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

Designs for a negative friction coefficient

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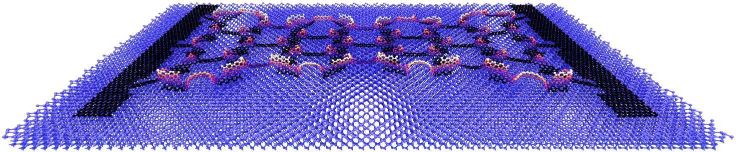

Outline

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   - Motivation
2. Creating a graphene Kirigami system
   - System setup
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3. Pilot study
   - Friction metrics
   - Out-of-plane buckling
   - Strain profiles
   - Negative friction coefficient
4. Kirigami configuration search
   - Machine learning
   - Accelerated search for new designs
5. Summary and outlook

Thesis overview
System preview

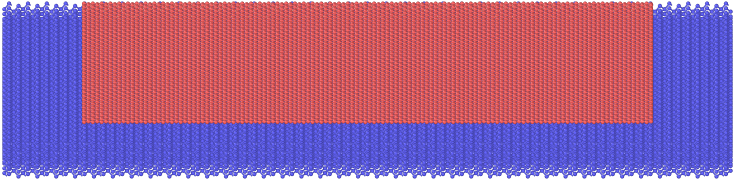


Figure: System of choice: Graphene sheet (red) on a silicon substrate (blue).

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

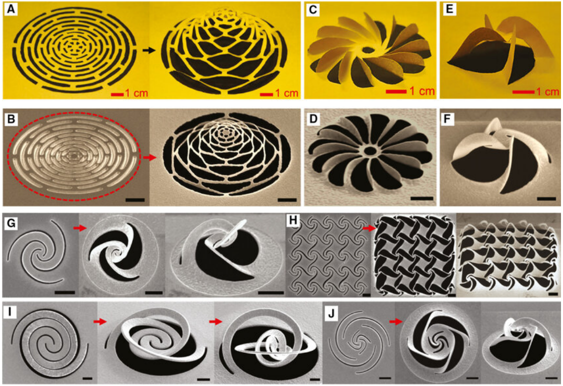
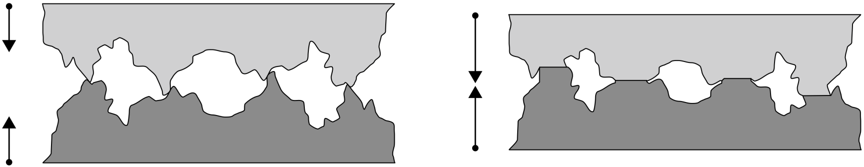


Figure: Example of macroscale Kirigami designs implemented on a microscale using a focused ion beam. Black scale bars: 1 μm. Reproduced from [1].

- 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

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System setup

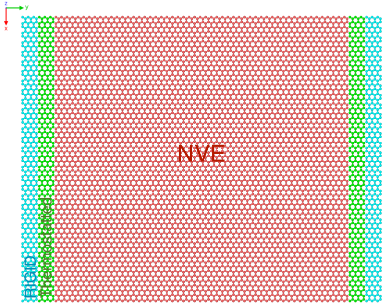
Regions

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

System size

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

(a) Side view.



(b) Top view.

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

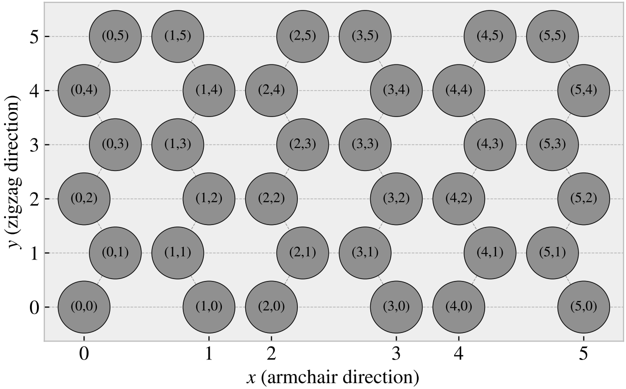


Figure: Graphene atom site indexing.

