

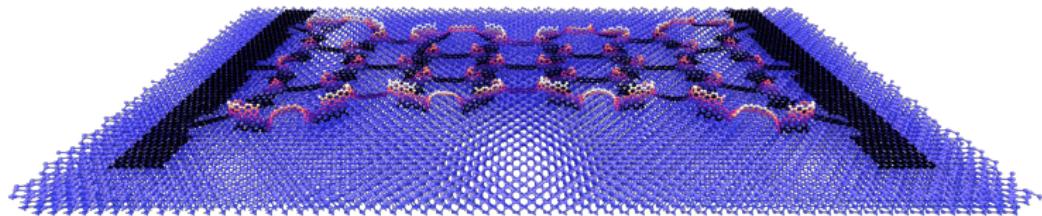
Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

Designs for a negative friction coefficient

Mikkel Metzsch Jensen

University of Oslo

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Outline

- ① Introduction
- ② Creating a graphene Kirigami system
- ③ Friction behaviour
- ④ Kirigami pattern search
- ⑤ Summary and outlook

Thesis overview

System preview

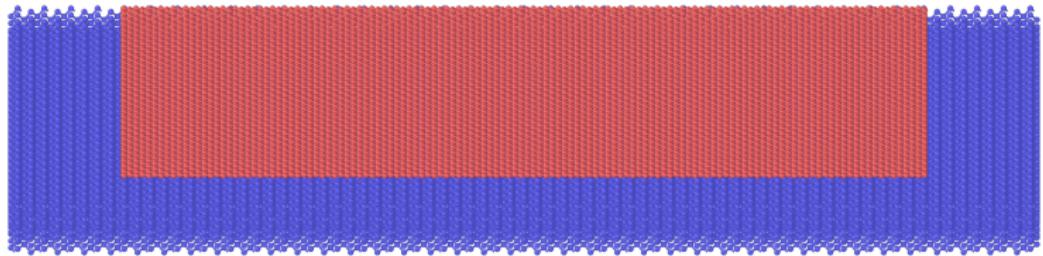


Figure: System of choice: Graphene sheet (red) on a silicon substrate (blue).

Thesis overview

- ① **Sheet modification:** Atomic-scale cuts and stretching
- ② **Forward simulation:** Simulate system and measure friction
- ③ **Pattern 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 stretching of the sheet?

Motivation

Kirigami

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

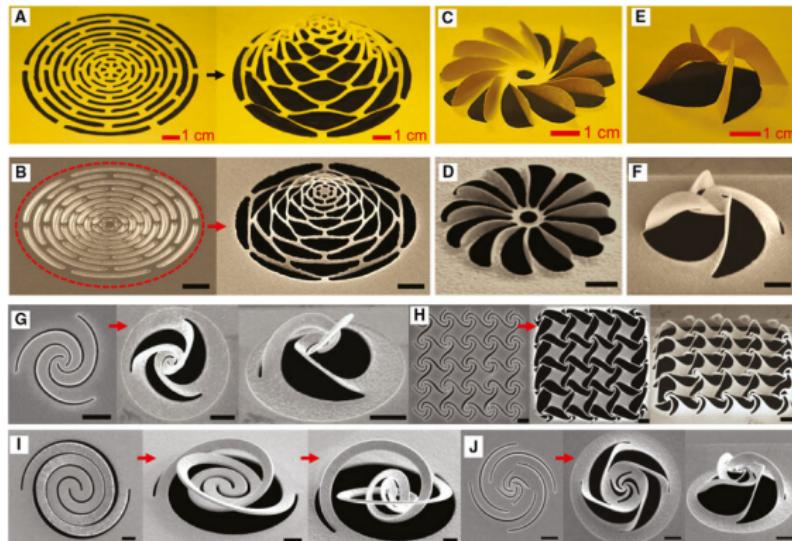
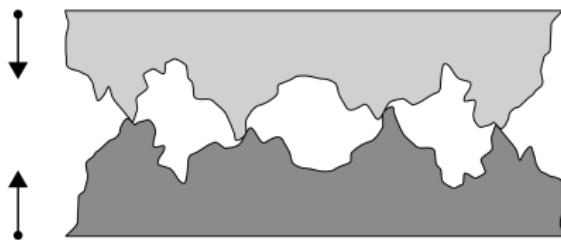


Figure: Example of macroscale Kirigami designs implemented on a microscale using a focused ion beam. Black scale bars: $1 \mu\text{m}$. Reproduced from [1].

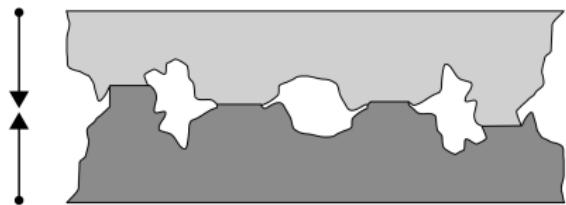
Motivation

Out-of-plane buckling

- Out-of-plane buckling
- Surface properties are important for friction
 - Asperity theory: Contact area



(a) Small load.



(b) High load.

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

Creating a graphene Kirigami system

① Introduction

② Creating a graphene Kirigami system

③ Friction behaviour

④ Kirigami pattern search

⑤ Summary and outlook

System setup

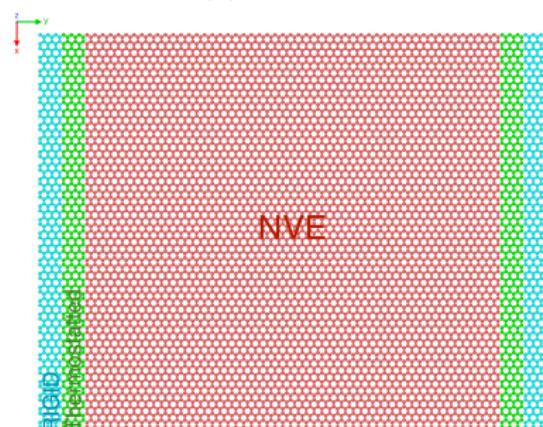


Regions

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

System size

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



(b) Top view.

