Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

Designs for a negative friction coefficient

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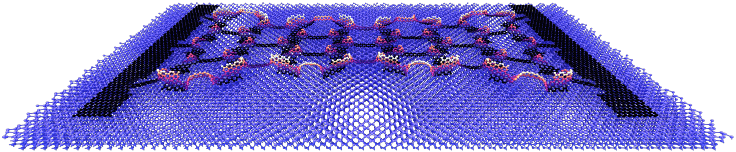
Juni 02, 2023



Outline

Thesis overview

System preview

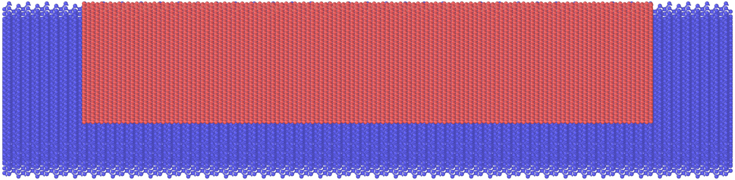


Figure: System of choice: Graphene sheet (red) on a silicon substrate (blue).

Thesis overview

1. **Sheet modification**: Atomic-scale cuts and stretching
2. **Forward simulation**: Simulate system and measure friction
3. **Accelerated search**: Use machine learning to search for new designs

Main research question

Can we control the friction of a nanoscale Kirigami sheet with pattern design and straining of the sheet?

- Kirigami: Variation of origami with cuts permitted
- Desgins: Macroscale → nanoscale

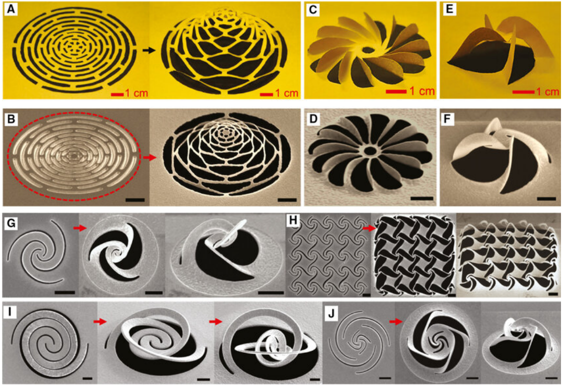
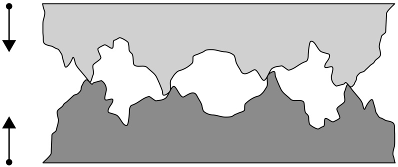
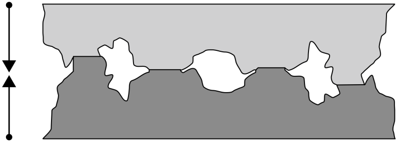


Figure: Example of macroscale Kirigami designs implemented on a microscale using a focused ion beam. Black scale bars: 1 μm. Reproduced from [1].

- Out-of-plane buckling
- Surface properties are important for friction
  - Asperity theory: Contact area
  - Frenkel–Kontorova models: Commensurability



(a) Small load.



(b) High load.

Figure: Qualitative illustration of microscopic asperity deformation under increasing load. Reproduced from [2].

Creating a graphene Kirigami system

System setup

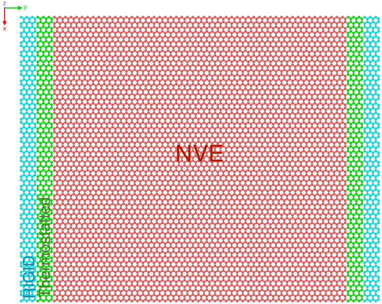
Regions

- Red: *NVE*
- Green: Thermostat *NVT*
- Blue: Rigid

System size

- Atoms $\sim 60,000$
- Sheet $\sim 130 \times 165\,\text{Å}$

(a) Side view.



(b) Top view.