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

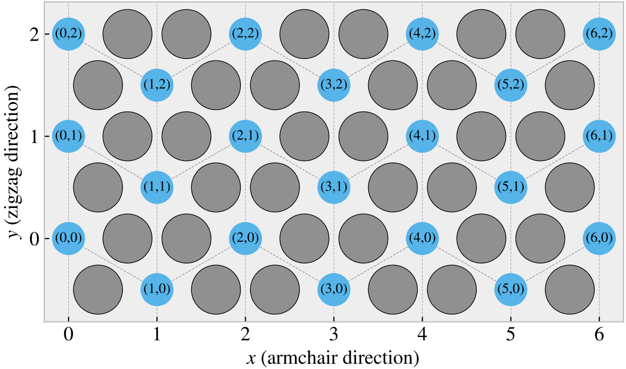
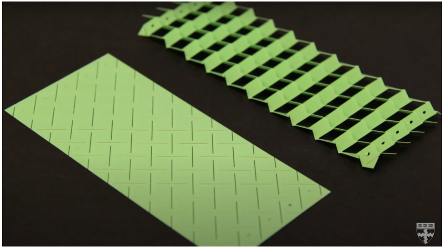
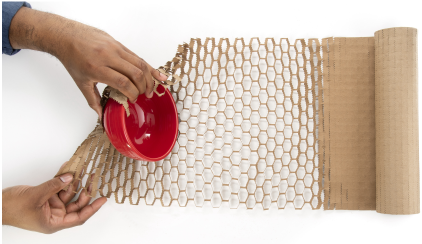


Figure: Graphene *center element* indexing.

Sheet Kirigami
Macroscale inspiration



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

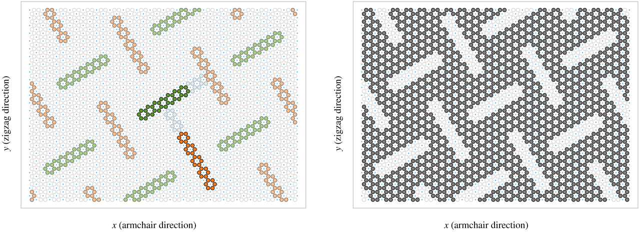


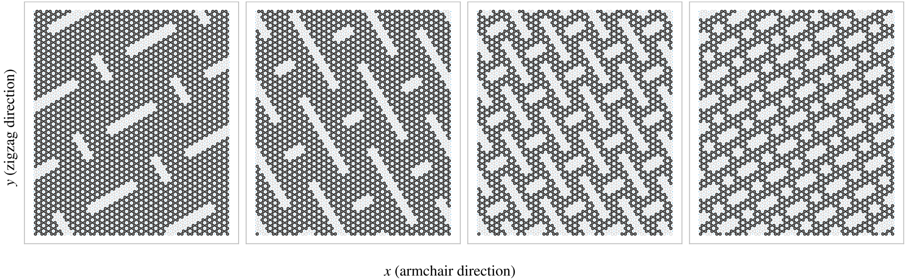
(b) Honeycomb: Scotch™ Cushion Lock™ [4] producing a honeycomb-shaped surface buckling when stretched. Reproduced from [4].

