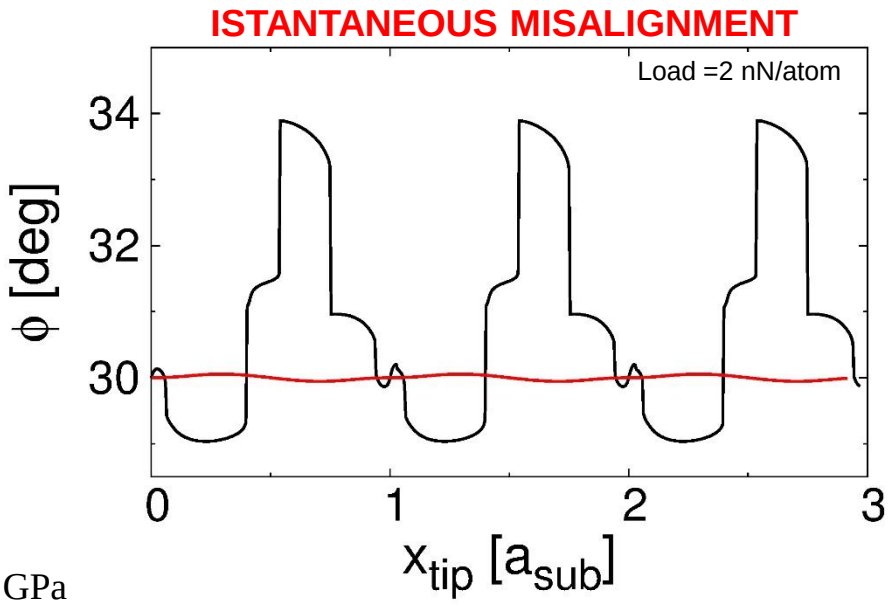
Heterogeneous junction

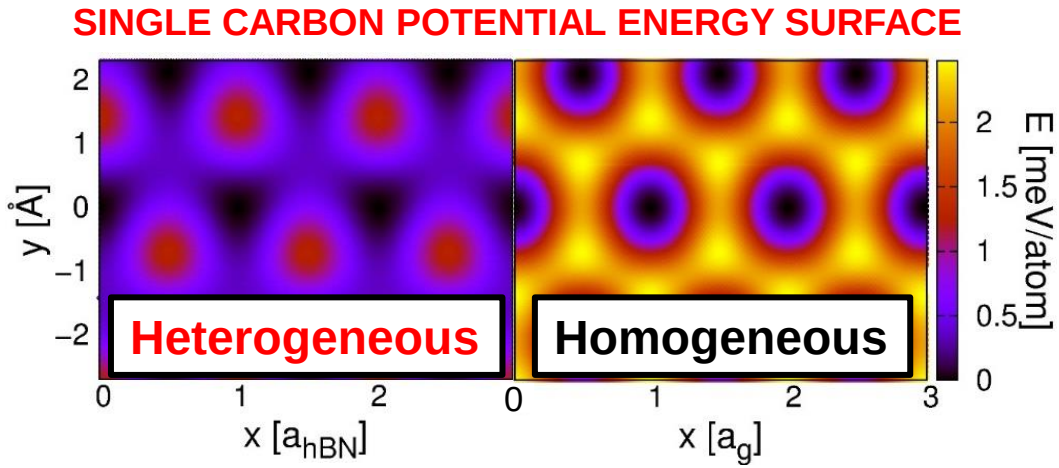
Up to the highest load investigated we always observe a smooth-sliding regime.

SIZE 2.4 nm^2

Results: misaligned interfaces θ=30°





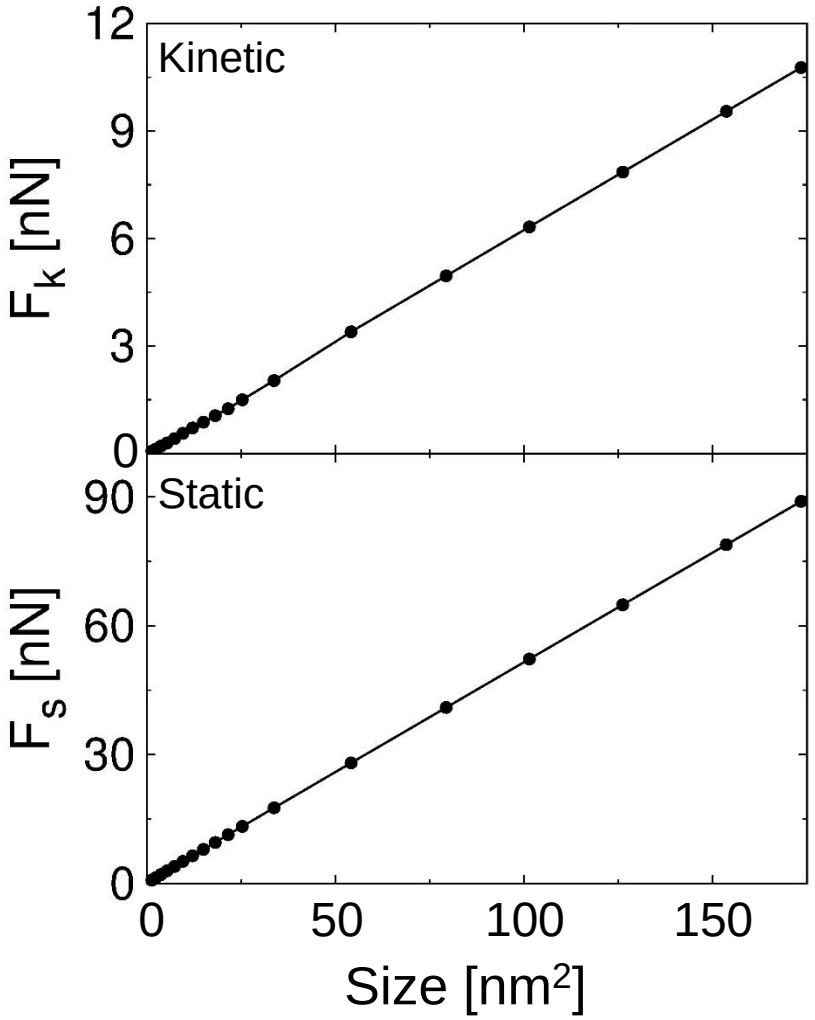


Over graphene edge carbons explore a more corrugated potential.

SIZE 2.4 nm^2

Results: aligned interfaces θ=0

FRICTION FORCE VERSUS SIZE



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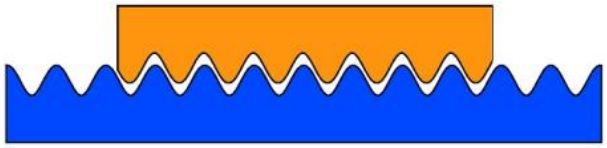
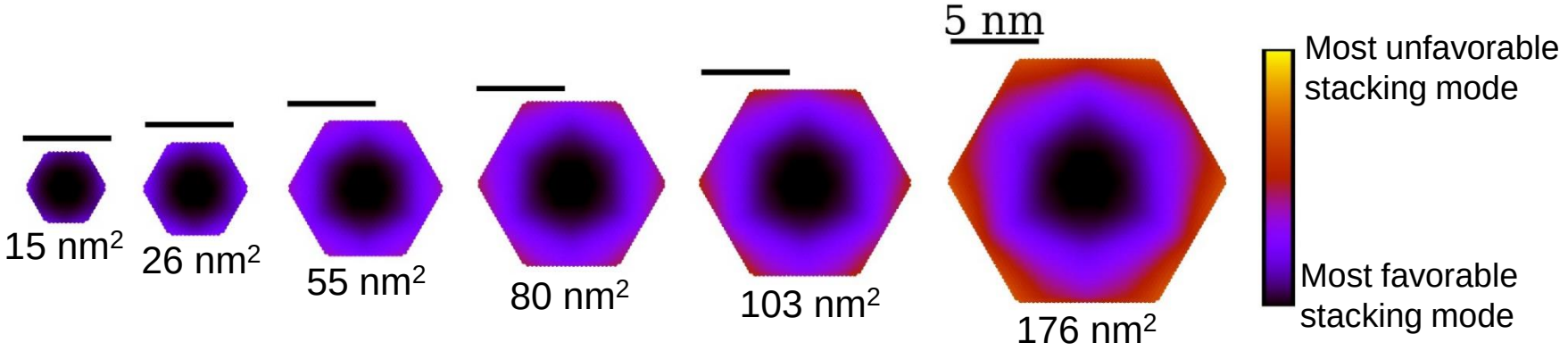


Commensurate contact:

Highly dissipative stick-slip motion.
F_k, F_s grow linearly with size.

