Tuning friction properties of graphene sheets using kirigami cuts and inverse design

Optional Subtitle

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Presentation Overview

Project description - 3 stages

1. Alter graphene sheet by making selected cuts on an atomic scale.
2. Calculate the effects on frictional properties using MD simulations.
3. Use inverse design on data to predict cut patterns for desirable properties.
    - E.g. coupling stretch and friction to achieve negative friction coefficients in nanomachines with coupling of normal force and stretch.

Stage 1 - Kirigami cuts

- Accelerated Search and Design of Stretchable Graphene Kirigami Using Machine Learning, Paul Z. Hanakata
- Reported tunability of yield stress and yield strain, as a function of cutting pattern

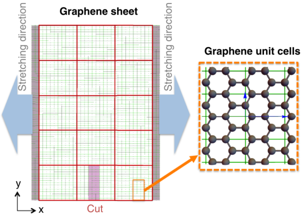

Figure: Schematic diagrams of a graphene sheet and rectangular graphene unit cells. Each of the grid (colored red) consists of 10 × 16 rectangular graphene unit cells (colored green).

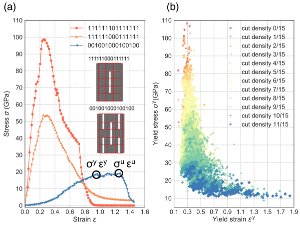

Figure: (a) Stress-strain plot of three representative kirigamis. Inset shows the “typical” kirigami cuts. (b) Yield stress as a function of yield strain for different configurations. Data are colored based on their cut density.

Stage 1 - Kirigami cuts

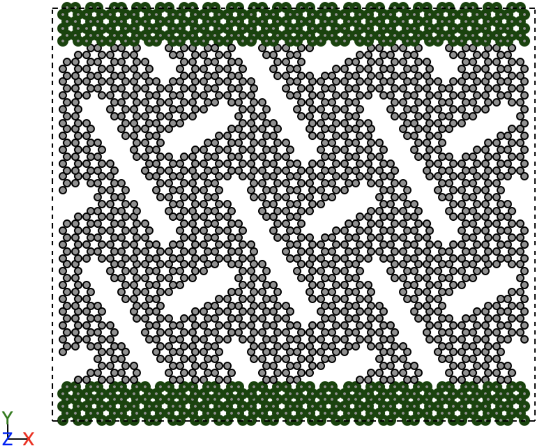

Figure: Example of cut pattern. The grey color marks the cutable sheet while green marks added blocks for stetching and dragging the sheet.

Stage 1 - Kirigami cuts

- Kirigami design on macroscale.

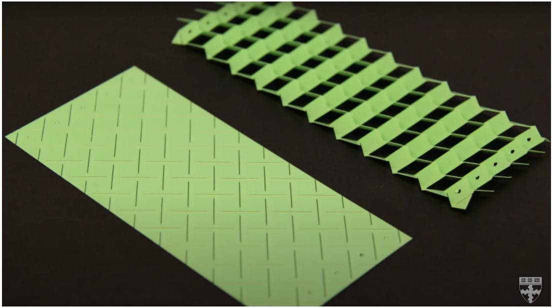

Figure: New pop-up strategy inspired by cuts, not folds - Leah Burrows, Harvard John A. Paulson School of Engineering and Applied Sciences

Stage 1 - Kirigami cuts

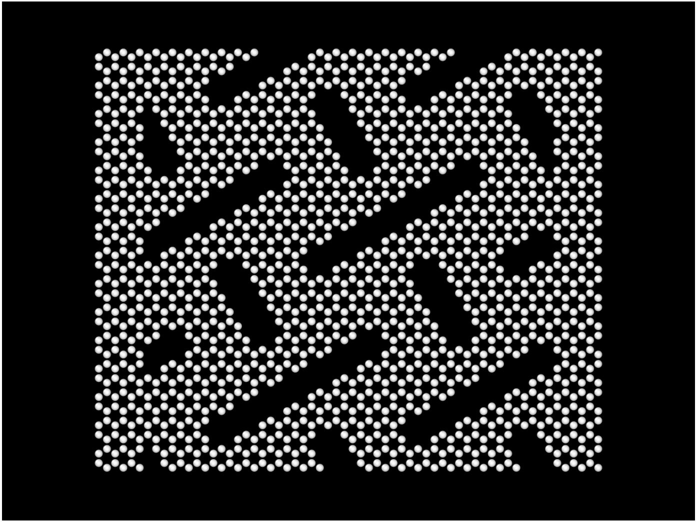

Figure: Kirigami sheet stretch in vaccuum.

