Tuning frictional properties of graphene sheets using kirigami inspired cuts and inverse design

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Project description
3 stages

1. Sheet kirigami: Alter graphene sheet using atomic scale cuts.
2. Forward simulation: Calculate frictional properties of the sheet using MD simulations.
3. Inverse design: Predict cut patterns based on frictional properties and optimize for desired properties using machine learning.
   - Low / high friction coefficient.
   - Coupling between stretch and friction.

Kirigami: Variation of origami with cuts permitted.

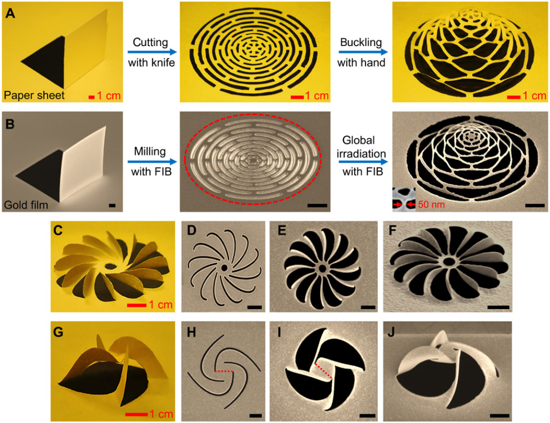

Figure: Example of transistion from macro- to nano-kirigami using a focused ion-beam (FIB) (Nano-kirigami with giant optical chirality, ZHIGUANG LIU, 2018).

Motivation

Kirigami inspired cuts

Accelerated Search and Design of Stretchable Graphene Kirigami Using Machine Learning, Paul Z. Hanakata, 2018.

- Kirigami inspired cuts is used to tune **yield stress** and **yield strain** as a function of cutting pattern.
- A side effect is buckling into the third dimension.

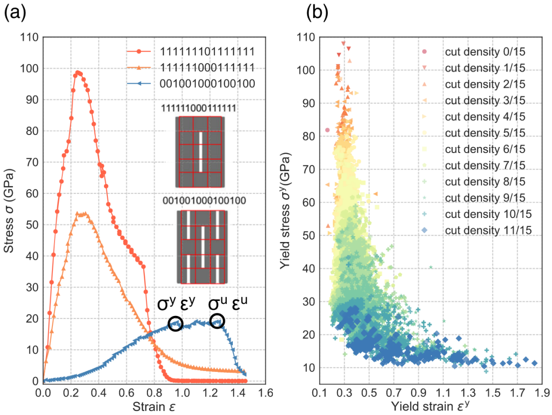

Figure: (a) Stress-strain plot of three representative kirigamis. Inset shows the “typical” kirigami cuts. (b) Yield stress as a function of yield strain for different configurations.

- Friction laws at different scales:

$$\begin{aligned} \text{Microscopic: } F_f &= \mu \cdot F_N \quad (\text{ independent of } A), \\ \text{Nanoscale: } F_f &\propto A = N_c \cdot A_c, \end{aligned}$$

where F_f is friction force, μ is the friction coefficient, F_N is the normal force, A is the contact area and N_c is the average number of atoms in contact with an average contact area A_c.

Motivation

Nanomachine for negative friction coefficient

$$\left.\begin{aligned} \text{Contact area}: A_0 &= k \cdot F_N \\ \text{Kirigami}: A &= A_0 - s_1 \cdot \text{stretch} \\ \text{Nanomachine}: \text{stretch} &= s_2 \cdot F_n \end{aligned}\right\} \implies F_f \propto A = \underbrace{(k - s_1 \cdot s_2)}_{\mu} \cdot F_N$$

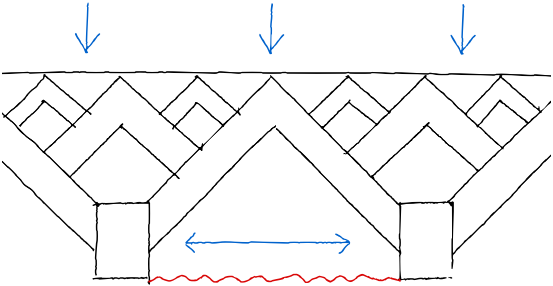

Figure: Sketch for nanomachine coupling normal force and stretch.