Load =0.1 nN/atom =4 GPa



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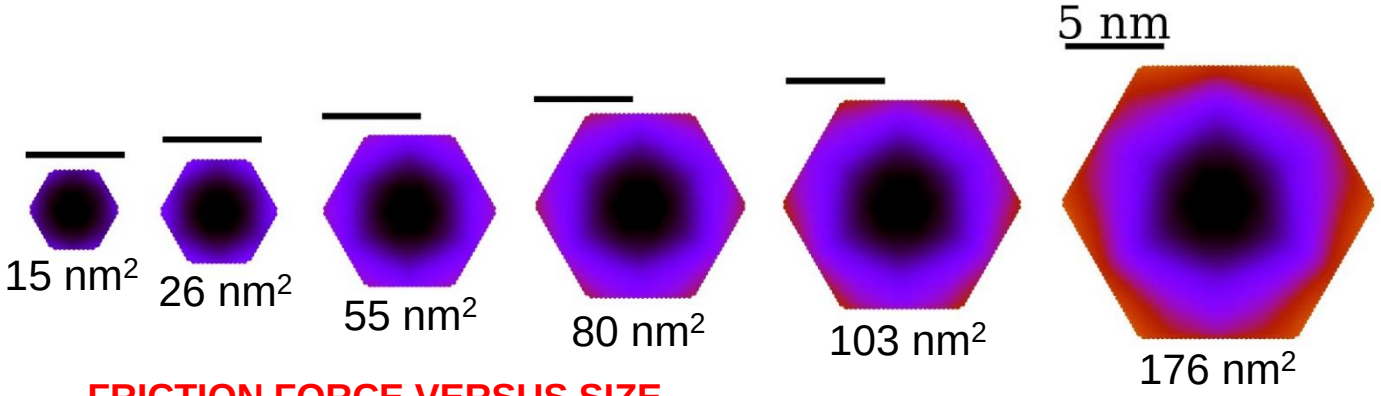
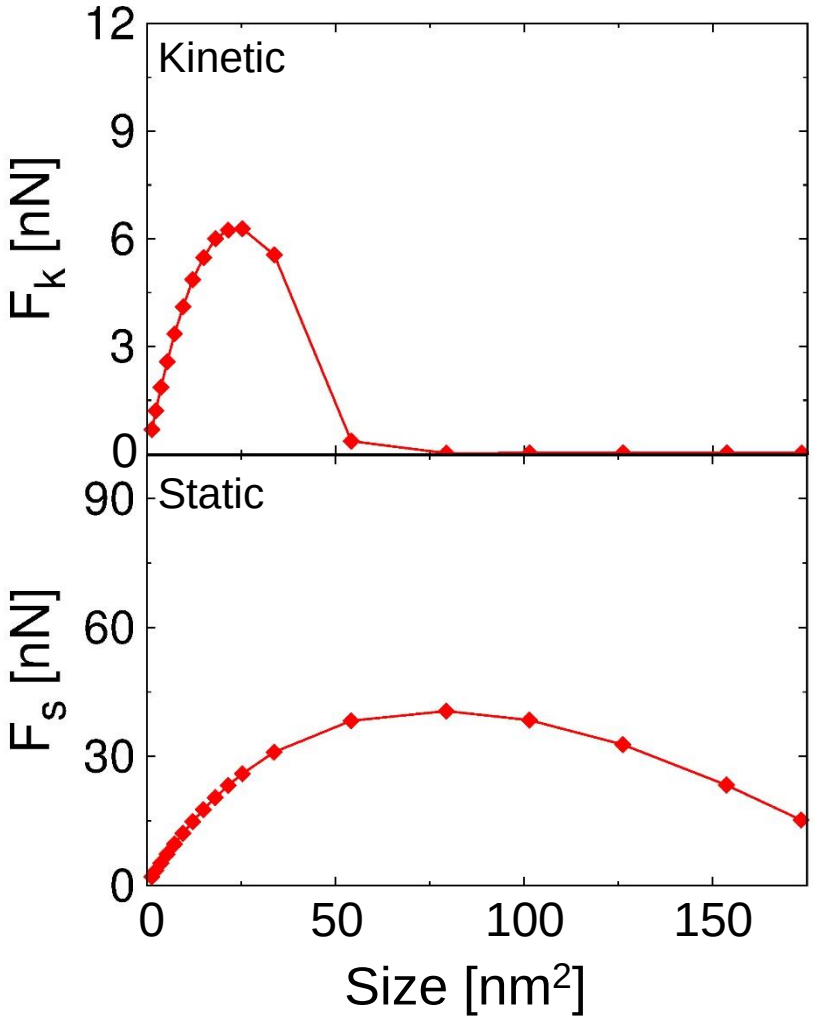


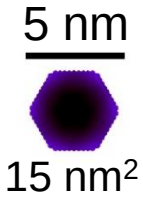
FRICTION FORCE VERSUS SIZE



Heterogeneous junction

Non-monotonic behavior of kinetic and static friction due to the progressive appearance of Moiré.

Load =0.1 nN/atom =4 GPa



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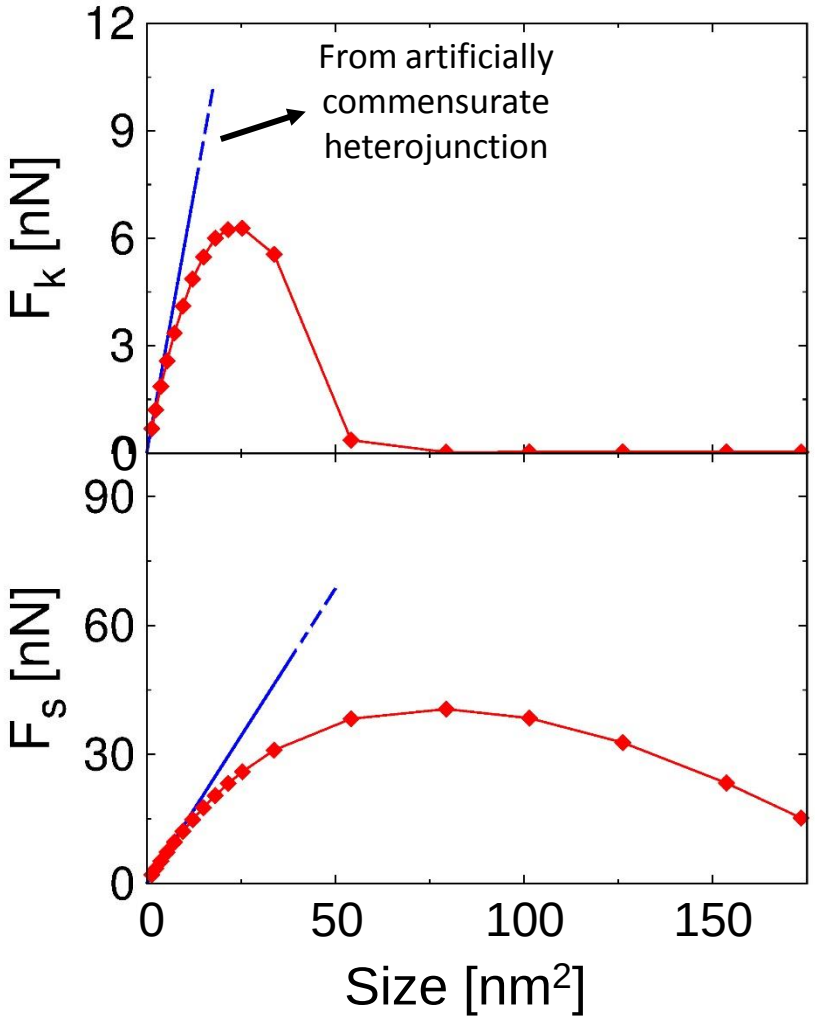
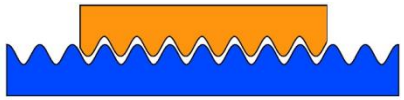
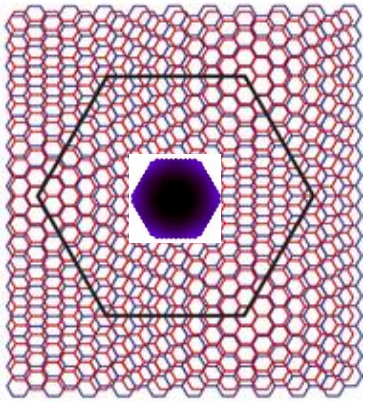
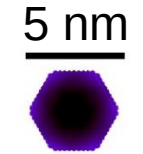