Stage 1 - Kirigami cuts

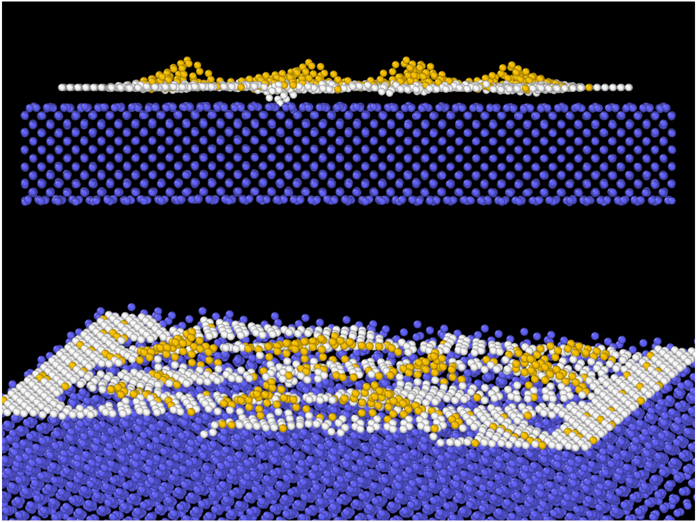

Figure: ...

Stage 1 - Kirigami cuts

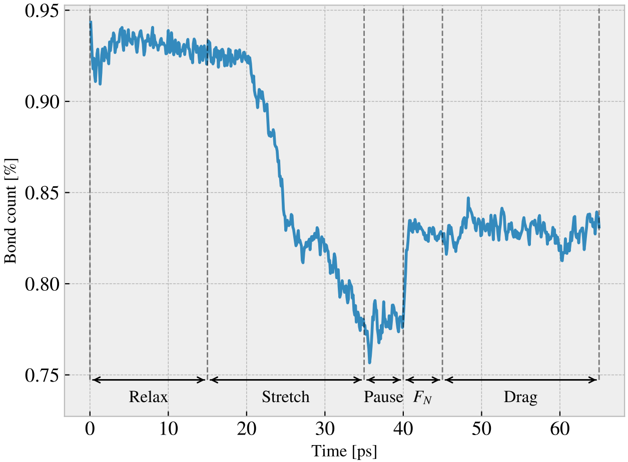

Figure: Bond threshold is defined as 110% of equlibrium distance in LJ potential.

Stage 2 - MD measurements

Friction force

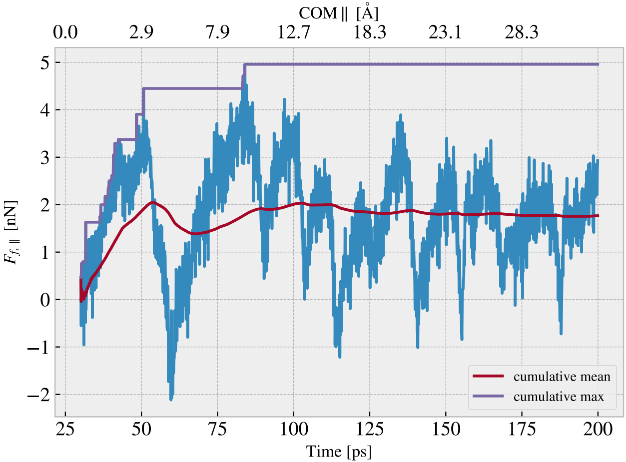

Figure: Friction force parallel to drag direction with normal force $F_N = 200$ nN. Drag distance = 40 Å

Stage 2 - MD measurements

Friction force

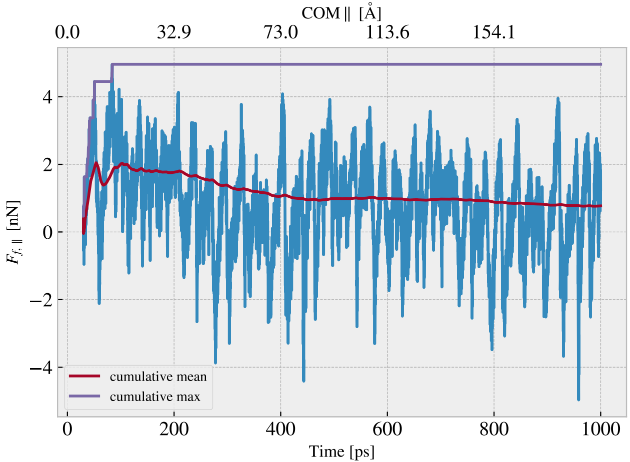

Figure: Friction force parallel to drag direction with normal force $F_N = 200$ nN. Drag distance = 200 Å