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

Sheet Kirigami

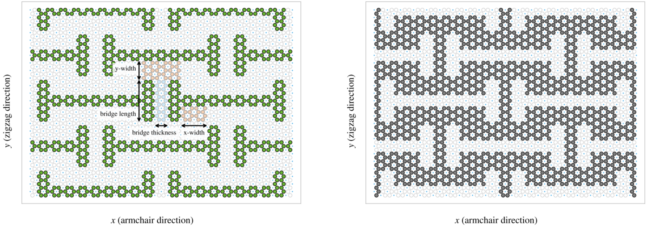
Tetrahedron patterns

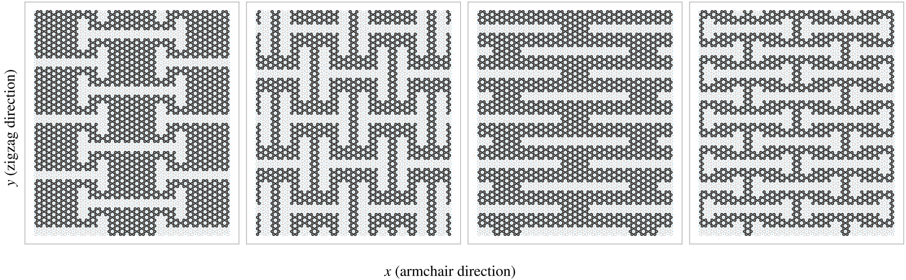




Sheet Kirigami

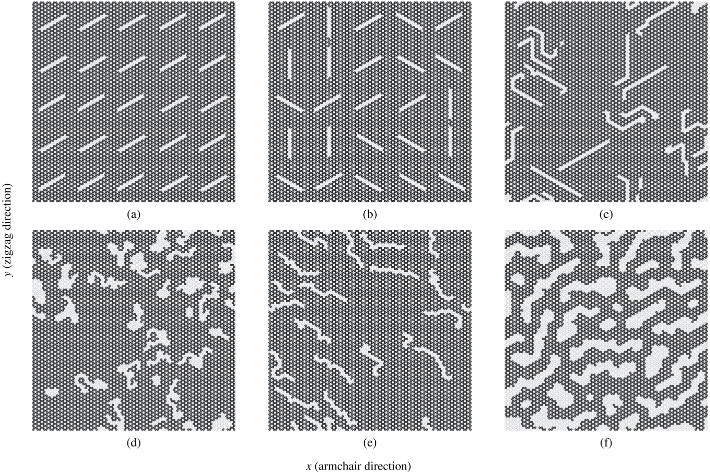
Honeycomb patterns





Sheet Kirigami

Random walk patterns



Pilot study

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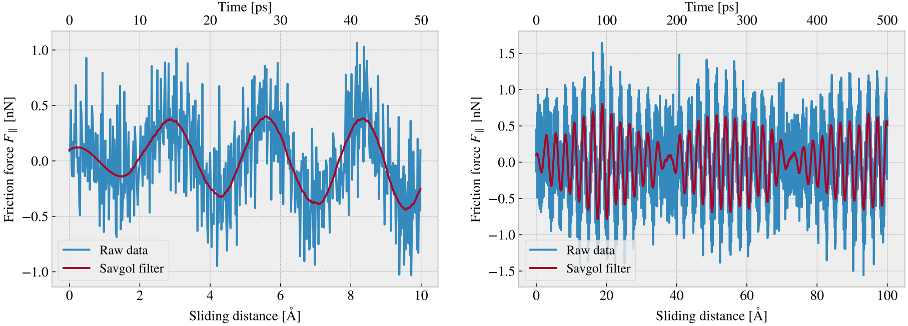
Friction metrics



(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

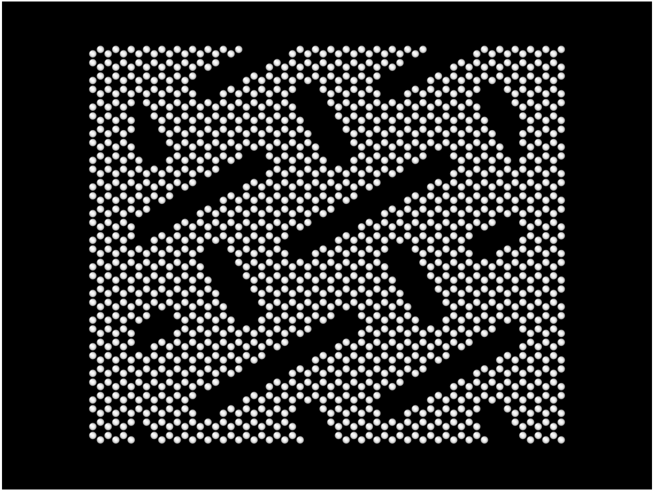


Figure: Kirigami sheet stretch in a vacuum.

Out-of-plane buckling

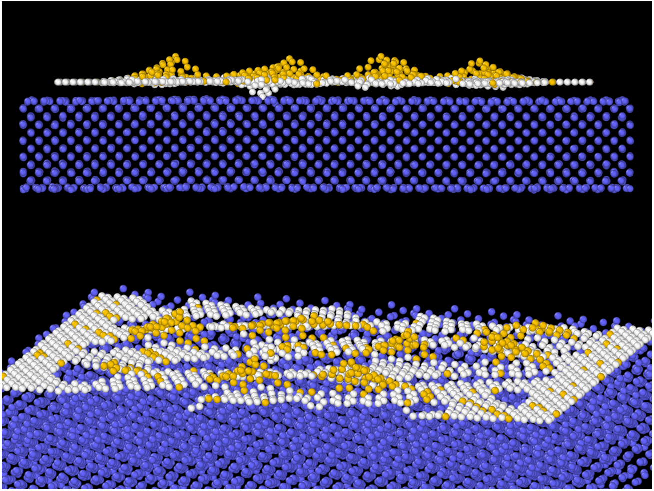


Figure: Kirigami stretch in contact with the substrate.