Designing complex architectured materials with generative adversarial networks, YUNWEI MAO, 2020.

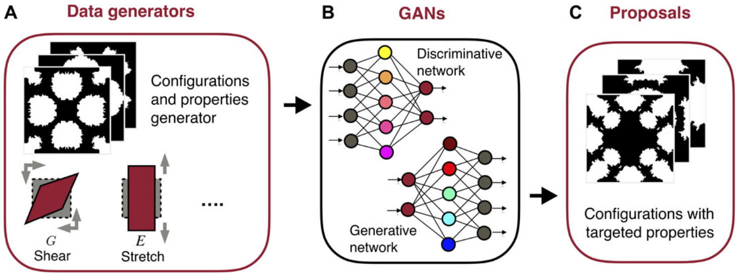

Figure: (A) Data generators to generate datasets of configurations and properties of architectured materials. (B) GANs trained by the datasets. (C) New designs of architectured materials with the targeted properties proposed by the GANs.

Stage 1 - Kirigami cuts

Choosing a cut pattern

- Kirigami design on macroscale.

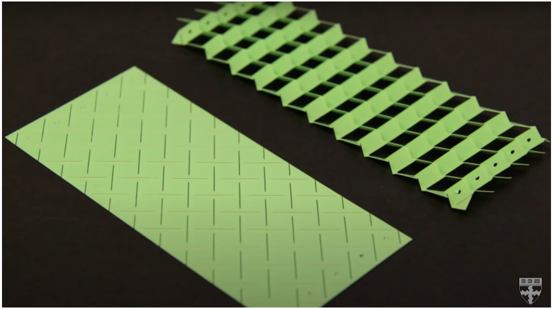

Figure: New pop-up strategy inspired by cuts, not folds - Leah Burrows, Harvard John A. Paulson School of Engineering and Applied Sciences

Stage 1 - Kirigami cuts

Choosing a cut pattern

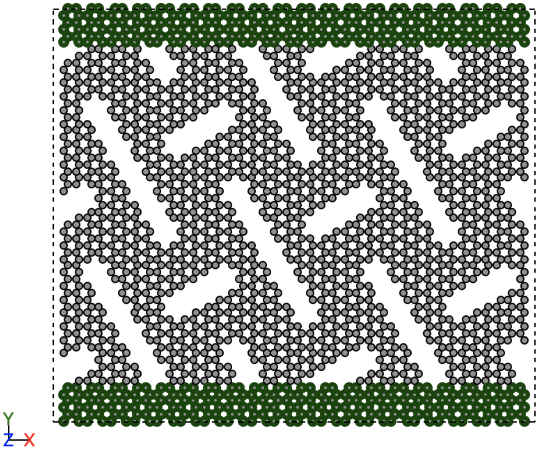

Figure: Example of cut pattern. The grey color marks the cutable sheet while green marks added blocks for stetching and dragging the sheet.

Stage 1 - Kirigami cuts

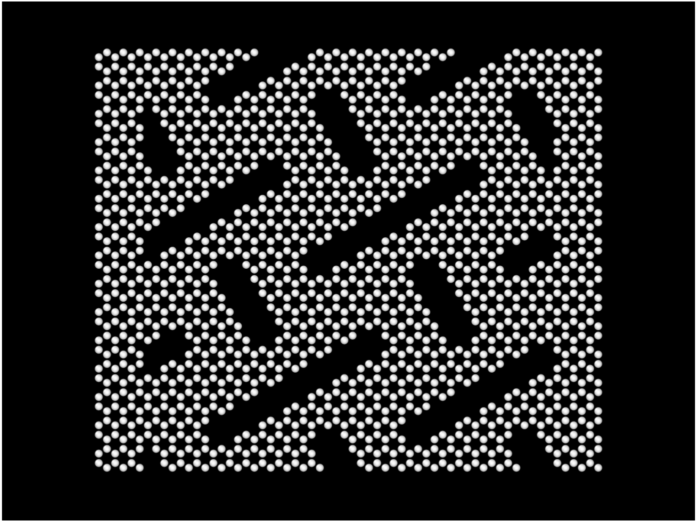

Figure: Kirigami sheet stretch in vaccuum.