Stage 2 - MD measurements
Contact area

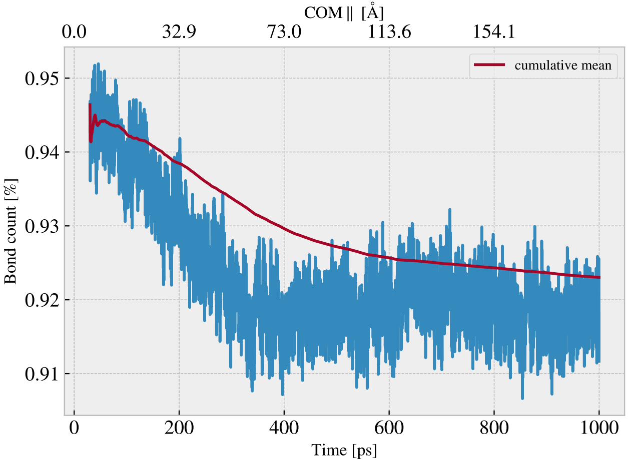

Figure: Contact bond count with normal force $F_N = 200$ nN. Drag distance = 200 Å

Stage 2 - MD measurements
Contact area

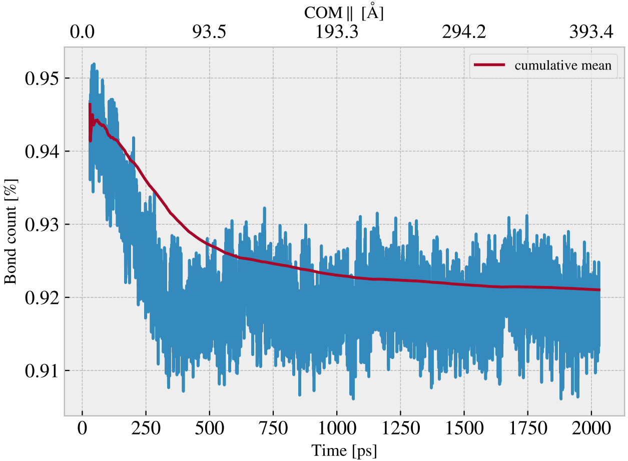

Figure: Contact bond count with normal force $F_N = 200$ nN. Drag distance = 400 Å

Stage 2 - MD measurements

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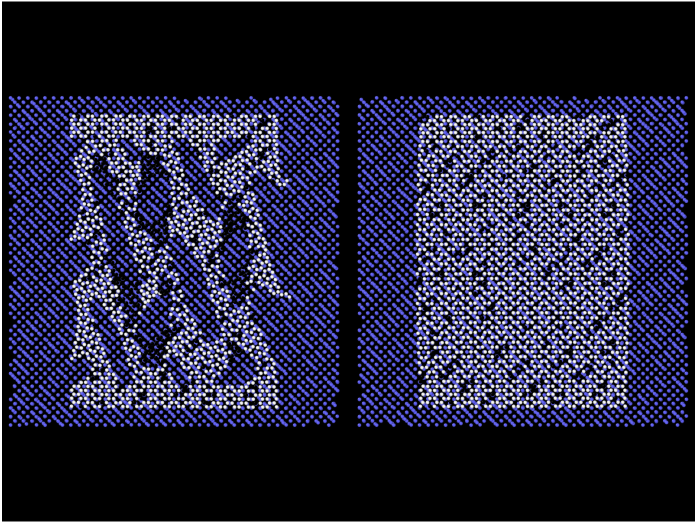

Figure: Stretch = 22 %, $F_N = 200$ nN, Drag length = 200 Å.