Sheet Kirigami

Indexing

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

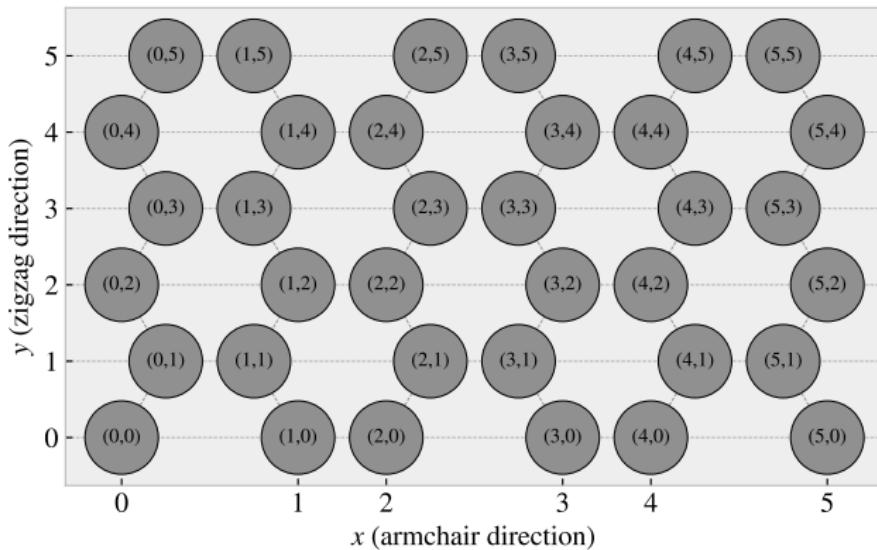
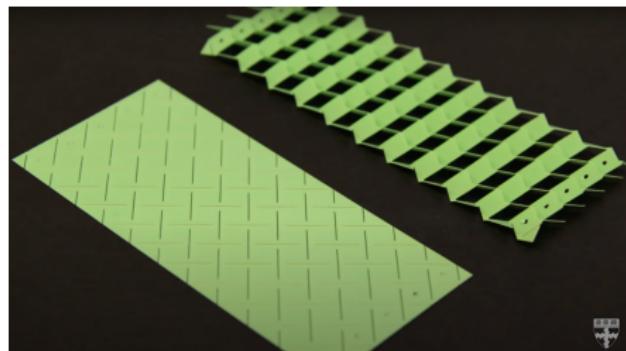


Figure: Graphene atom site indexing.

Sheet Kirigami

Macroscale inspiration



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

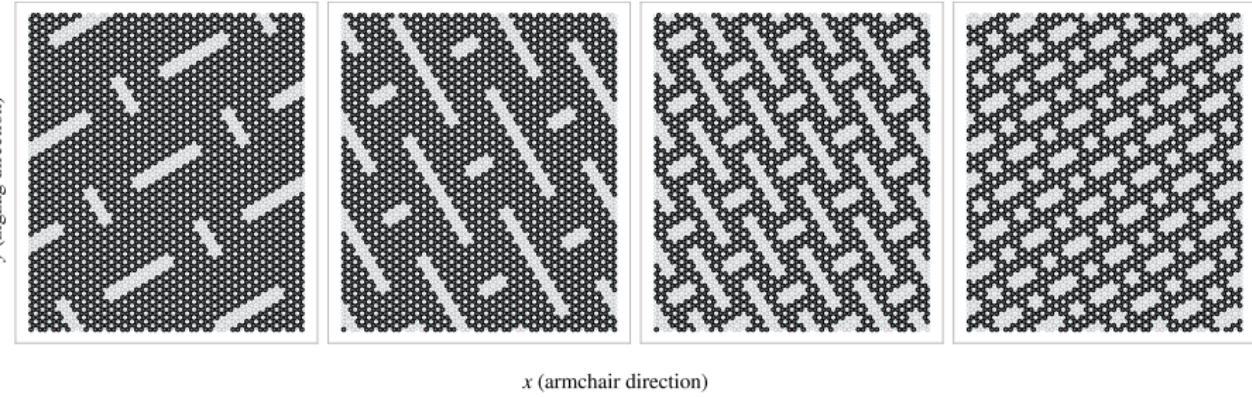
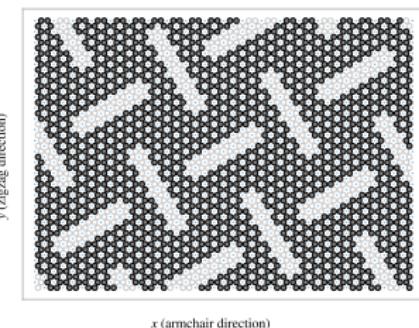
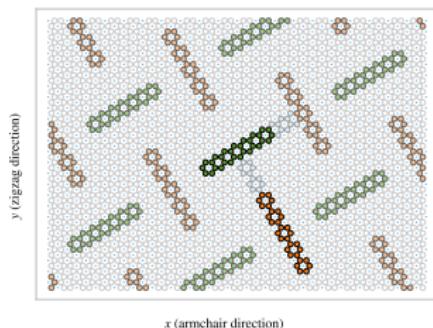


(b) Honeycomb: ScotchTM Cushion LockTM [4] producing a honeycomb-shaped surface buckling when stretched. Reproduced from [4].