Sheet Kirigami
Indexing

$$M \in \mathbb{Z}_2^{62\times 106}, \qquad \text{Combinations} = 2^{6572} = 10^{1978}$$

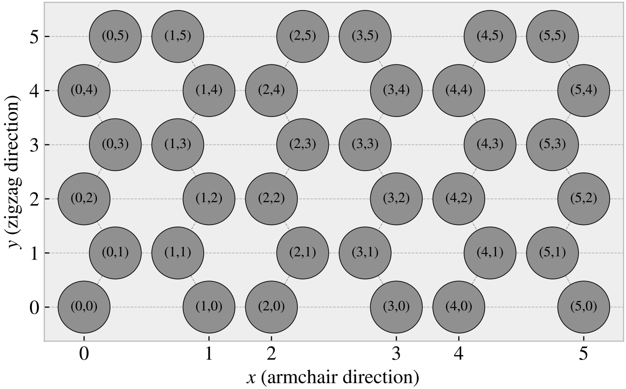


Figure: Graphene atom site indexing.

$$M \in \mathbb{Z}_2^{62\times 106}, \qquad \text{Combinations} = 2^{6572} = 10^{1978}$$

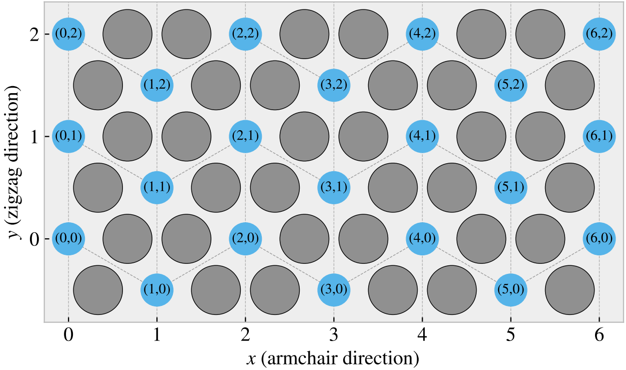
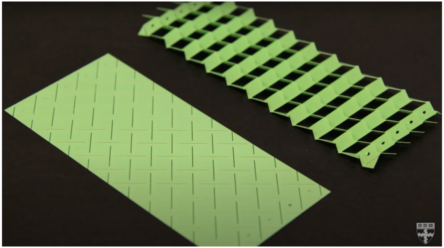


Figure: Graphene *center element* indexing.

Sheet Kirigami

Macroscale inspiration



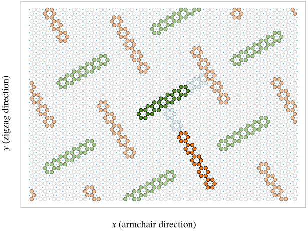
(a) Tetrahedron: Alternating perpendicular cuts producing a tetrahedron-shaped surface buckling when stretched. Reproduced from [3].

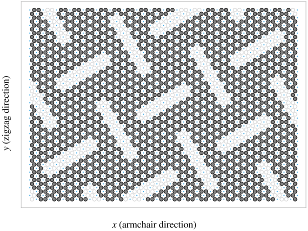
(b) Honeycomb: Scotch™ Cushion Lock™ [4] producing a honeycomb-shaped surface buckling when stretched. Reproduced from [4].

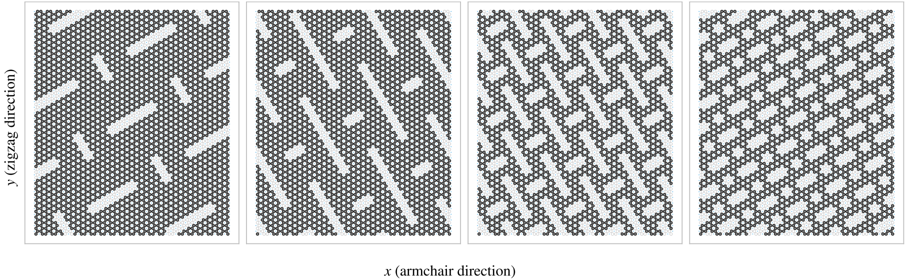
Figure: Macroscale kirigami cut patterns used as inspiration for the nanoscale implementation.