Stage 1 - Kirigami cuts

Investigating 3D buckling

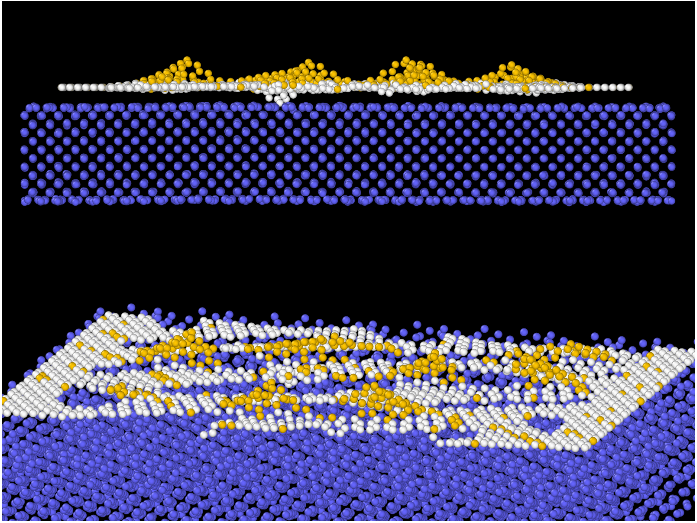

Figure: Kirigami stretch in contact with Si-substrate.

Stage 1 - Kirigami cuts

Investigating 3D buckling

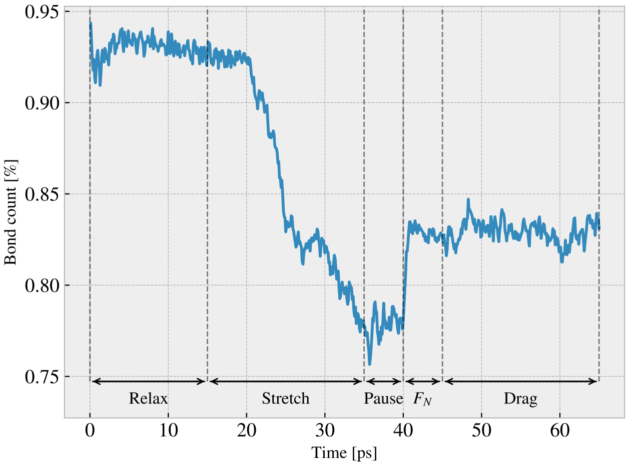

Figure: Contact area: number of C-Si bonds within a threshold distance of 110% the equlibrium distance in LJ the potential.

Stage 2 - MD measurements
Friction force

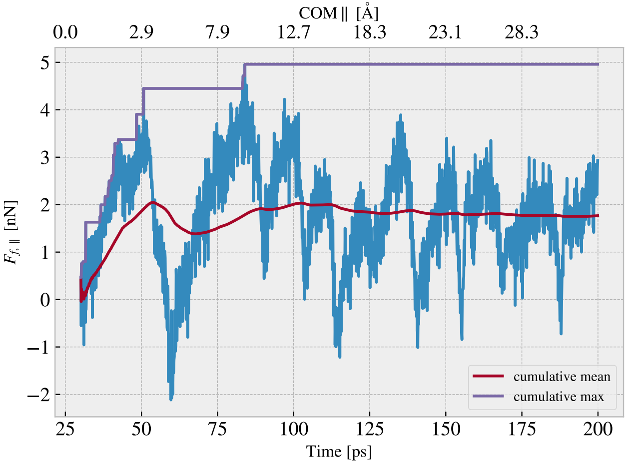

Figure: Friction force parallel to drag direction with normal force $F_N = 200$ nN. Drag distance = 40 Å