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

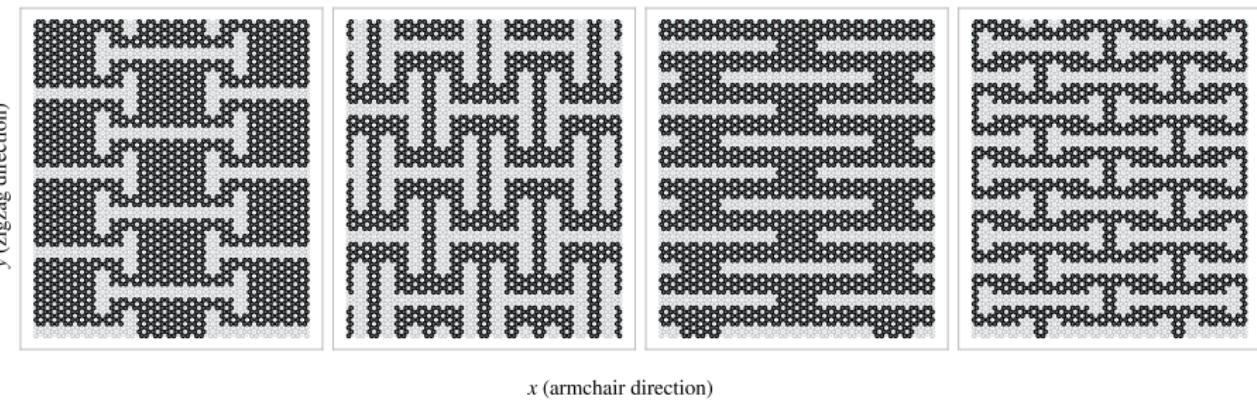
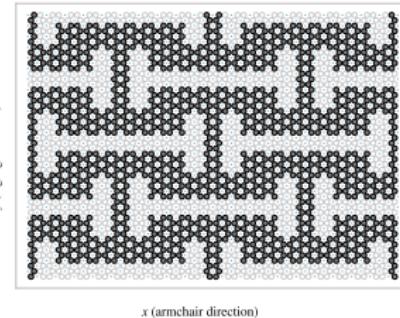
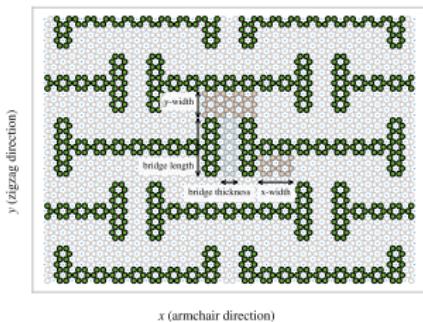
Sheet Kirigami