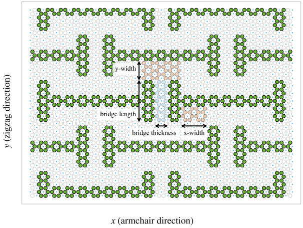
Sheet Kirigami

Tetrahedron patterns

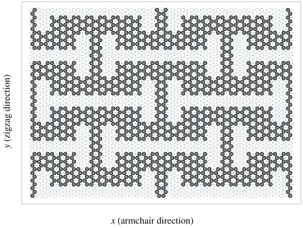




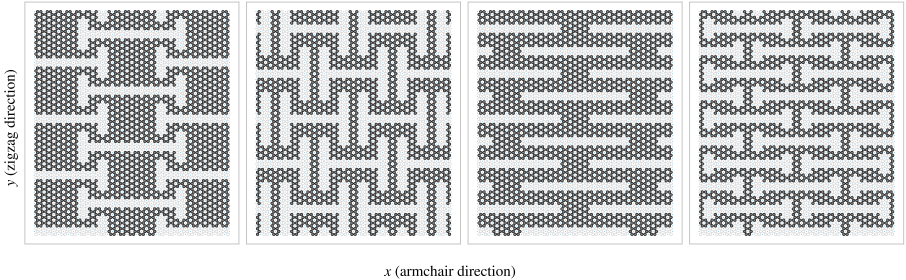




y-width
bridge length
bridge thickness
x-width
y (zigzag direction)
x (armchair direction)

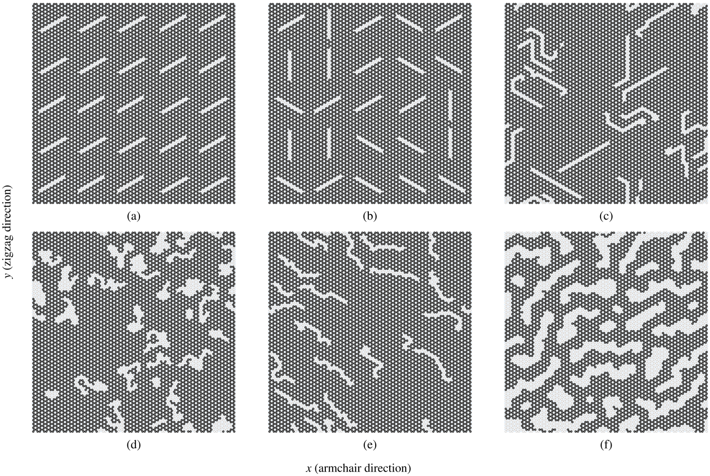


y (zigzag direction)
x (armchair direction)

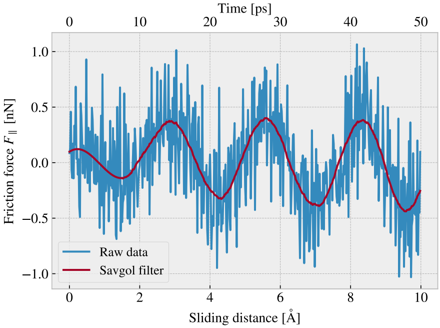


y (zigzag direction)
x (armchair direction)

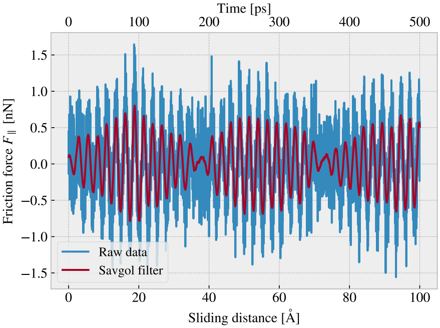
Sheet Kirigami
Random walk patterns



Friction metrics



(a) 10 Å sliding.



(b) 100 Å sliding.