0 < size < 20 nm² stick-slip, linear increase of F_k, F_s





Load =0.1 nN/atom =4 GPa

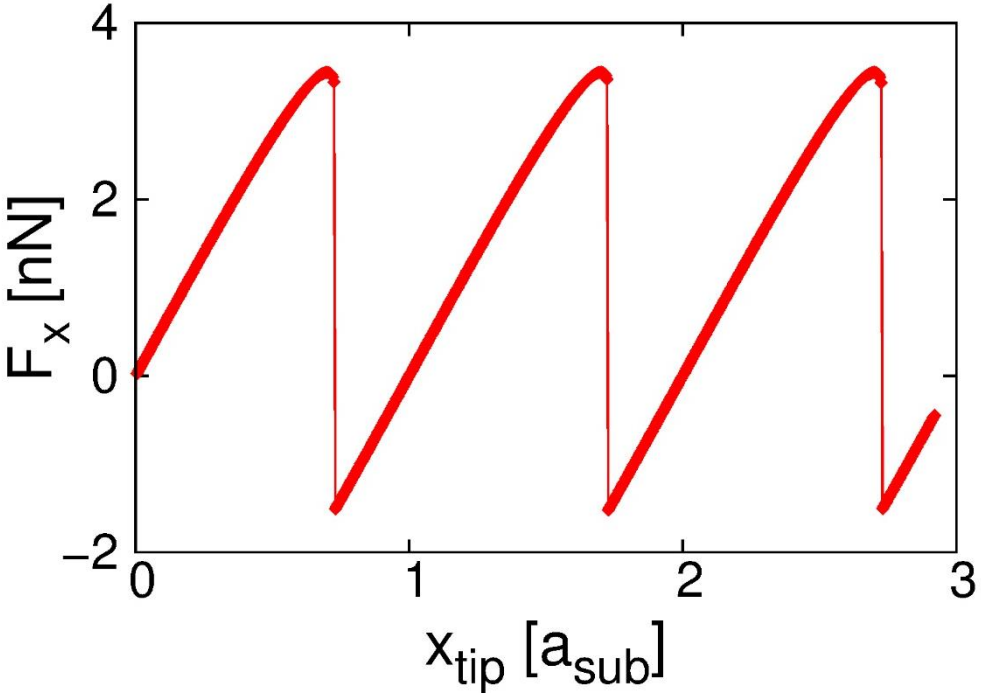


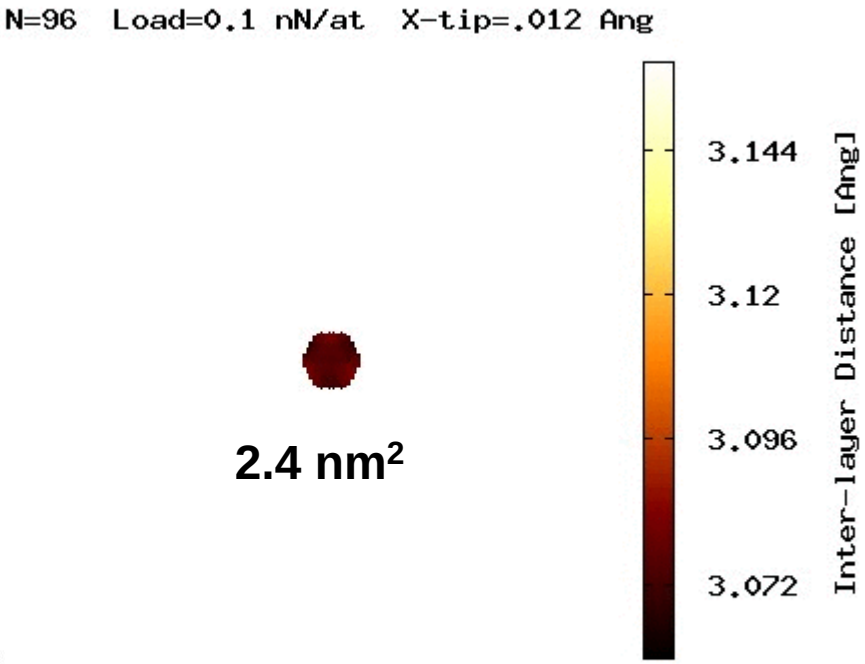
15 nm^2

Diameter d < 5 nm
Nearly commensurate contact

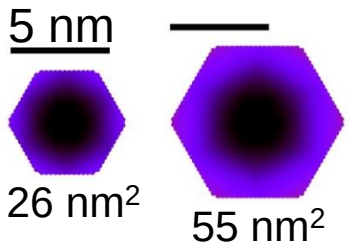
Most unfavorable stacking mode

Most favorable stacking mode

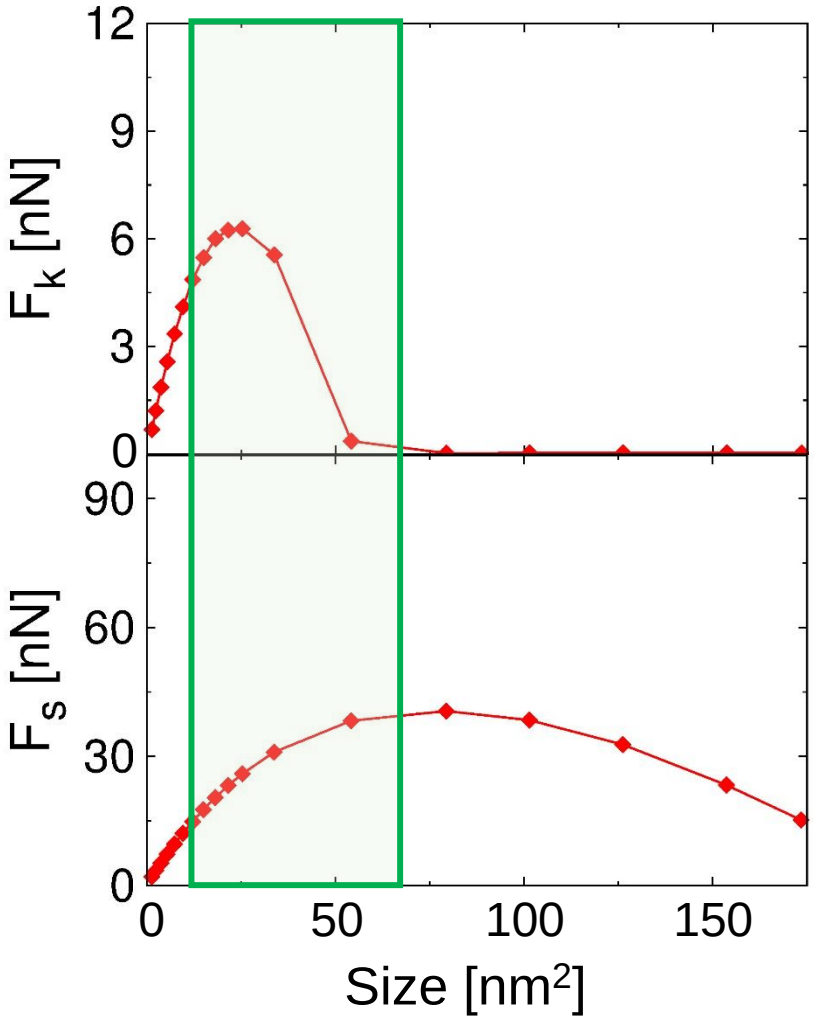




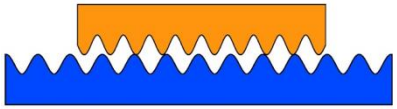
Load=0.1 nN/atom

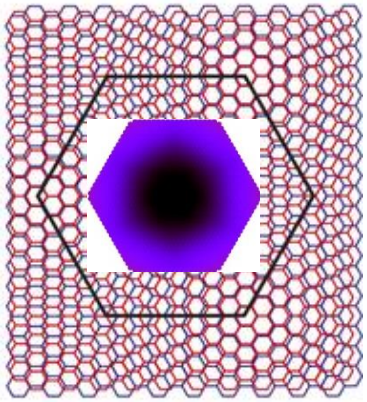


FRICTION FORCE VERSUS SIZE

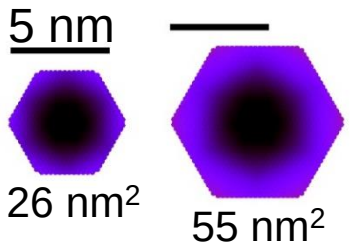


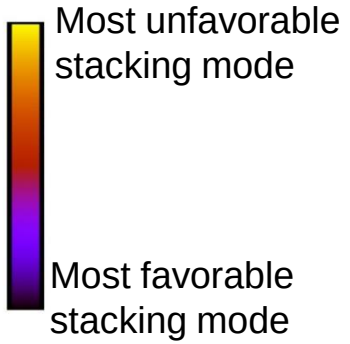
20 < size < 70 nm² stick-slip, deviation from linearity.