Stage 2 - MD measurements

Friction force

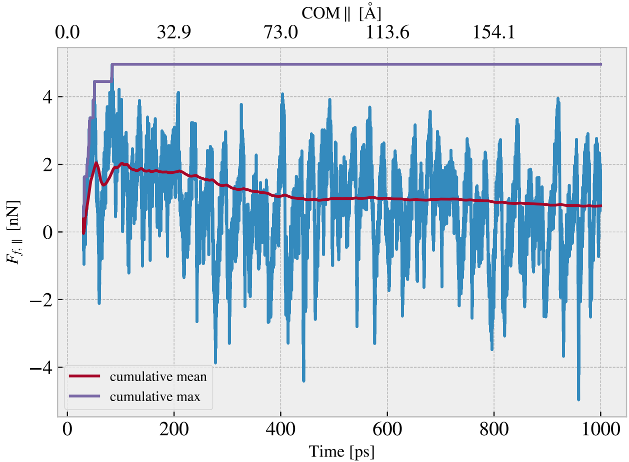

Figure: Friction force parallel to drag direction with normal force $F_N = 200$ nN. Drag distance = 200 Å.

Stage 2 - MD measurements
Contact area

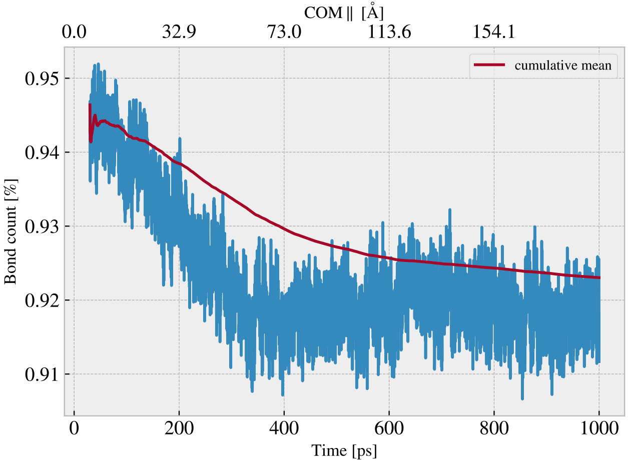

Figure: Contact bond count with normal force $F_N = 200$ nN. Drag distance = 200 Å.

Stage 2 - MD measurements

Contact area

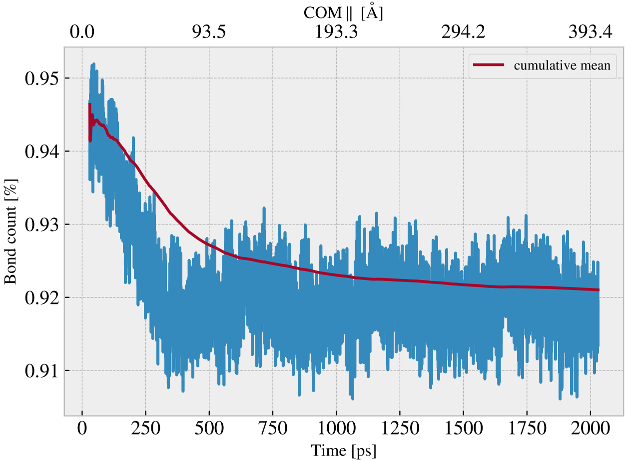

Figure: Contact bond count with normal force $F_N = 200$ nN. Drag distance = 400 Å.

Category	**Parameter**	**Range**
Physical (free)	Temperatur	[0, 300] K
	Drag speed	$[1, 20]$ m/s
Physical (ML input)	Cut configuration	No ruptures
	Scan angle	$[0, 90^\circ]$
	Stretch amount	$[0, 20]$ %
	Normal force	$[10, 200]$ nN
MD settings	Relax and pauses	$\sim$ 10 ps
	Stretch speed	$[0.5, 0.1]$ %/ps
	Drag spring constant	$[10, \infty]$ N/m
	Drag length	$[50, 400]$ Å
	Sheet size	$\sim 62 \times 75$ Å

Table: Relevant parameters of MD simulation and approximate ranges.