Tetrahedron patterns



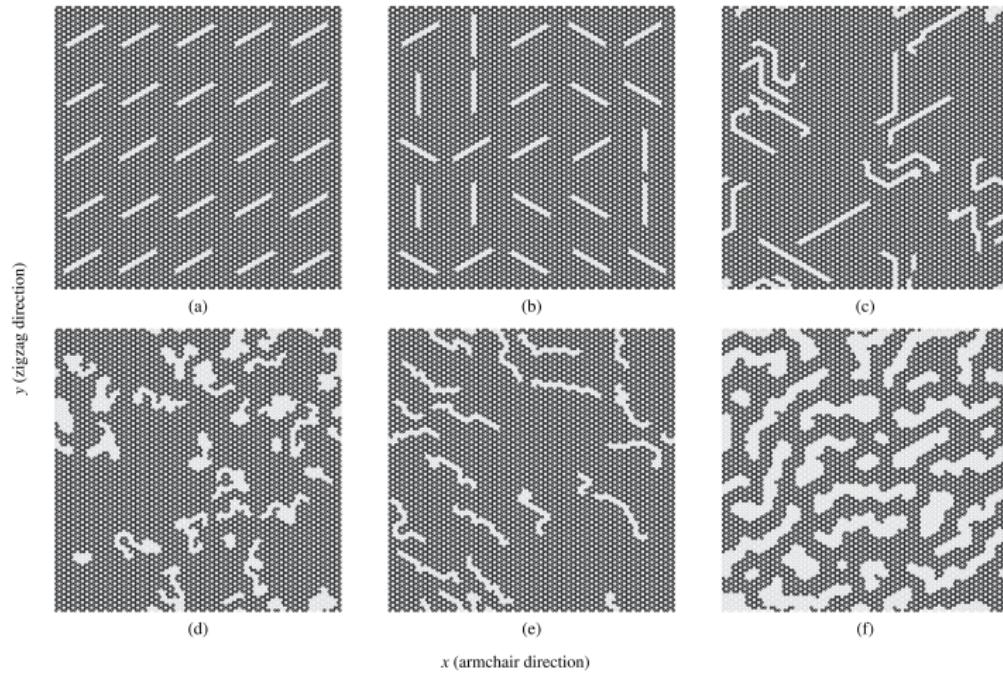
Sheet Kirigami

Honeycomb patterns



Sheet Kirigami

Random walk patterns



Friction behaviour

① Introduction

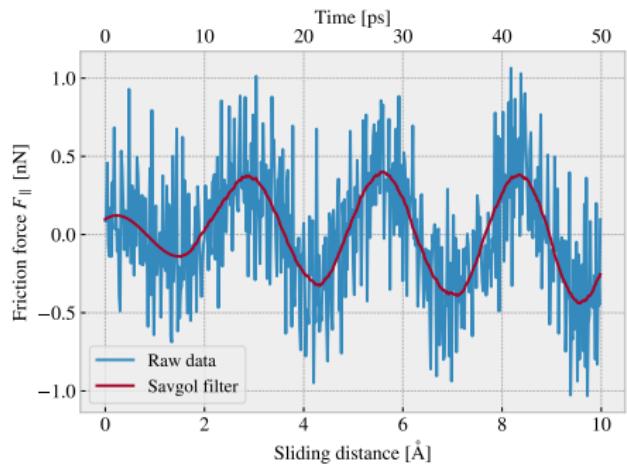
② Creating a graphene Kirigami system

③ Friction behaviour

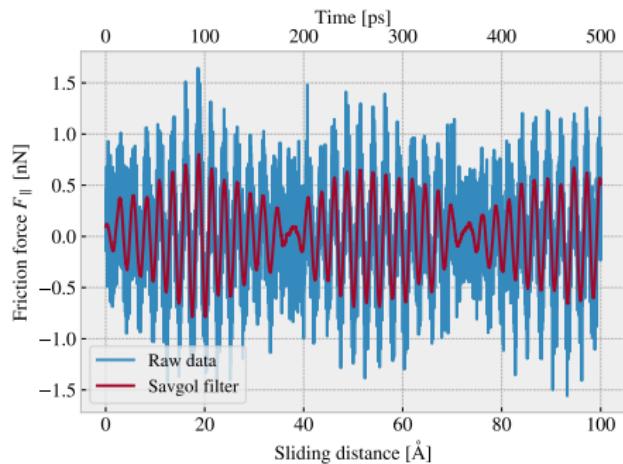
④ Kirigami pattern search

⑤ Summary and outlook

Friction metrics



(a) 10 \AA sliding.



(b) 100 \AA sliding.

Figure: Friction force traces. The red line represents a Savgol filter.

Out-of-plane buckling

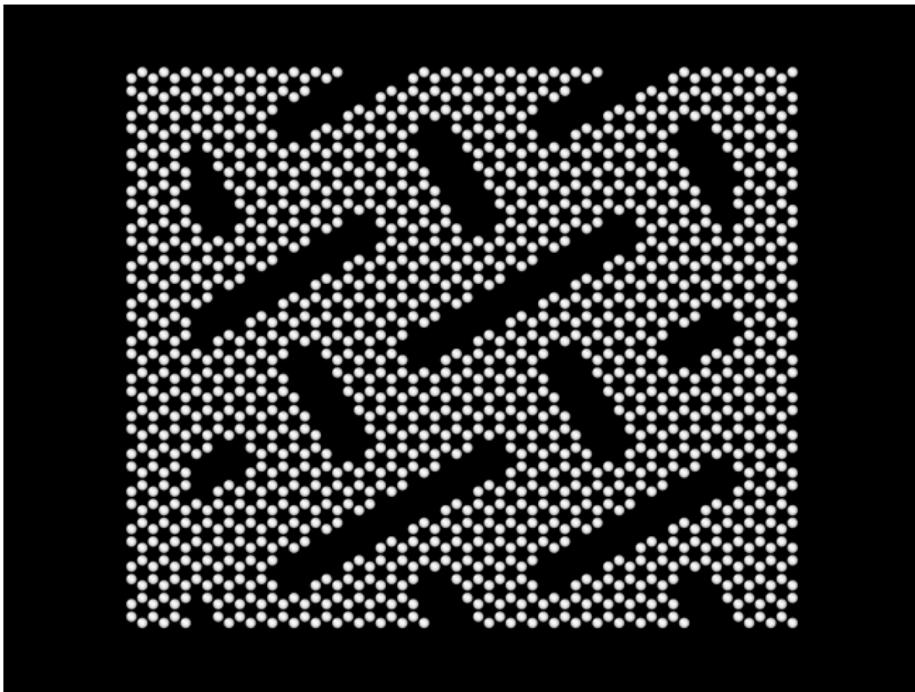


Figure: Kirigami sheet stretch in a vacuum.

Out-of-plane buckling

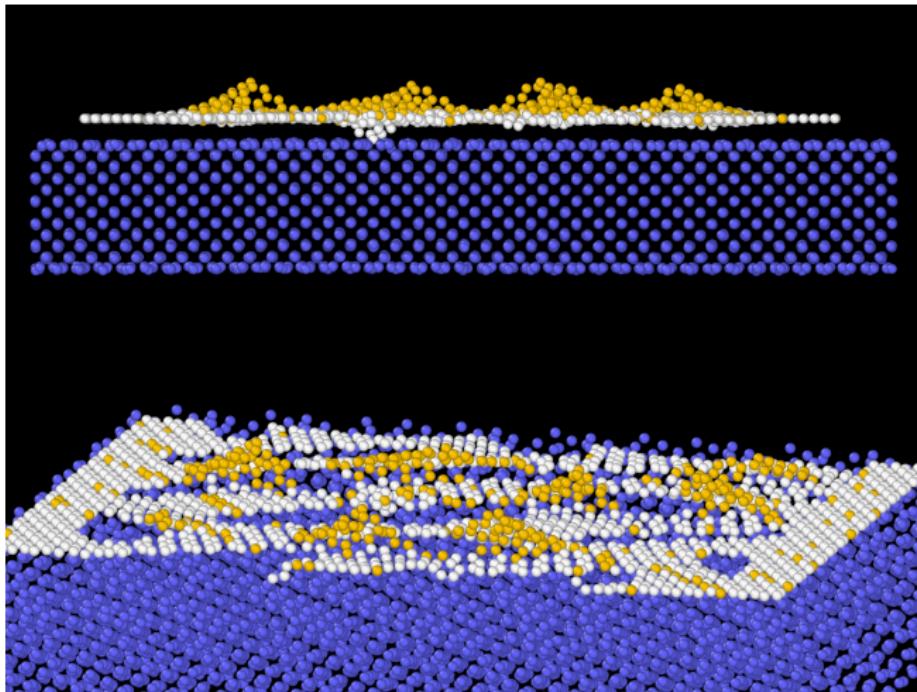


Figure: Kirigami stretch in contact with the substrate.