Figure: Friction force traces. The red line represents a Savgol filter.
$T = 300\,\mathrm{K}$, $v = 20\,\mathrm{m/s}$, $K = \infty$.

Out-of-plane buckling

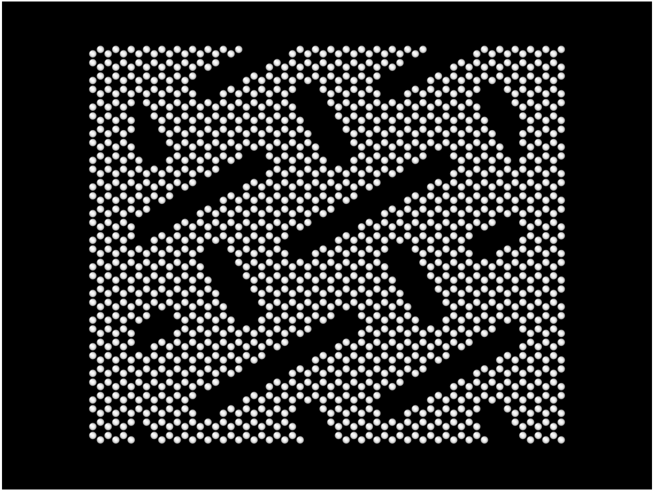


Figure: Kirigami sheet stretch in a vacuum.

Out-of-plane buckling

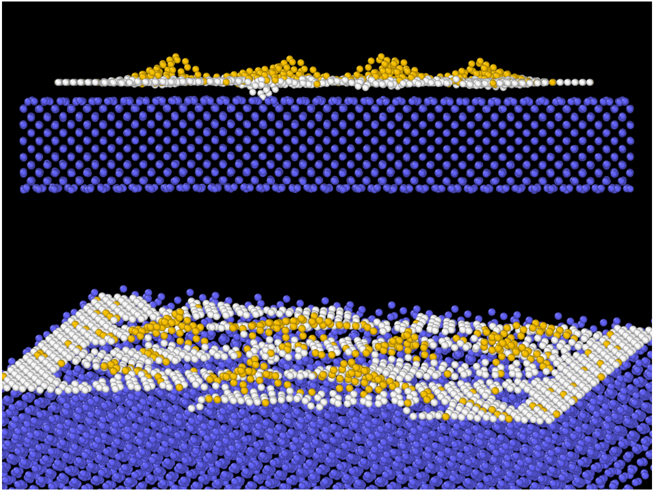


Figure: Kirigami stretch in contact with the substrate.

Out-of-plane buckling

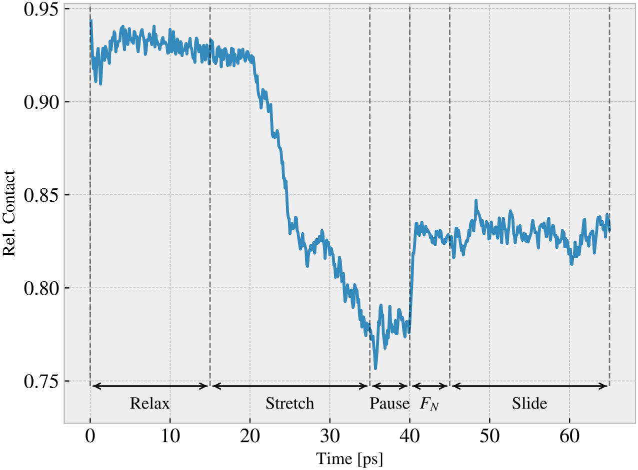


Figure: Contact area approximation: Number of C–Si bonds within a threshold distance of 110% the LJ interaction equilibrium distance.