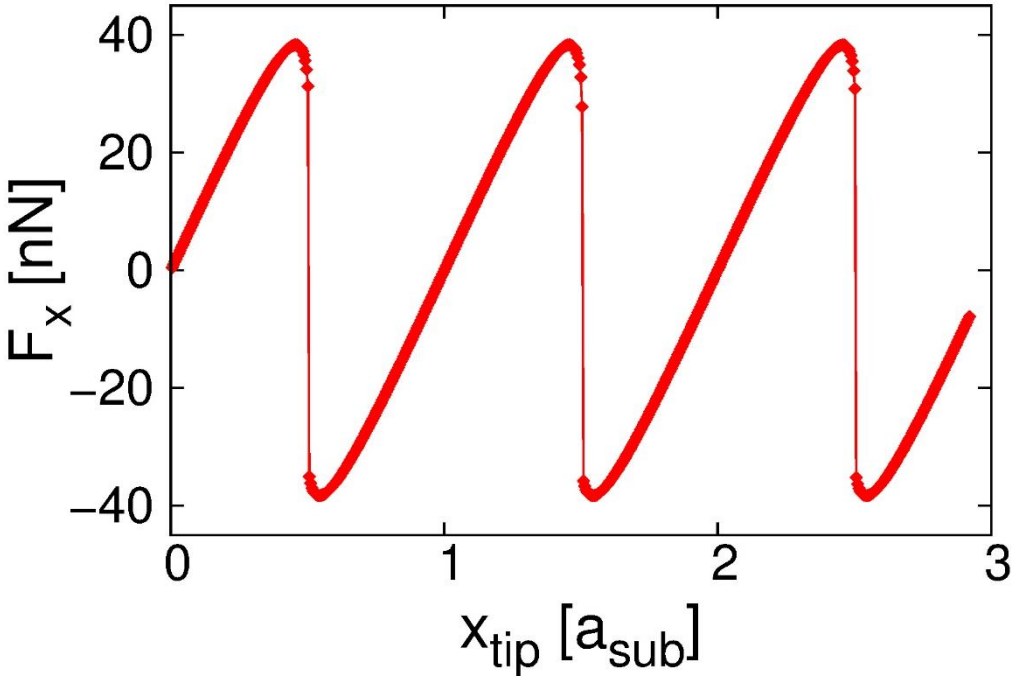
Load=0.1 nN/atom

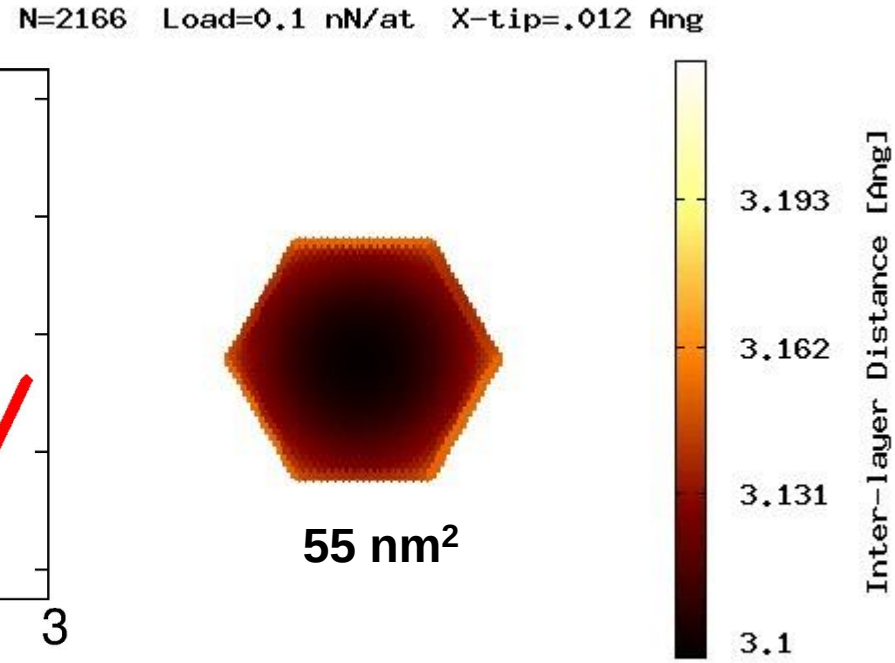




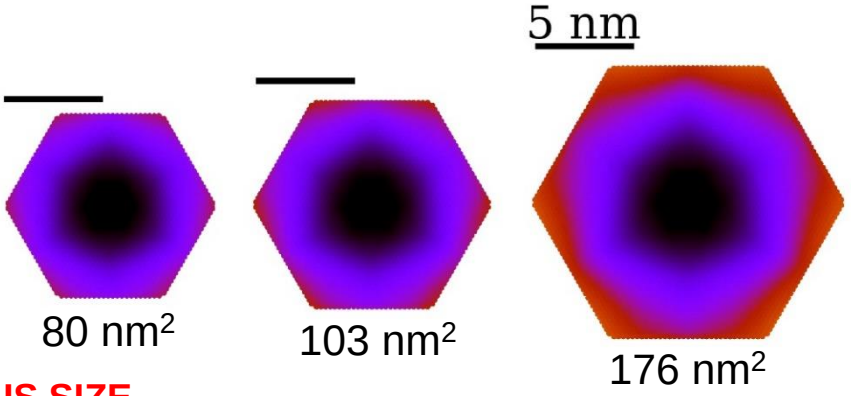
Diameter d ≈ soliton-width ≈ 5 nm

Stick-slip instability
triggered by the soliton

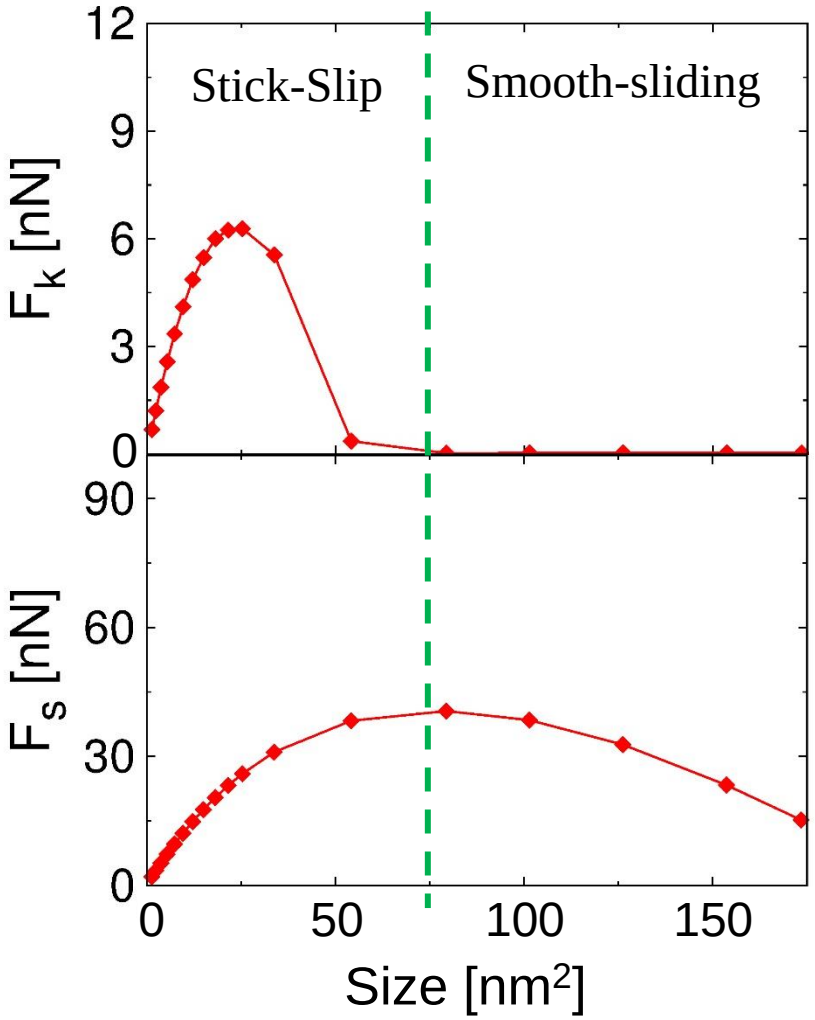




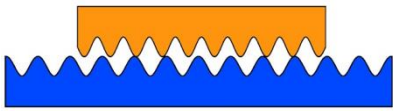
55 nm²

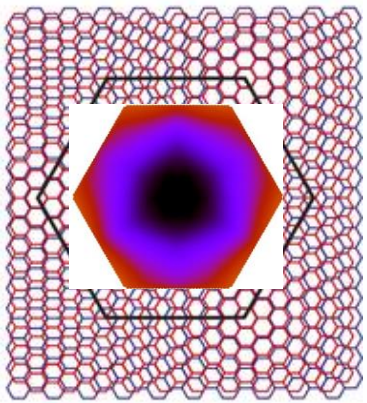


FRICTION FORCE VERSUS SIZE

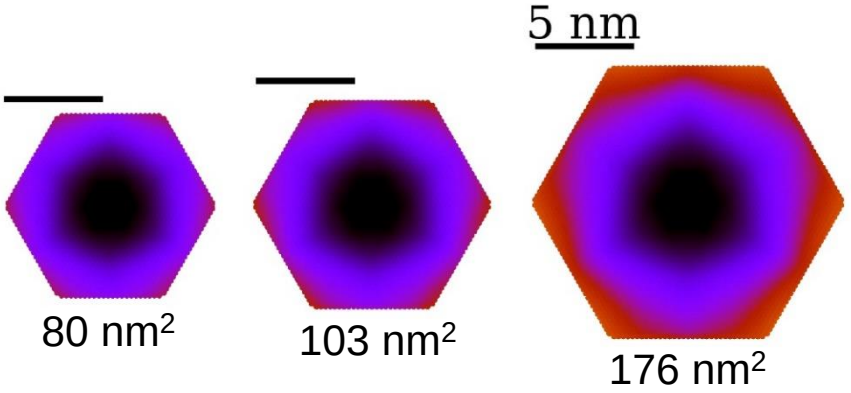


Size > 70 nm² smooth sliding.