Stage 2 - MD measurements

Varying normal force and stretch

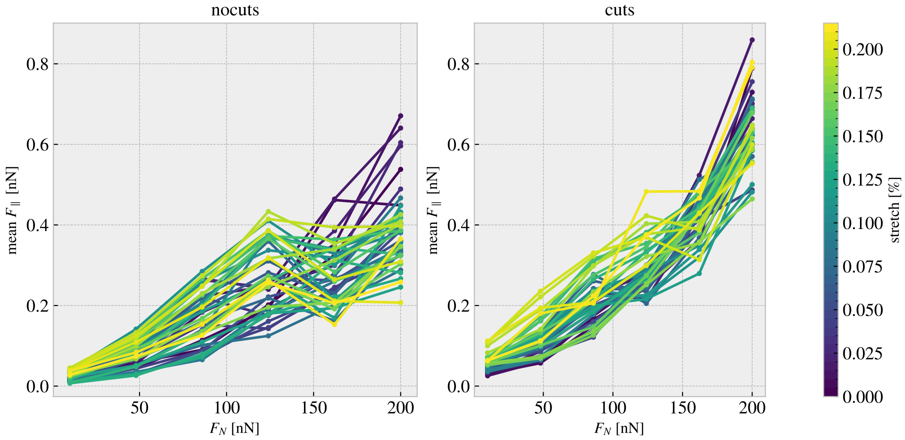

Figure: Mean friction force $F_{\parallel}$ parallel to drag direction versus applied normal force (F_N) with and without cuts.

Stage 2 - MD measurements

Varying normal force and stretch

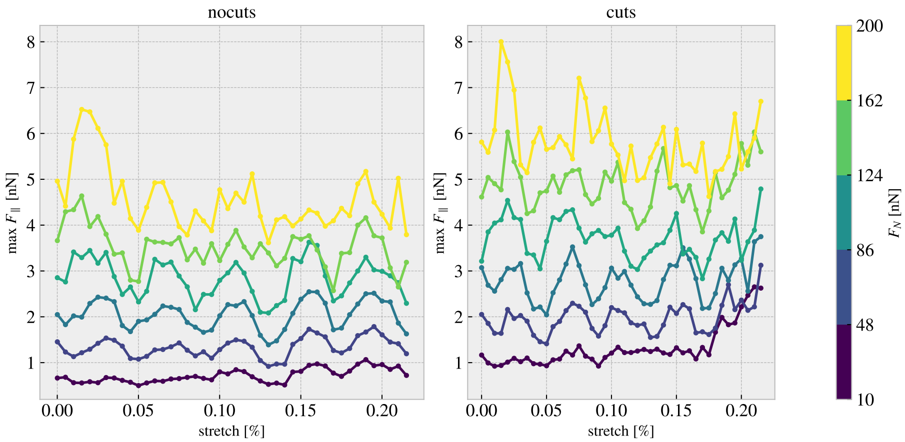

Figure: Max friction force $F_{\parallel}$ parallel to drag direction versus stretch of the sheet with and without cuts.

Stage 2 - MD measurements

Varying normal force and stretch

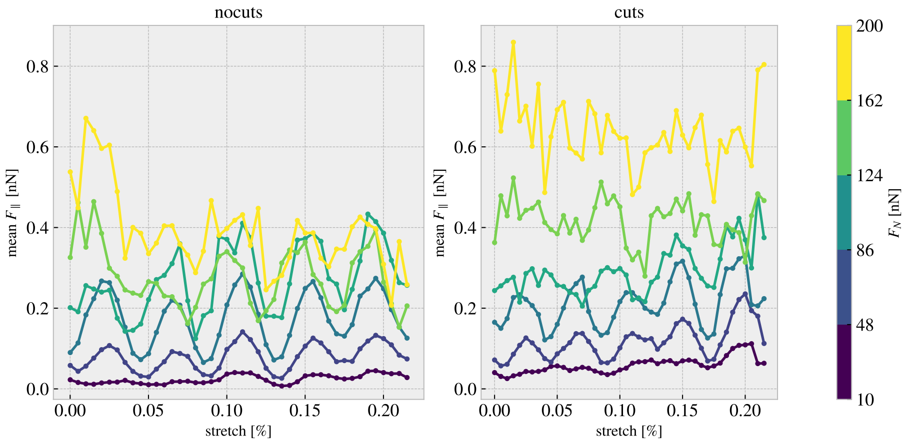

Figure: Mean friction force $F_{\parallel}$ parallel to drag direction versus stretch of the sheet with and without cuts.