Out-of-plane buckling

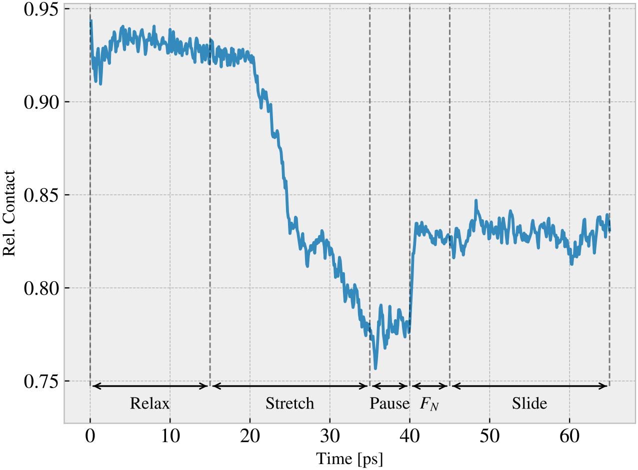


Figure: Contact area approximation: Number of C–Si bonds within a threshold distance of 110% the LJ interaction equilibrium distance.

Contact-strain profile

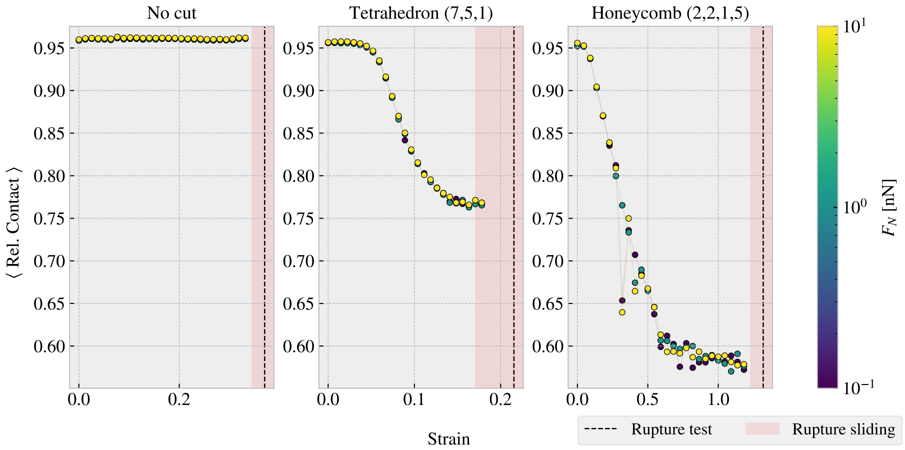


Figure: Contact-strain profile for $F_N = \{0.1, 1, 10\}$nN.

Friction-strain profile

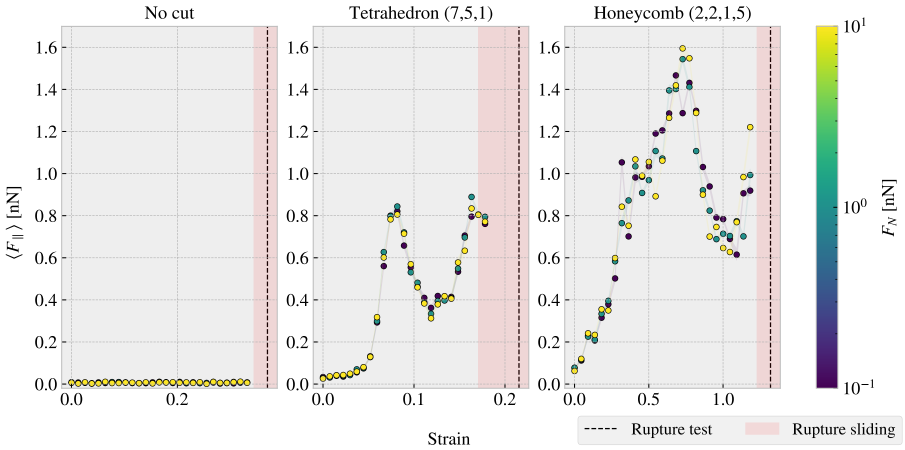


Figure: Friction-strain profile for $F_N = \{0.1, 1, 10\}$nN.

Negative friction coefficient

Coupling of load to sheet tension

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

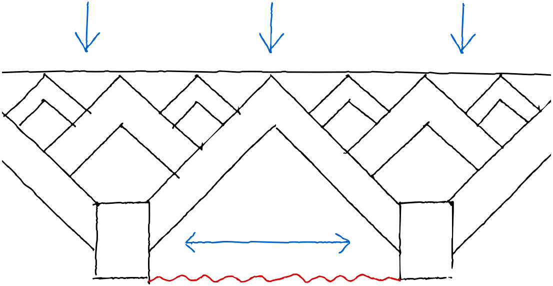


Figure: Working sketch for a nanomachine design translating applied load (from the top of the figure) to a straining of the graphene sheet (shown in red).