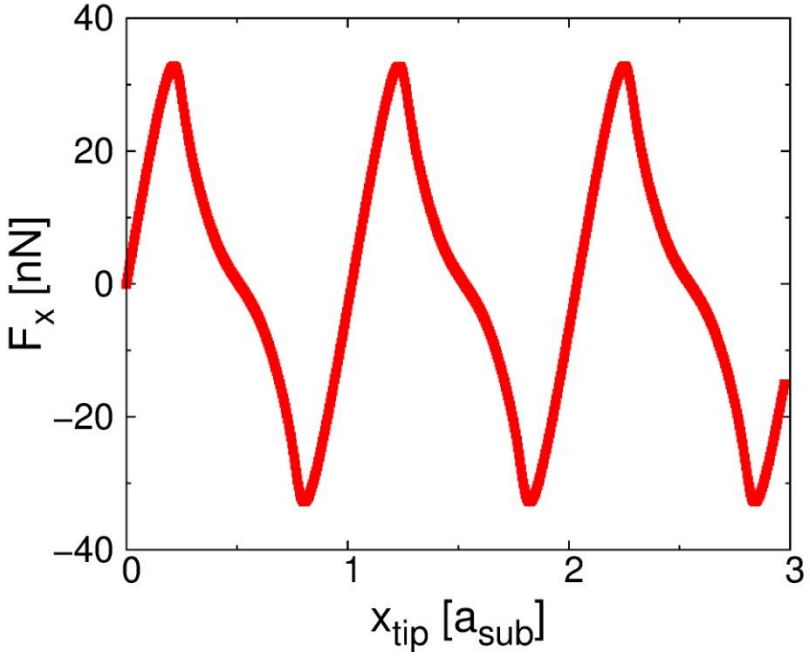


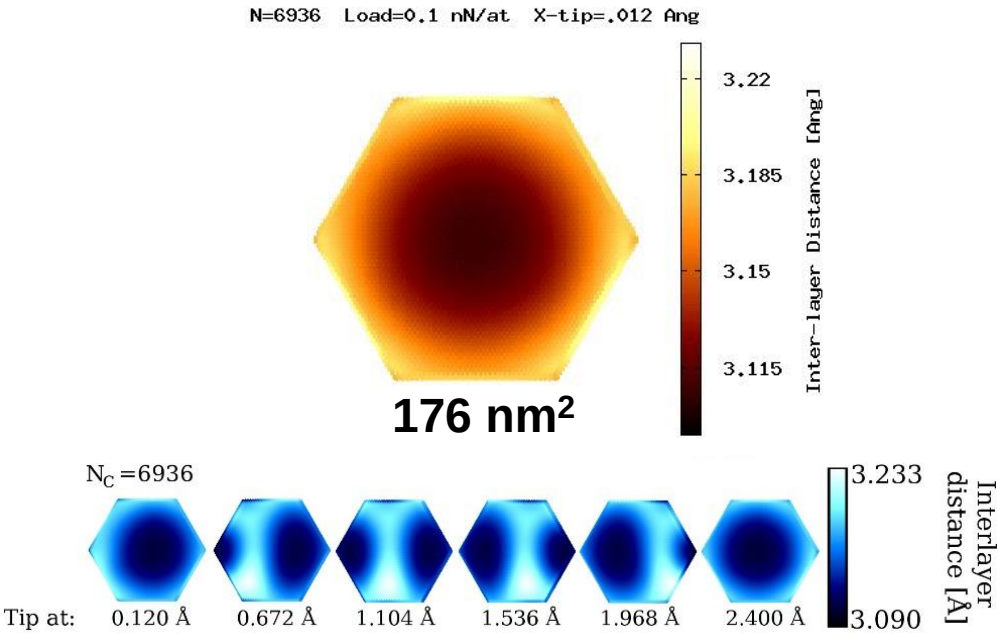
Load=0.1 nN/atom



Diameter d > soliton-width

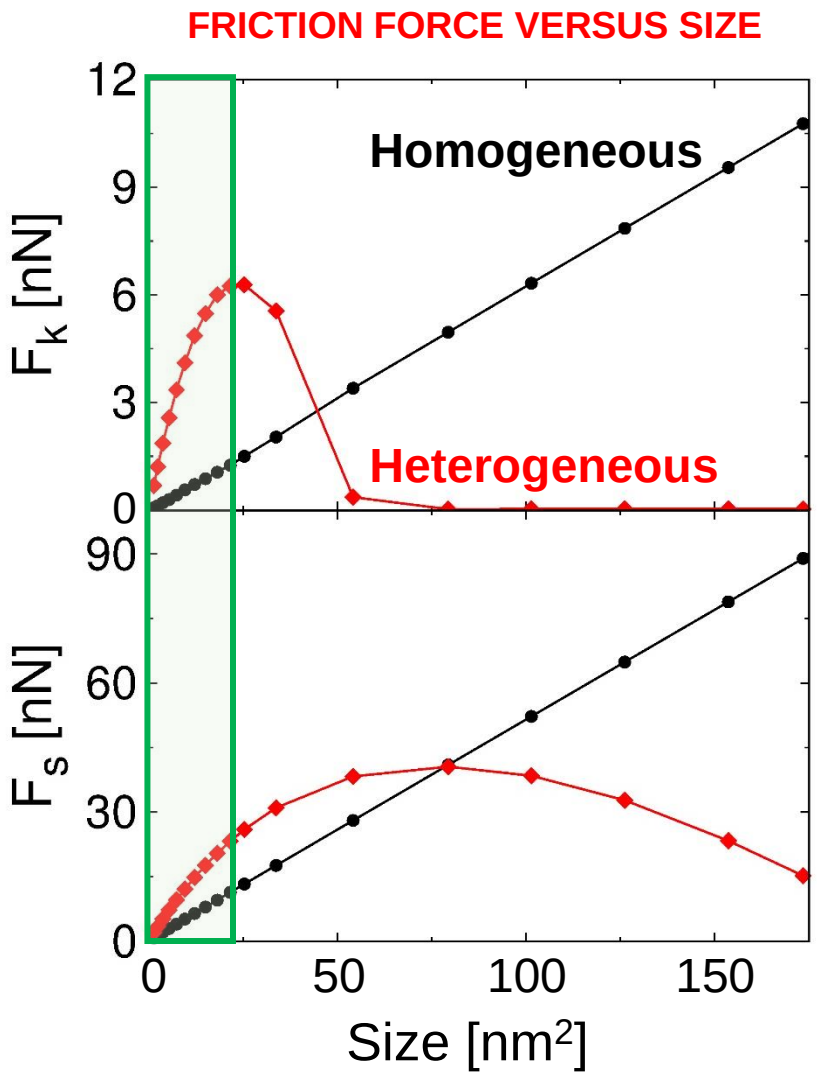
SMOOTH SLIDING

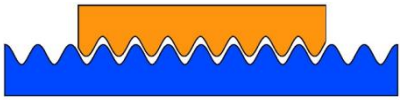




Load=0.1 nN/atom

Results: aligned interfaces θ=0

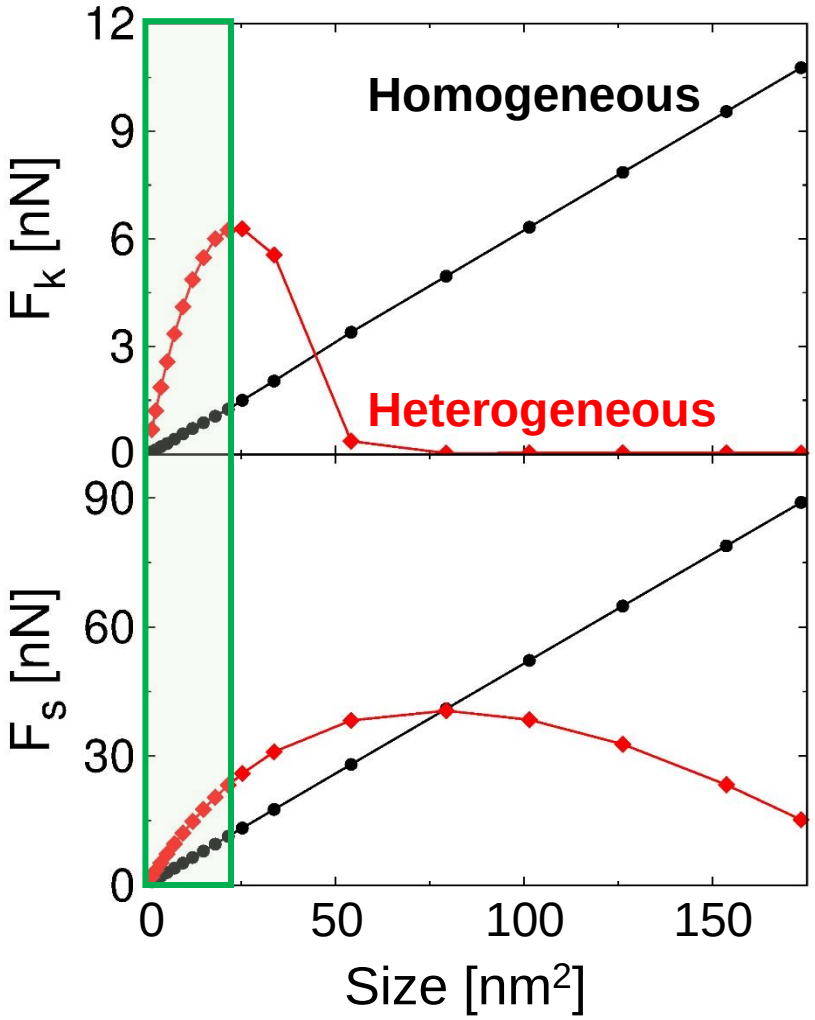


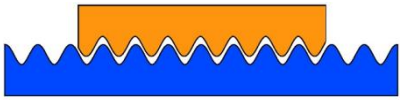


Load =0.1 nN/atom =4 GPa

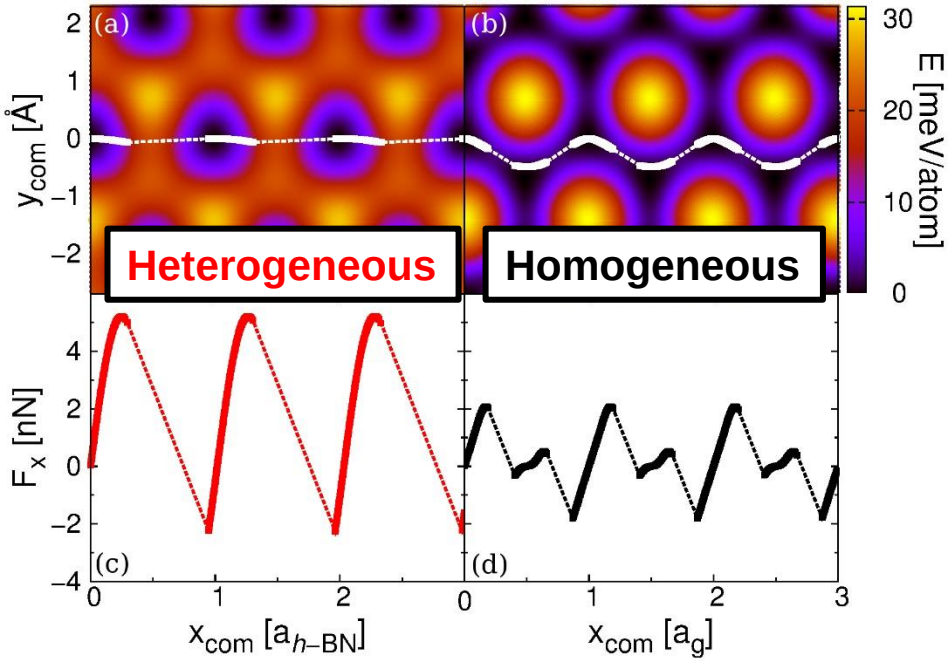
Results: aligned interfaces θ=0

FRICTION FORCE VERSUS SIZE





POTENTIAL ENERGY SURFACE

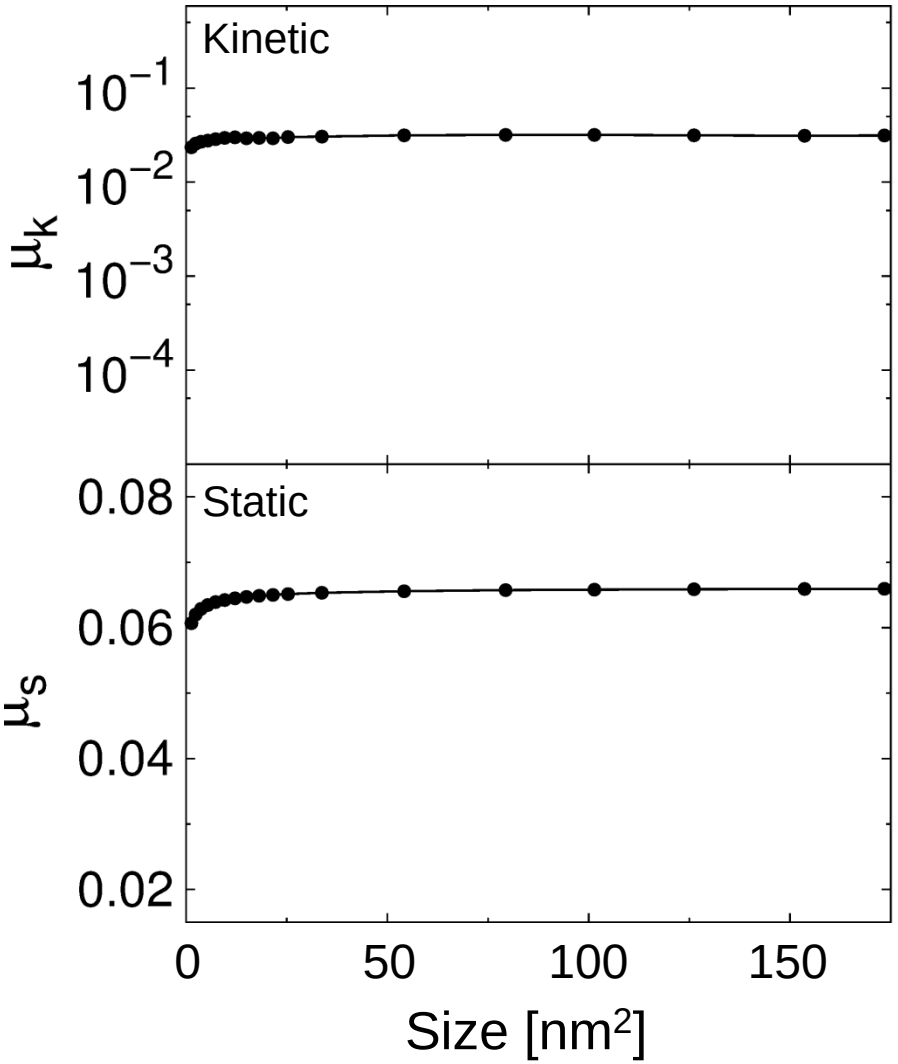


Load =0.1 nN/atom =4 GPa

SIZE 2.4 nm^2

Results: aligned junctions θ=0

FRICTION COEFFICIENT VERSUS SIZE