Stage 2 - MD measurements

Varying normal force and stretch

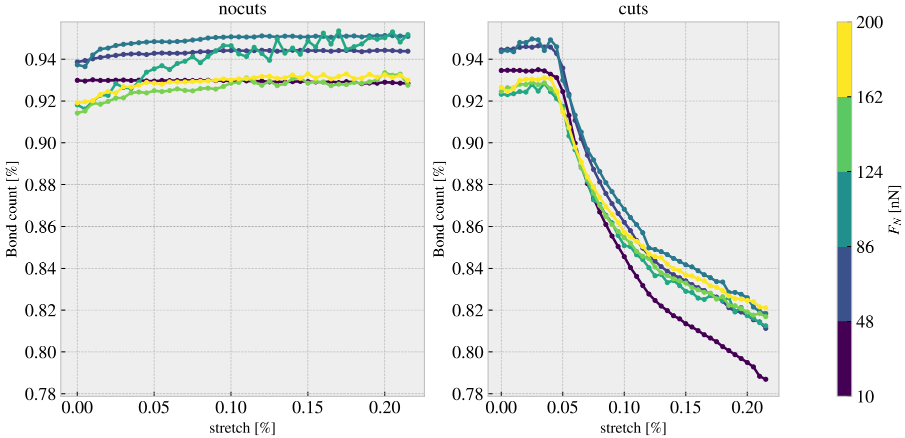

Figure: Contact bonds versus stretch of the sheet with and without cuts.

Stage 2 - MD measurements

Varying normal force and stretch

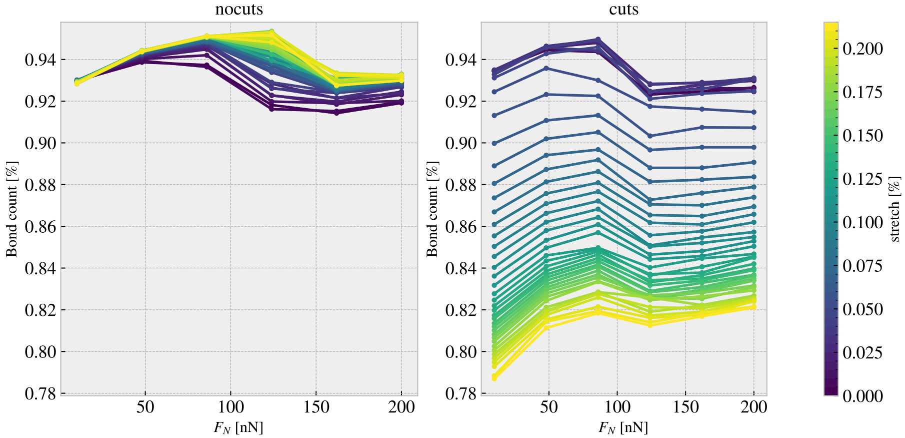

Figure: Contact bonds versus normal force F_N of the sheet with and without cuts.

Stage 2 - MD measurements

Varying normal force and stretch

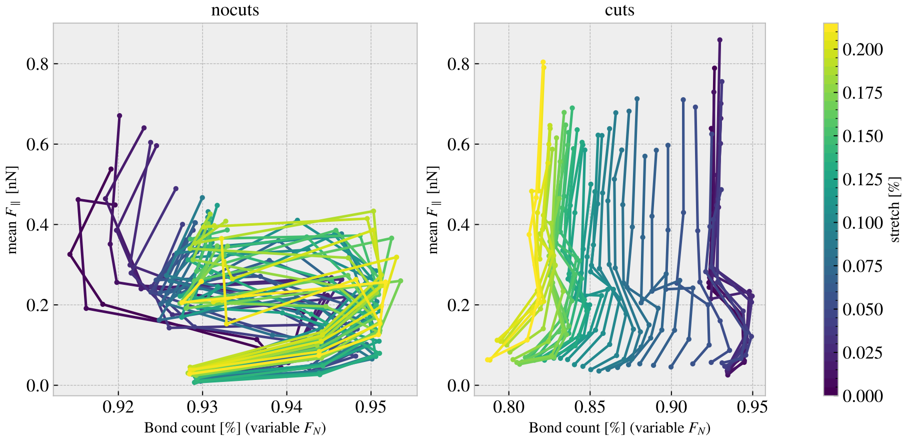

Figure: Mean friction force $F_{||}$ parallel to drag direction versus contact bonds (varied by normal force F_N) with and without cuts.