Contact-strain profile

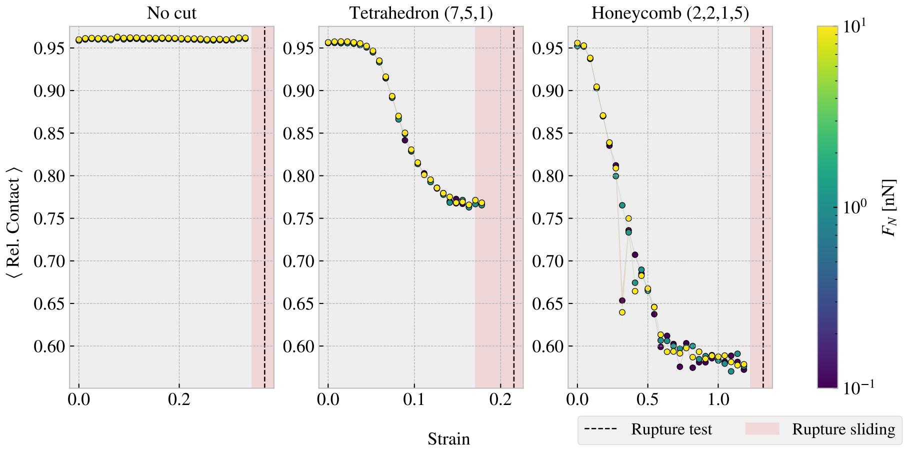


Figure: Contact-strain profile for $F_N = \{0.1, 1, 10\}$nN.

Friction-strain profile

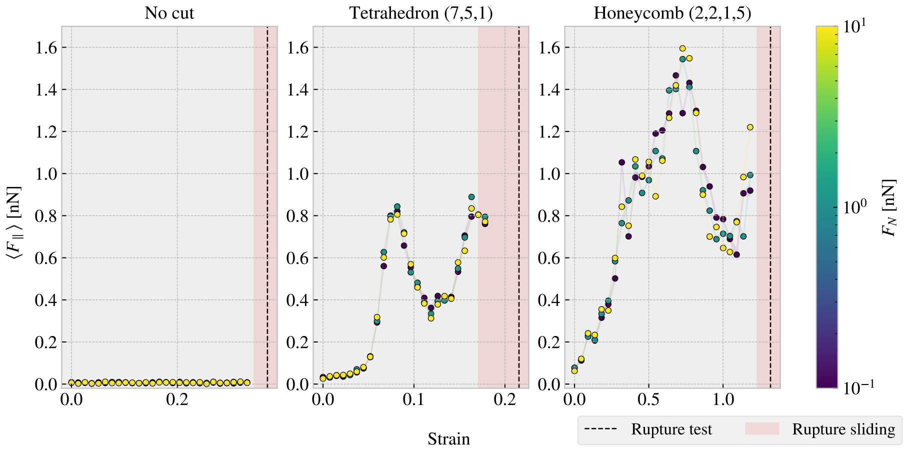


Figure: Friction-strain profile for $F_N = \{0.1, 1, 10\}$nN.

Negative friction coefficient

Coupling of load to sheet tension

$$F_t = TF_N, \qquad T = 6$$

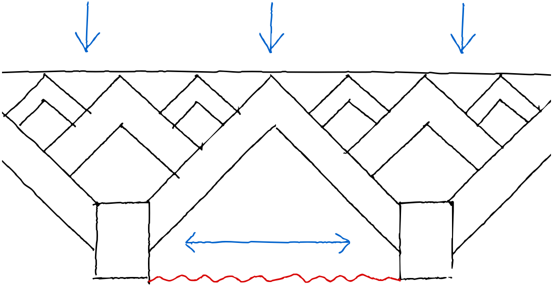


Figure: Working sketch for a nanomachine design translating applied load (from the top of the figure) to a straining of the graphene sheet (shown in red).