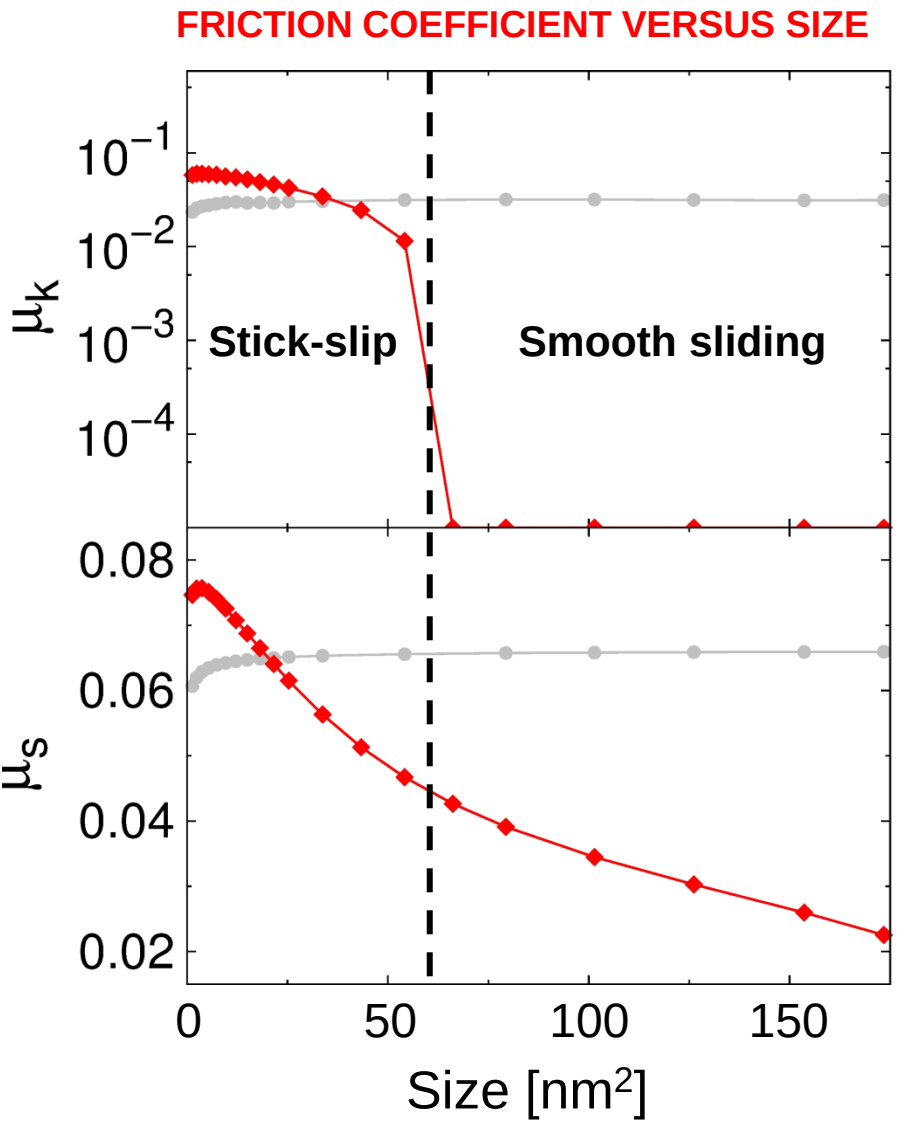
Homogeneous

Friction coefficient saturates at large sizes. $\mu_k \approx 0.03$ is in good agreement with typical exp. values for microscale graphitic contacts.

Edge effects account for the initial growth.

1. D. Marchetto *et al.*, Tribol. Lett. **48**, 77 (2012).

Results: aligned junctions θ=0



Heterogeneous

Crossover between stick-slip to superlubric smooth sliding.

Onset of superlubricity at contact size ≈ 60 nm^2.
Well below the size of the Moiré ≈ 200 nm^2.

Dependence on $k_{||}$:
The crossover occurs at sizes < Moiré in the whole estimated experimental range of $k_{||}$≈11-30 meV/Å^2.

Conclusions