Out-of-plane buckling

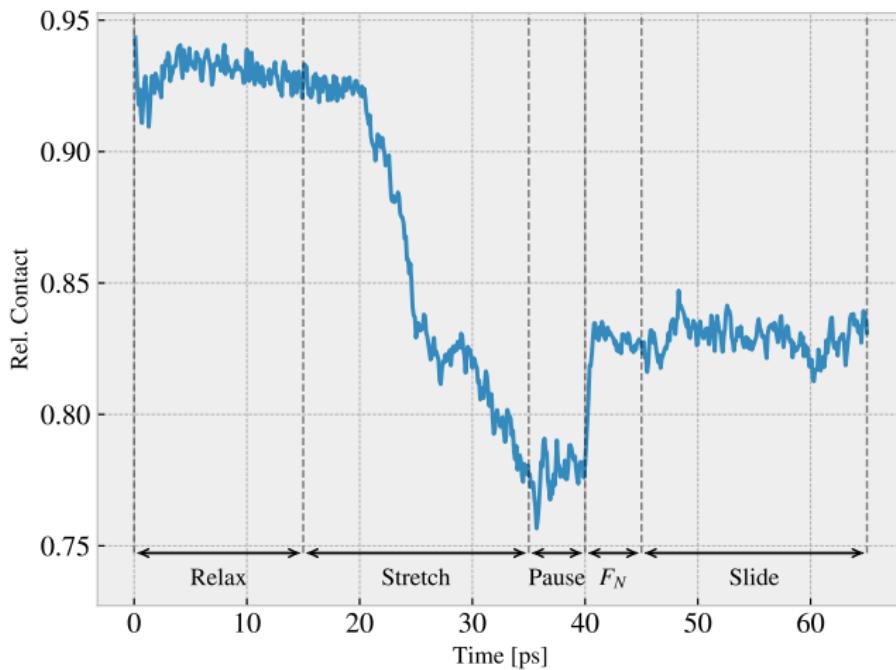


Figure: Contact area approximation: Number of C–Si bonds within a threshold distance of 110% the LJ interaction equilibrium distance.

Contact-strain profile

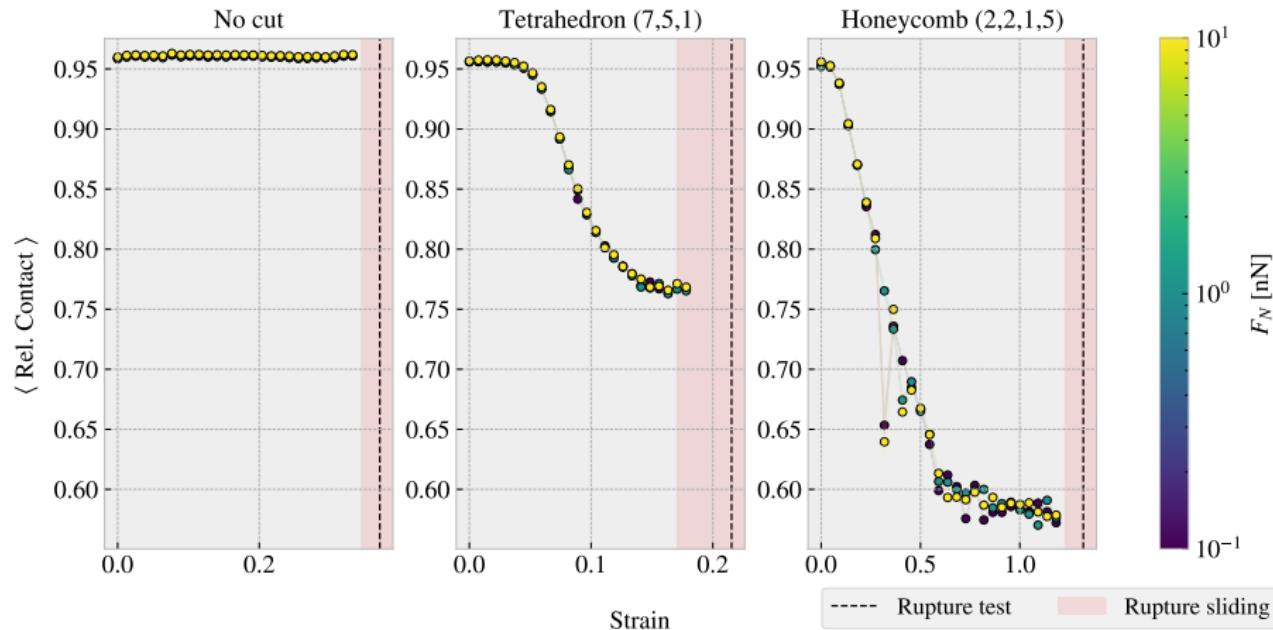


Figure: Contact-strain profile for $F_N = \{0.1, 1, 10\}$ nN.