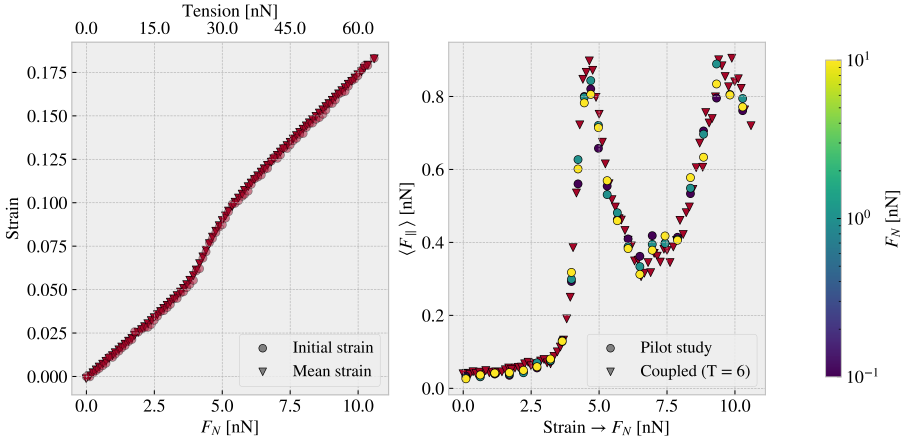


Figure: Tetrahedron $(7, 5, 1)$

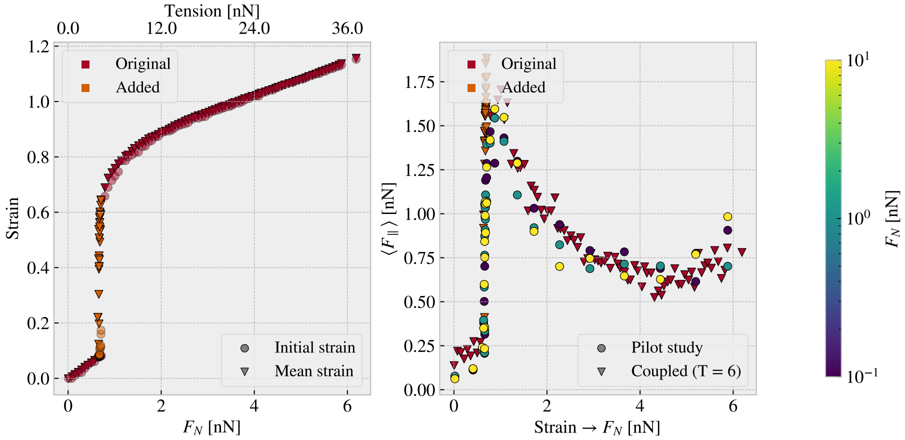


Figure: Honeycomb $(2, 2, 1, 5)$

Negative friction coefficient
Honeycomb deformations

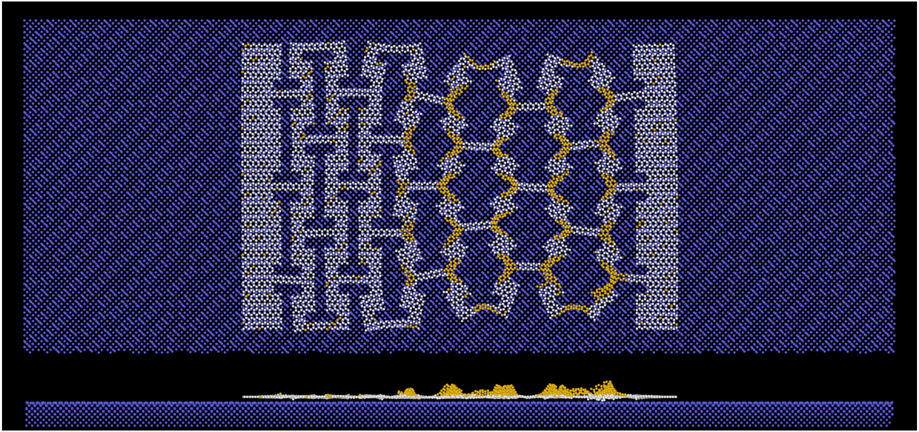


Figure: Honeycomb $(2, 2, 1, 5)$ stretch.