MISALIGNED INTERFACE, θ=30°

Small loads:
Superlubric smooth sliding;
Static and kinetic friction force independent of size;
No significant difference between homogeneous and heterogenous contacts;

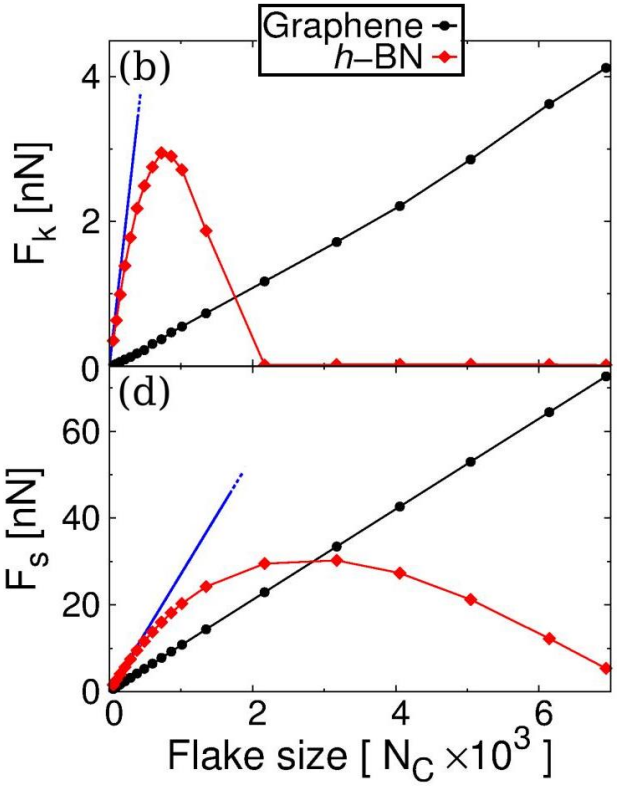
High loads:
The smoother potential energy surface at small interlayer distances makes superlubricity more robust against load in heterogeneous nano-contacts when compared with their homogeneous counterparts.

ALIGNED INTERFACE, θ=0°

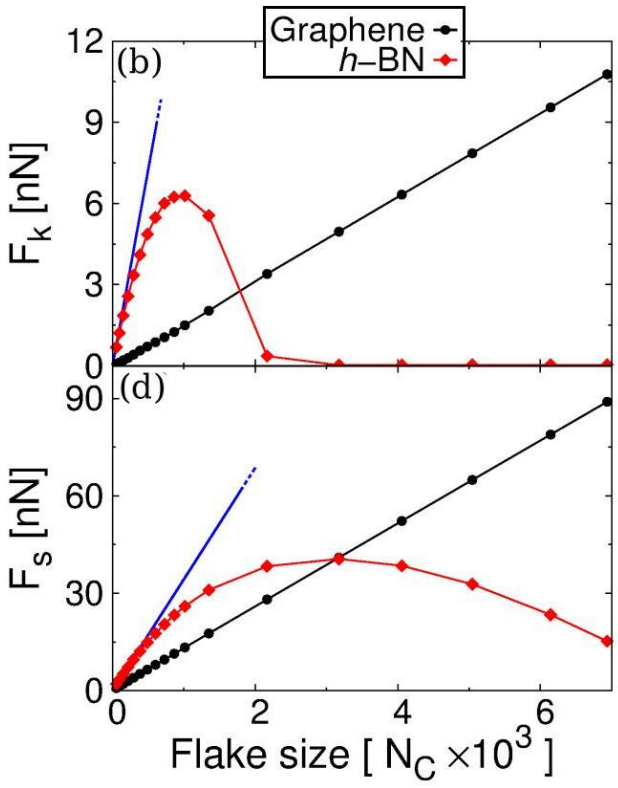
Crossover from stick-slip to superlubricity at contact size ≈80 nm^2, significantly smaller than the size ≈200 nm^2 of one full Moiré “primitive cell”.