Friction-strain profile

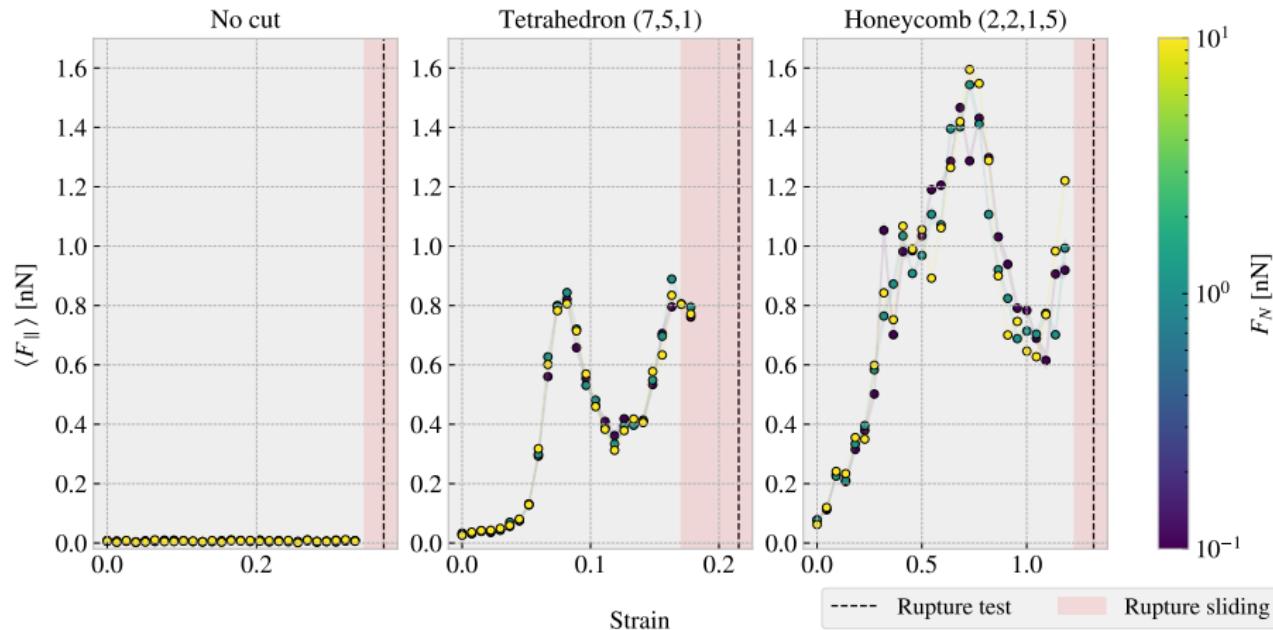


Figure: Friction-strain profile for $F_N = \{0.1, 1, 10\}$ nN.

Negative friction coefficient

Coupling of load to sheet tension

$$F_t = T \cdot F_N, \quad T = 6$$

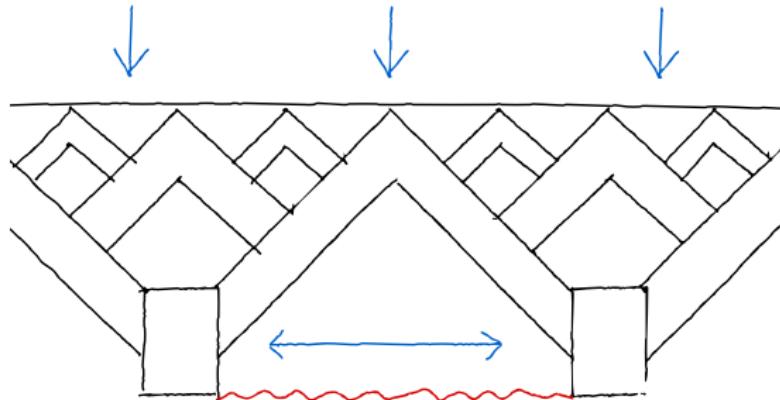


Figure: Working sketch for a nanomachine design translating applied load to a strain of the sheet (shown in red).

Negative friction coefficient

Tetrahedron results

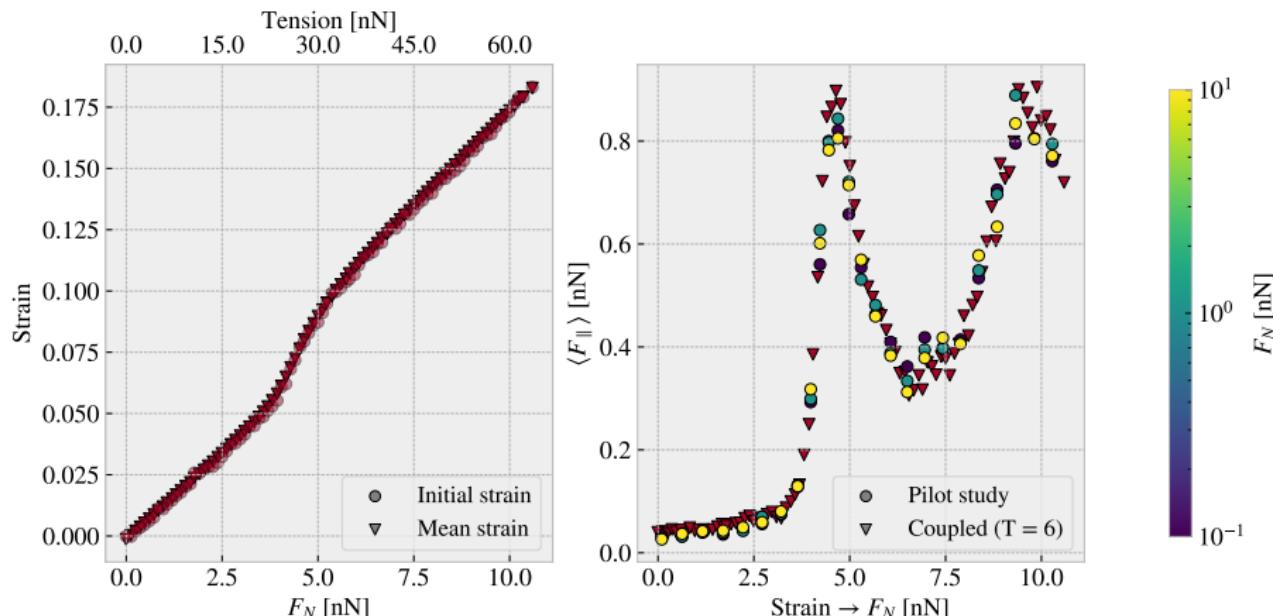


Figure: Tetrahedron (7, 5, 1)