Machine learning

Dataset

- 216 Kirigami configurations ($\sim 10,000$ data points)

Machine learning

- Input: Kirigami configuration, strain and load
- Output: Mean F_{fric}, max F_{fric}, contact area, porosity, rupture, rupture strain

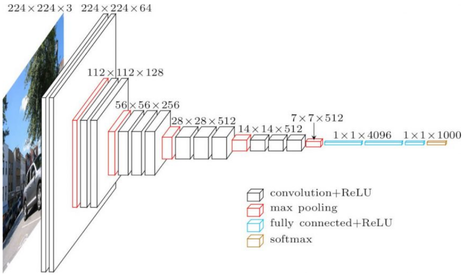


Figure: Convolutional network architecture. Reproduced from [5].

- Good validation performance
- R^2 score

Properties of interest

$$(1)\ \min F_{\text{fric}}, \qquad (2)\ \max F_{\text{fric}}, \qquad (3)\ \max \Delta F_{\text{fric}}, \qquad (4)\ \max \text{drop}.$$

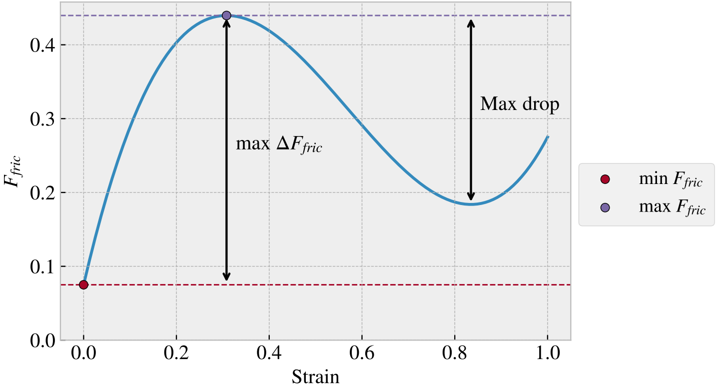


Figure: Properties of interest.

Accelerated search for new designs

Two search approaches

1. Extended dataset search

   Tetrahedron: 1.35×10^5 Honeycomb: 2.025×10^6 Random walk: 10^4

2. Genetic algorithm
   - Survival of the fittest
   - Max drop property optimization

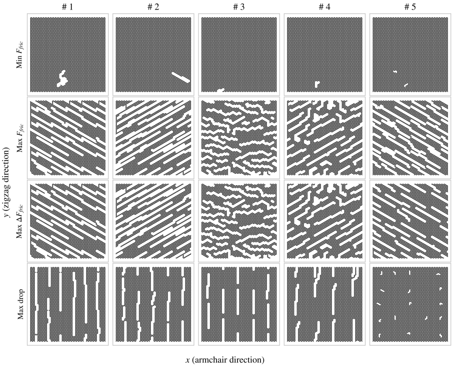


Table: Evaluation of the final model performance.

	R^2 [10^2]			Abs. [10^2]	Rel. [10^2]	Acc. [10^2]
	Mean F_f	Max F_f	Contact	Porosity	Rup. Strain	Rupture
Validation	98.067	93.558	94.598	2.325	12.958	96.102
Tetrahedron	88.662	85.836	64.683	1.207	5.880	99.762
Honeycomb	96.627	89.696	97.171	1.040	1.483	99.111