Results: aligned interface θ=0

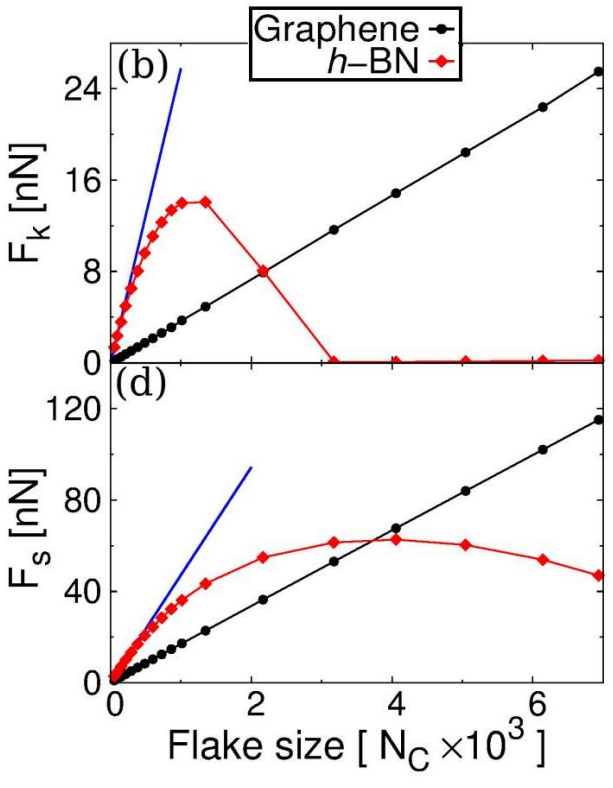
LOAD=0.05 nN/atom



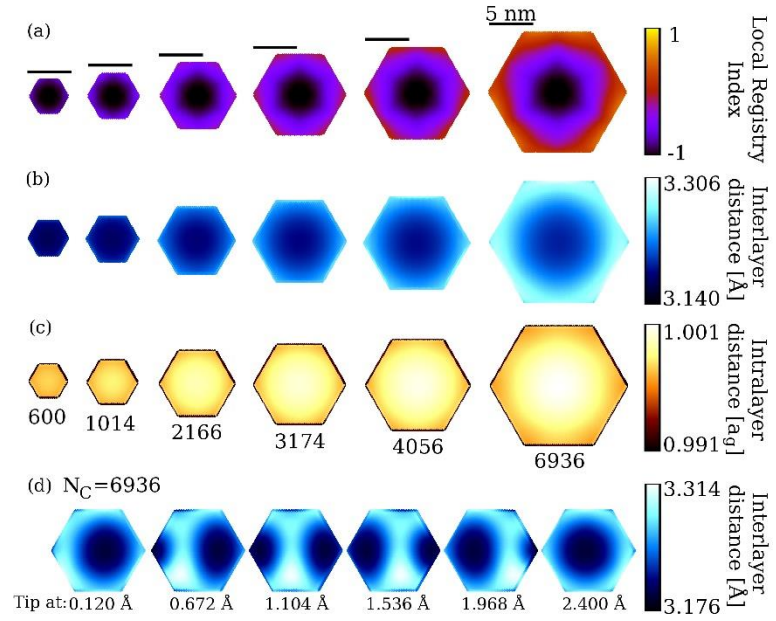
LOAD=0.1 nN/atom



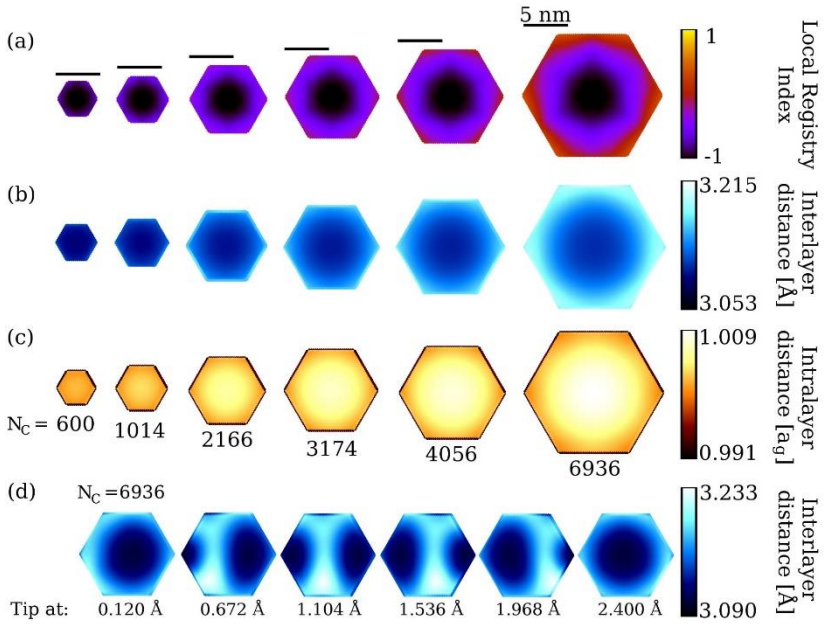
LOAD=0.2 nN/atom



Results: aligned interface θ=0

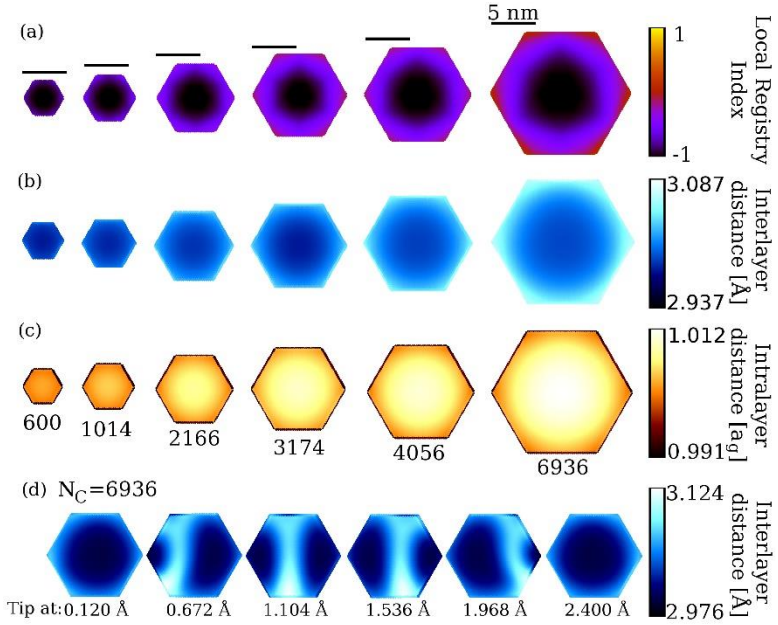


L=0.05

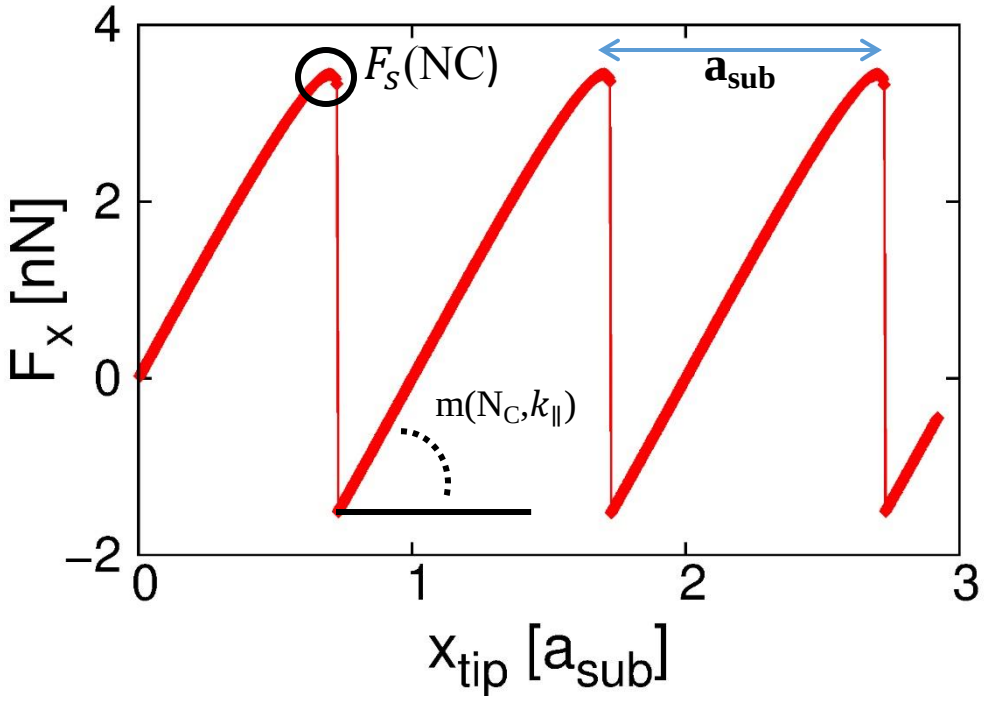


L=0.1

L=0.2



Results: aligned interface θ=0



$$F_k = F_s(N_C) - a_{sub} m(N_C, k_\parallel) \text{ [1]}$$

$m(N_C, k_\parallel) \propto N_C, k_\parallel$

Using estimates of '*m*' eq.[1] reproduces the position of the maximum of F_k.