Negative friction coefficient

Honeycomb results

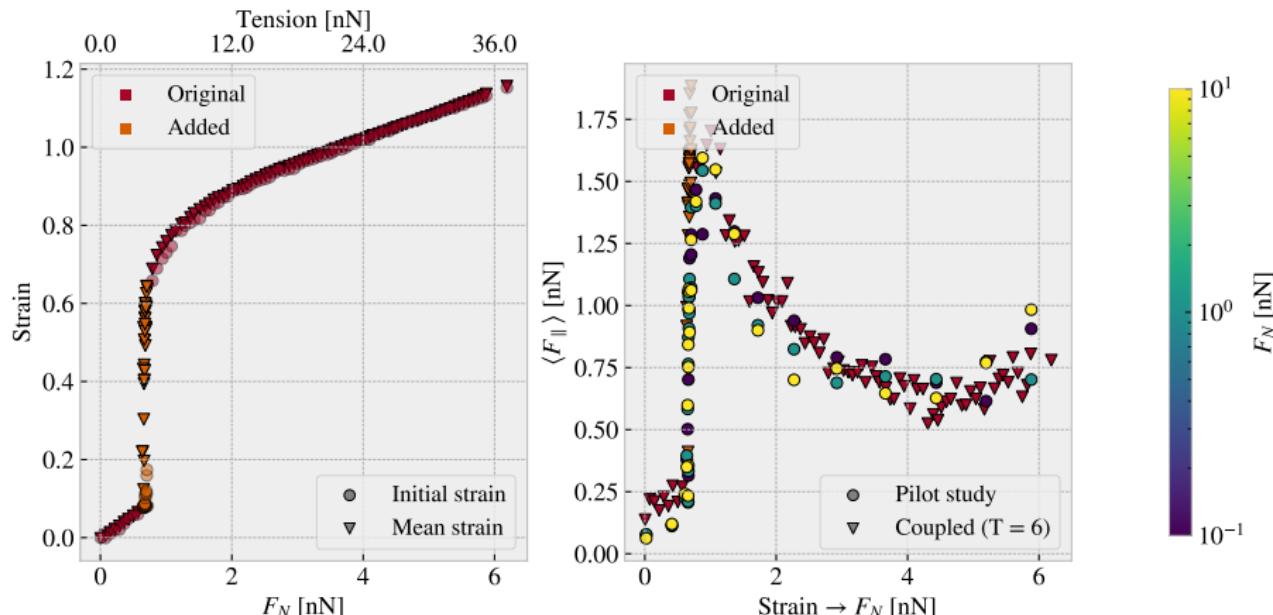
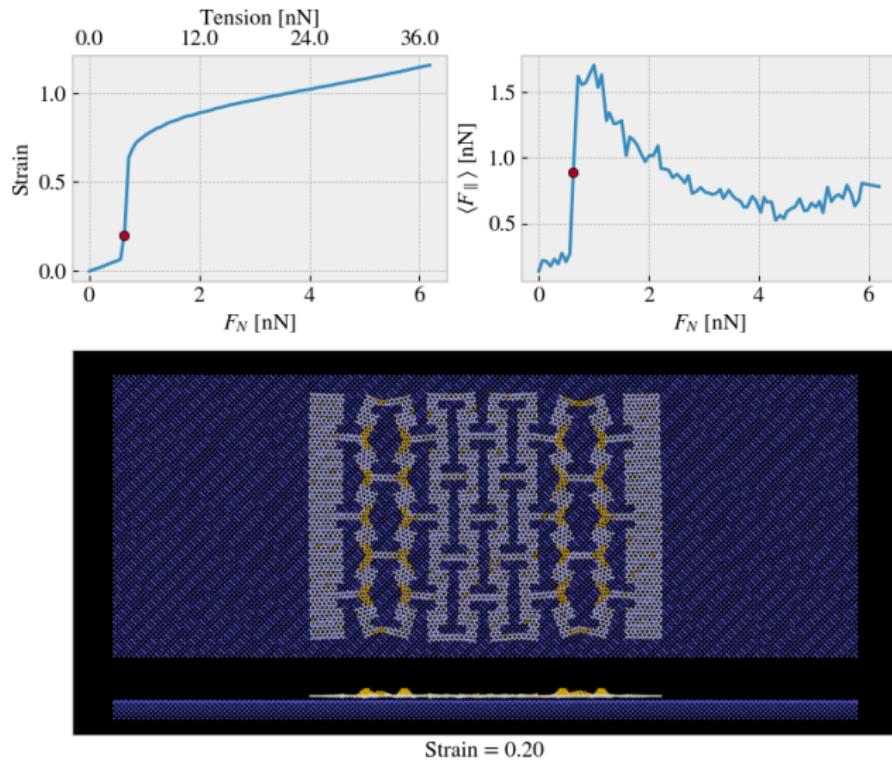


Figure: Honeycomb (2, 2, 1, 5)

Negative friction coefficient

Honeycomb deformations



Kirigami pattern 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 friction, rupture

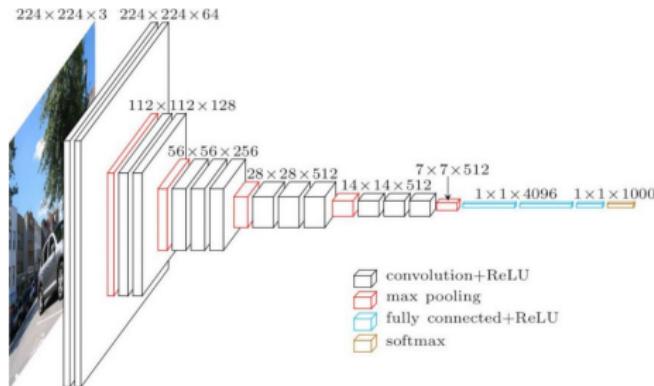


Figure: Convolutional neural network. Reproduced from [5].