Stage 2 - MD measurements
Parameters

Category	Parameter	Range
Physical (free)	Temperatur	[0, 300] K
	Drag speed	$< 50m/s$
Physical (ML input)	Cut configuration	No ruptures
	Scan angle	$[0, 90^\circ]$
	Streth amount	$[0, 20]$ %
	Normal force	$[10, 200]$ nN
MD settings	Relax and pauses	$\sim$ 10 ps
	Sretch 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 and approximate ranges

Motivation

- Friction has a huge impact in various engineering applications.
- Most obvious advantages: Energy efficiency

> "The economic aspects of tribology are significant. Investigations by a number of countries arrived at figures of savings of 1.0% to 1.4% of the GNPs, obtainable by the application of tribological principles."
>
> — Professor H. Peter Jost, President, International Tribology Council

Inspiration

- Inverse Design of Inflatable Soft Membranes Through Machine Learning
- Accelerated Search and Design of Stretchable Graphene Kirigami Using Machine Learning
- Designing complex architectured materials with generative adversarial networks

Paragraphs of Text

Sed iaculis dapibus gravida. Morbi sed tortor erat, nec interdum arcu. Sed id lorem lectus. Quisque viverra augue id sem ornare non aliquam nibh tristique. Aenean in ligula nisl. Nulla sed tellus ipsum. Donec vestibulum ligula non lorem vulputate fermentum accumsan neque mollis.

> *Sed diam enim, sagittis nec condimentum sit amet, ullamcorper sit amet libero. Aliquam vel dui orci, a porta odio.*
> *— Someone, somewhere…*

Nullam id suscipit ipsum. Aenean lobortis commodo sem, ut commodo leo gravida vitae. Pellentesque vehicula ante iaculis arcu pretium rutrum eget sit amet purus. Integer ornare nulla quis neque ultrices lobortis.

Lists

Bullet Points and Numbered Lists

- Lorem ipsum dolor sit amet, consectetur adipiscing elit
- Aliquam blandit faucibus nisi, sit amet dapibus enim tempus
  - Lorem ipsum dolor sit amet, consectetur adipiscing elit
  - Nam cursus est eget velit posuere pellentesque
- Nulla commodo, erat quis gravida posuere, elit lacus lobortis est, quis porttitor odio mauris at libero

1. Nam cursus est eget velit posuere pellentesque
2. Vestibulum faucibus velit a augue condimentum quis convallis nulla gravida

Blocks of Highlighted Text

Block Title

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Integer lectus nisl, ultricies in feugiat rutrum, porttitor sit amet augue.

Example Block Title

Aliquam ut tortor mauris. Sed volutpat ante purus, quis accumsan.

Alert Block Title

Pellentesque sed tellus purus. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos himenaeos.

Suspendisse tincidunt sagittis gravida. Curabitur condimentum, enim sed venenatis rutrum, ipsum neque consectetur orci.

Multiple Columns

Subtitle

Heading

1. Statement
2. Explanation
3. Example

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Integer lectus nisl, ultricies in feugiat rutrum, porttitor sit amet augue. Aliquam ut tortor mauris. Sed volutpat ante purus, quis accumsan dolor.

Table

Subtitle

Treatments	Response 1	Response 2
Treatment 1	0.0003262	0.562
Treatment 2	0.0015681	0.910
Treatment 3	0.0009271	0.296

Table: Table caption

Definitions & Examples

Definition

A prime number is a number that has exactly two divisors.

Example

- 2 is prime (two divisors: 1 and 2).
- 3 is prime (two divisors: 1 and 3).
- 4 is not prime (three divisors: 1, 2, and 4).

You can also use the `theorem`, `lemma`, `proof` and `corollary` environments.

Theorem, Corollary & Proof

Theorem (Mass–energy equivalence)

$E = mc^2$

Corollary

$x + y = y + x$

Proof.

$\omega + \phi = \epsilon$ $\square$

Equation

$$\cos^3 \theta = \frac{1}{4} \cos \theta + \frac{3}{4} \cos 3\theta \tag{1}$$

Verbatim

Example (Theorem Slide Code)

```
\begin{frame}
\frametitle{Theorem}
\begin{theorem}[Mass--energy equivalence]
$E = mc^2$
\end{theorem}
\end{frame}
```

Slide without title.

Citing References

An example of the `\cite` command to cite within the presentation:

This statement requires citation [Smith, 2022, Kennedy, 2023].

References

John Smith (2022)
Publication title
Journal Name 12(3), 45 – 678.

Annabelle Kennedy (2023)
Publication title
Journal Name 12(3), 45 – 678.

Acknowledgements

Smith Lab

- Alice Smith
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- Yuan

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The End

Questions? Comments?