Stage 2 - MD measurements

Varying normal force and stretch

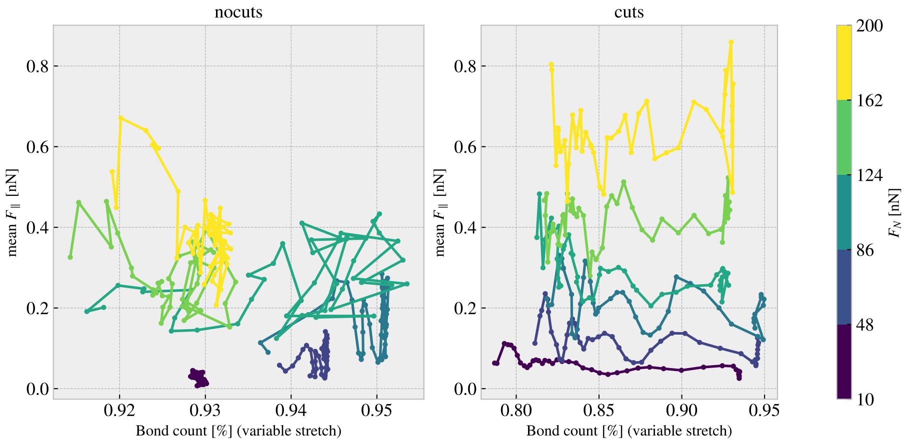

Figure: Mean friction force $F_\parallel$ parallel to drag direction versus contact bonds (varied by normal force stretch) with and without cuts.

Friction force dependence of stretch might be explained by simple friction models such as the Frenkel-Kontorova (FK) model.

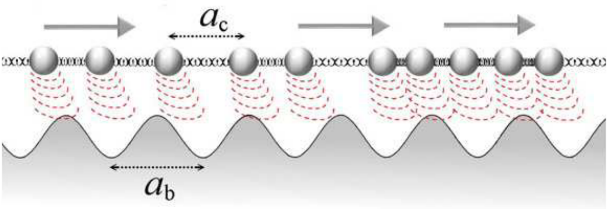

Figure: A sketch of the FK model, showing the two competing lengths: The average interparticle spacing and the lattice periodicity of the substrate. Friction and Nonlinear Dynamics, N. Manini, 2016.

Stage 2 - MD measurements
Static non-bonded regions

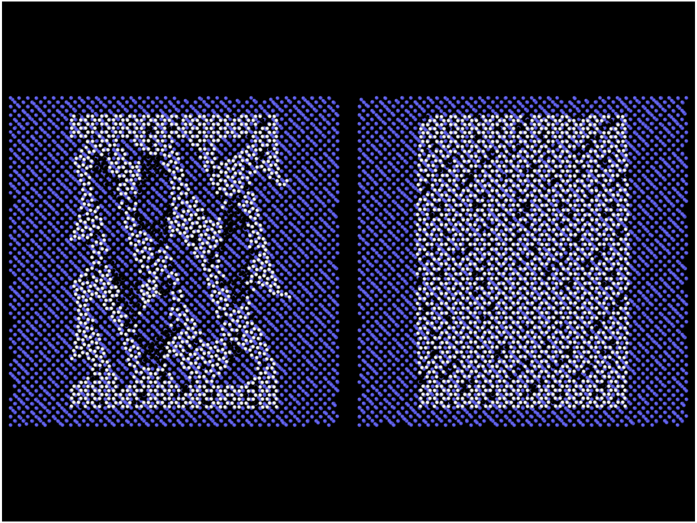

Figure: Stretch = 22 %, $F_N = 200$ nN, Drag length = 200 Å.

The End

Questions? Comments?