Machine learning
Model performance

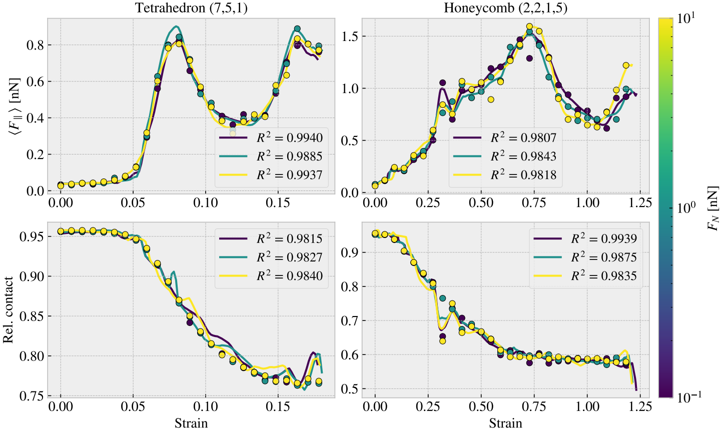


Figure: Visual evaluation of the final model predictions on the Tetrahedron $(7, 5, 1)$ and Honeycomb $(2, 2, 1, 5)$ used in the pilot study.

Accelerated search

Grad-CAM

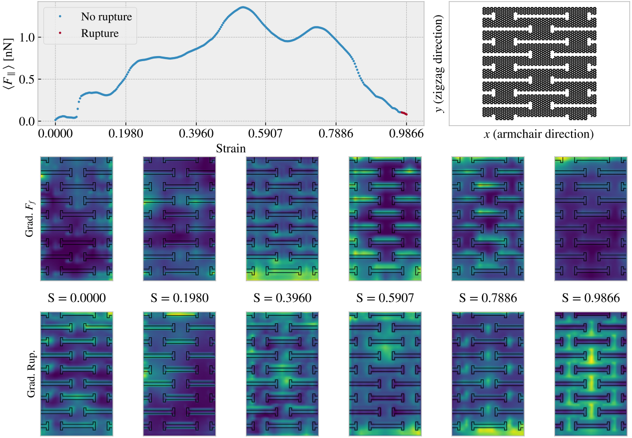


Figure: Honeycomb (3, 3, 5, 3). Top: Friction-strain curve and configuration. Bottom: Grad-CAM analysis.

Outline

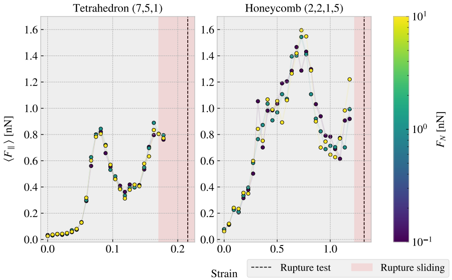
Summary and outlook

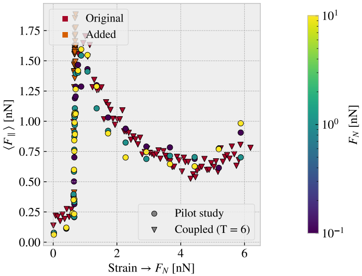
Key findings

- Non-monotonous friction-strain
- Coupled system → negative friction coefficient
- Machine learning needs more data

Further studies

- Investigate the underlying mechanism
  - Commensurability hypothesis
- Friction-strain relationship at different physical conditions
- Edge and thermostat effects.
- Improve dataset with active learning





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Designs for a negative friction coefficient

References I

[1] J. Li and L. Zhiguang, "Focused-ion-beam-based nano-kirigami: from art to photonics", Nanophotonics **7**, 10.1515/nanoph-2018-0117 (2018).

[2] W. Commons, *File:asperities.svg — wikimedia commons, the free media repository*, (2023) https://commons.wikimedia.org/w/index.php?title=File:Asperities.svg&oldid=659167170 (visited on 02/03/2023).

[3] L. Burrows, *New pop-up strategy inspired by cuts, not folds*, (Feb. 24, 2017) https://seas.harvard.edu/news/2017/02/new-pop-strategy-inspired-cuts-not-folds.

[4] *Scotch cushion lock protective wrap*, https://www.scotchbrand.com/3M/en_US/scotch-brand/products/catalog/~/Scotch-Cushion-Lock-Protective-Wrap/?N=4335+3288092498+3294529207&rt=rud.

[5] Neurohive, *VGG16 — Convolutional Network for Classification and Detection*, (2018) https://neurohive.io/en/popular-networks/vgg16/ (visited on 05/07/2023).