Properties of interest

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

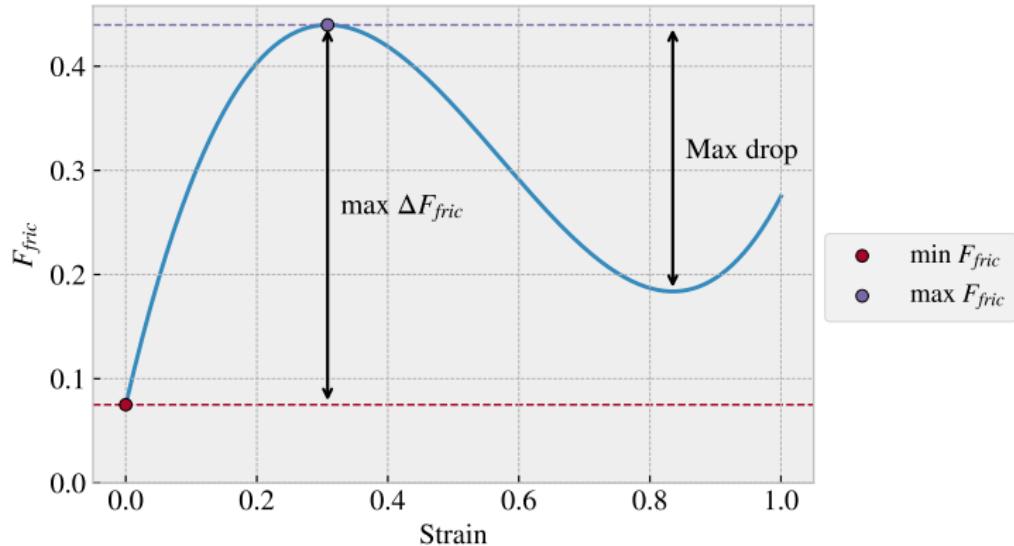


Figure: Properties of interest.

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

Accelerated search

Grad-CAM

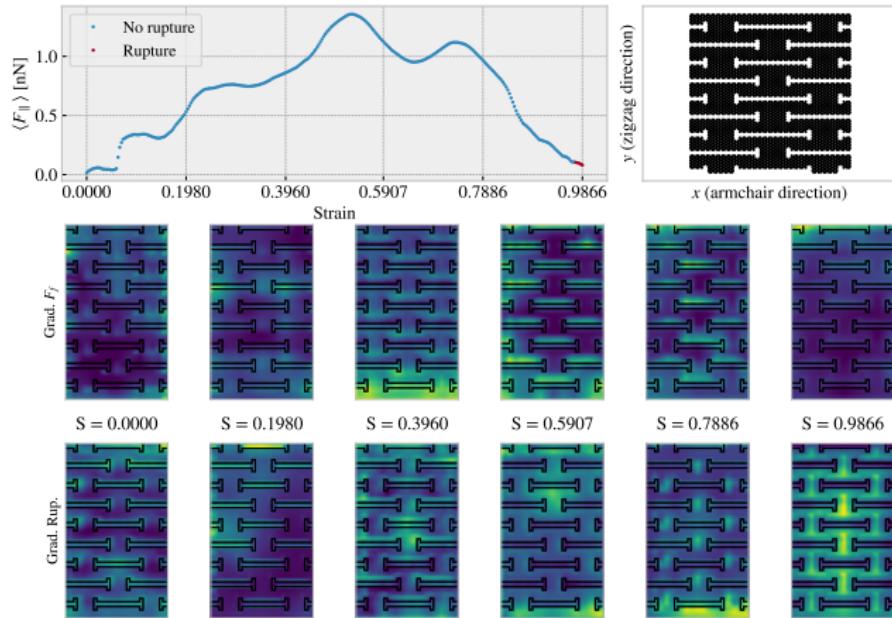


Figure: Honeycomb (3, 3, 5, 3). Top: Friction-strain curve and configuration. Bottom: Grad-CAM analysis.

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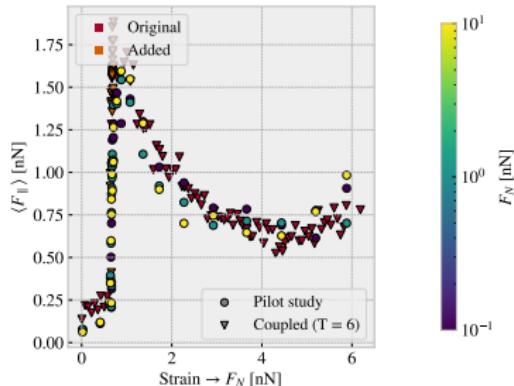
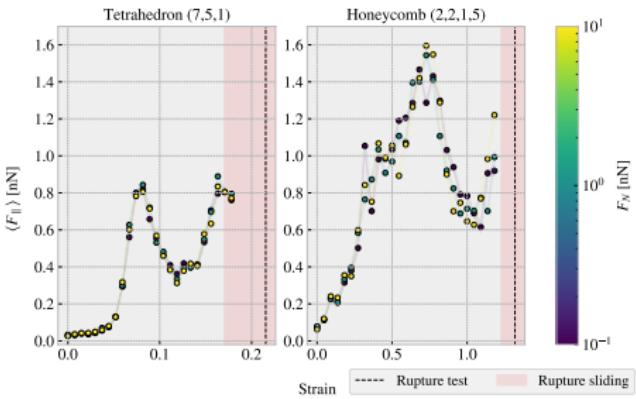
Summary and outlook

Key findings

- Non-monotonous friction-strain
- 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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Neural Networks

Designs for a negative friction coefficient

References

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