Negative friction coefficient
Tetrahedron results

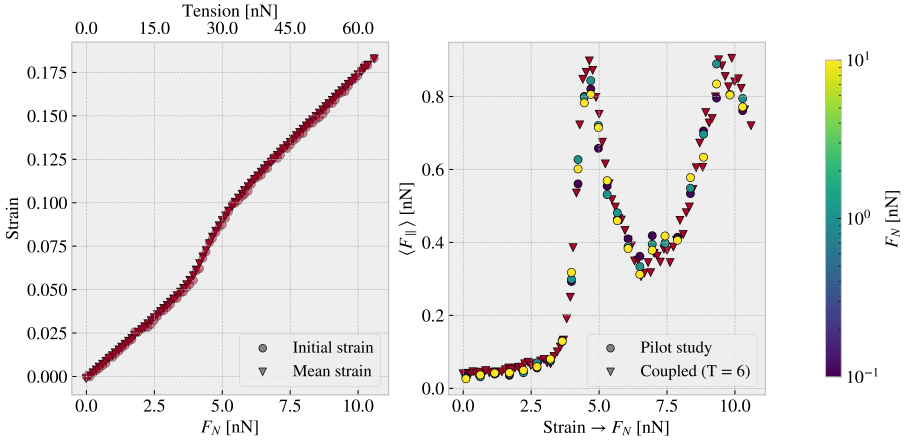


Figure: Tetrahedron $(7, 5, 1)$

Negative friction coefficient

Honeycomb results

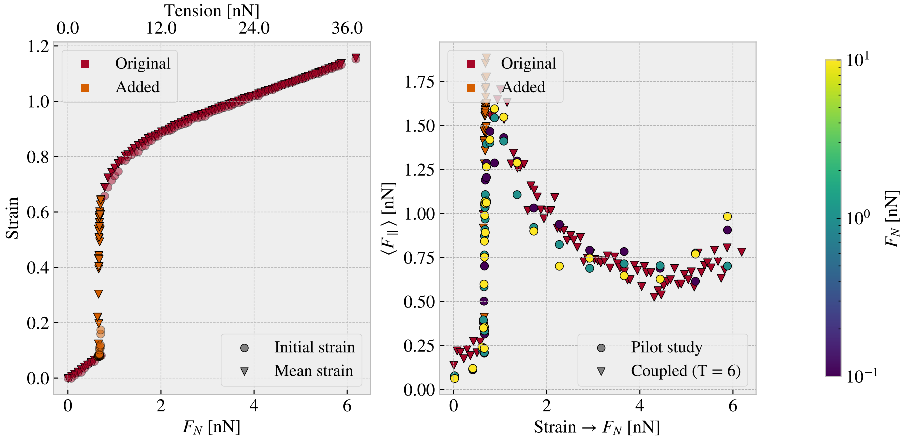


Figure: Honeycomb $(2, 2, 1, 5)$

Negative friction coefficient

Honeycomb deformations

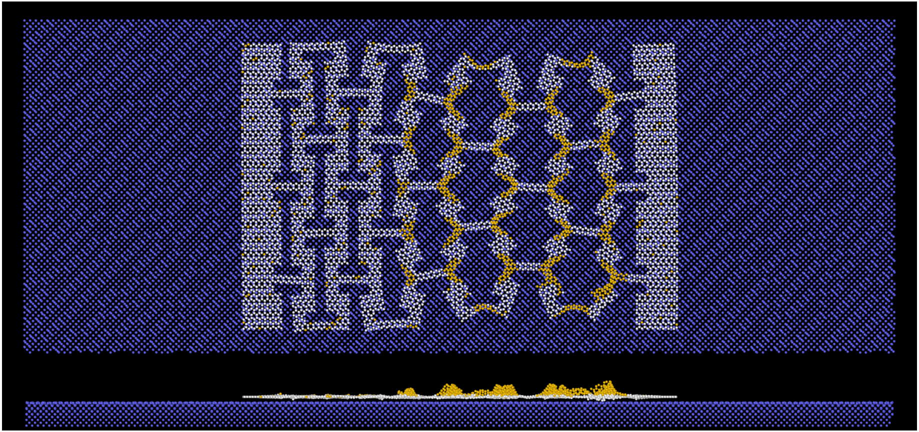


Figure: Honeycomb $(2, 2, 1, 5)$ stretch.

Kirigami configuration search

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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

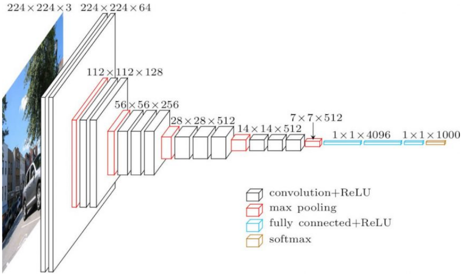

Figure: Convolutional network architecture. Reproduced from [5].

- Good validation performance
- R^2 score

Properties of interest

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

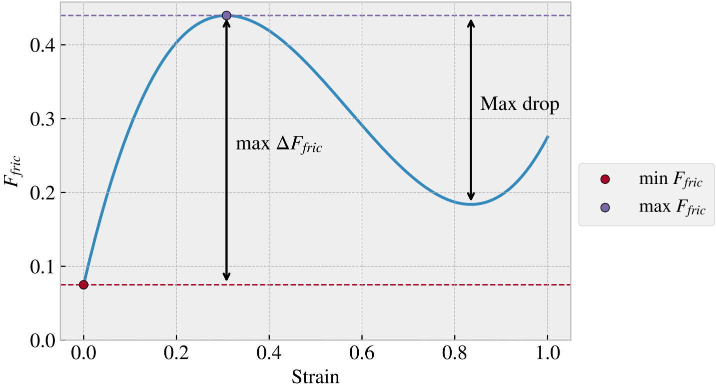

Figure: Properties of interest.

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

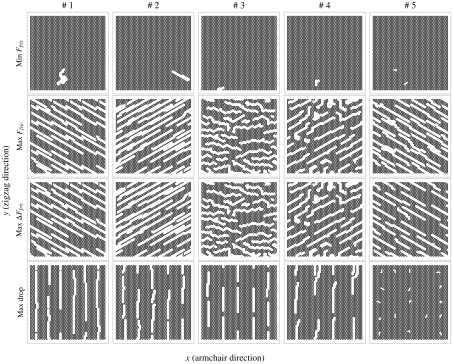

Figure: Top 5 candidates for random walk extended dataset accelerated search.

Accelerated search

Grad-CAM

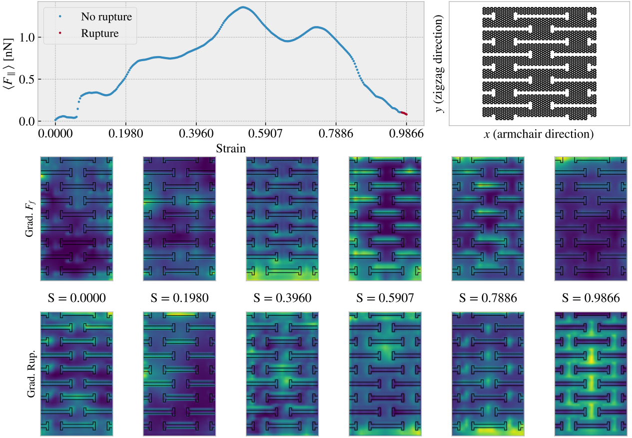

Figure: Honeycomb $(3, 3, 5, 3)$. Top: Friction-strain curve and configuration. Bottom: Grad-CAM analysis.

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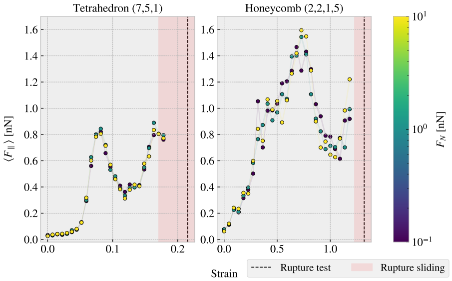
Summary and outlook

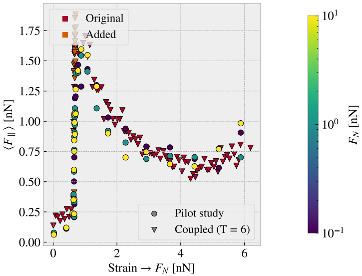
Key findings

- Non-monotonous friction-strain
- Coupled system $\rightarrow$ negative friction coefficient
- Machine learning needs more data



Further studies

- 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).