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

Designs for a negative friction coefficient

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Master's thesis

3 Phases

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

1. Sheet kirigami: Alter graphene sheet using atomic scale cuts
2. Forward simulation: Calculate frictional properties of the sheet using MD simulations
3. Accelerated search: Use machine learning to search for new Kirigami designs optimizing for various frictional properties
    - Low/high friction coefficient
    - Coupling between stretch and friction
    - Negative friction coefficients

Motivation

- Kirigami: Variation of origami with cuts permitted
- Macroscale $\rightarrow$ Nanoscale

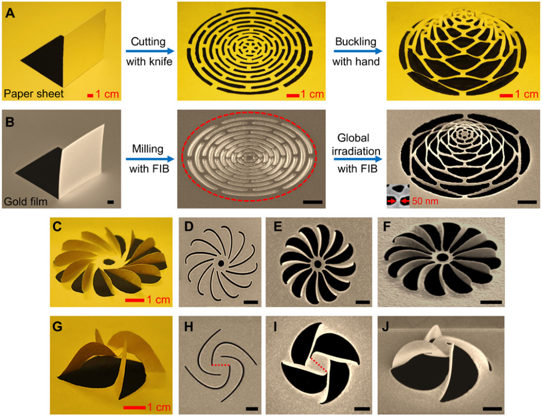

Figure: Example of transistion from macro- to nano-kirigami using a focused ion-beam (FIB) (Nano-kirigami with giant optical chirality, ZHIGUANG LIU, 2018).

Stage 1 - Sheet Kirigami

Choosing a cut pattern

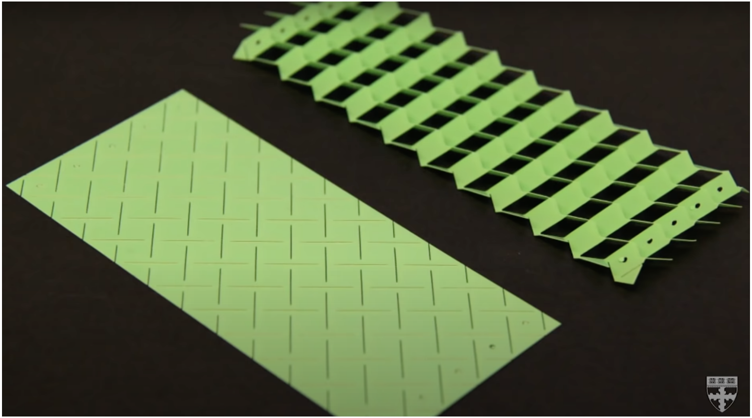

Figure: New pop-up strategy inspired by cuts, not folds - Leah Burrows, Harvard John A. Paulson School of Engineering and Applied Sciences.

Stage 1 - Sheet Kirigami

Choosing a cut pattern

Figure: Scotch Cushion Lock Protective Wrap.

Stage 1 - Sheet Kirigami

Implementation

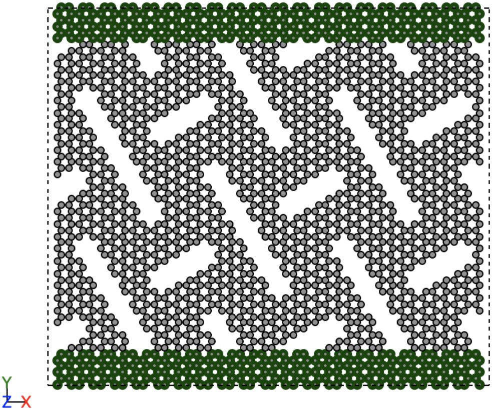

Figure: Example of “popup” cut pattern. Grey color marks the cuttable sheet while green marks added blocks for stretching and dragging the sheet.

Stage 1 - Sheet Kirigami

Investigating 3D buckling

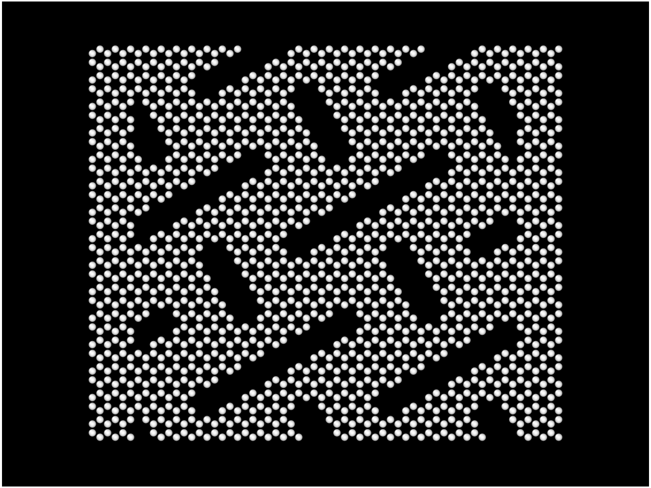

Figure: Kirigami sheet stretch in vaccuum.

Stage 2 - Forward Simulation

Contact vs. Stretch

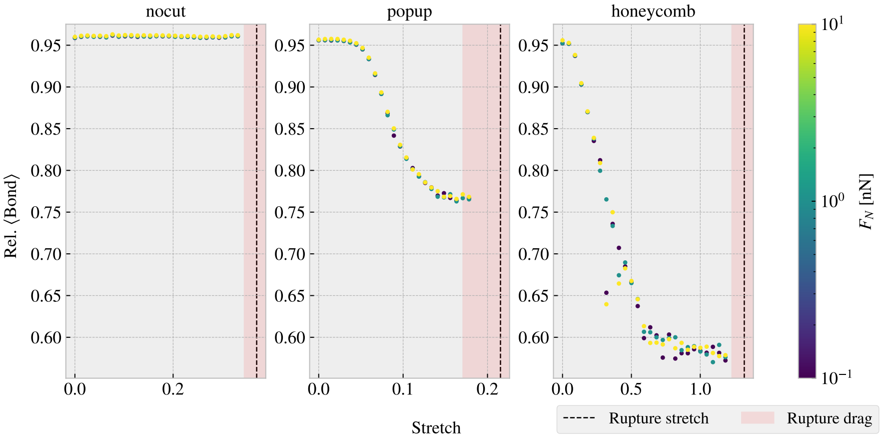

Figure: Average relative amount of bonds between sheet and substrate as a function of stretch for different cut configurations.

Stage 2 - Forward Simulation

Friction vs. Stretch

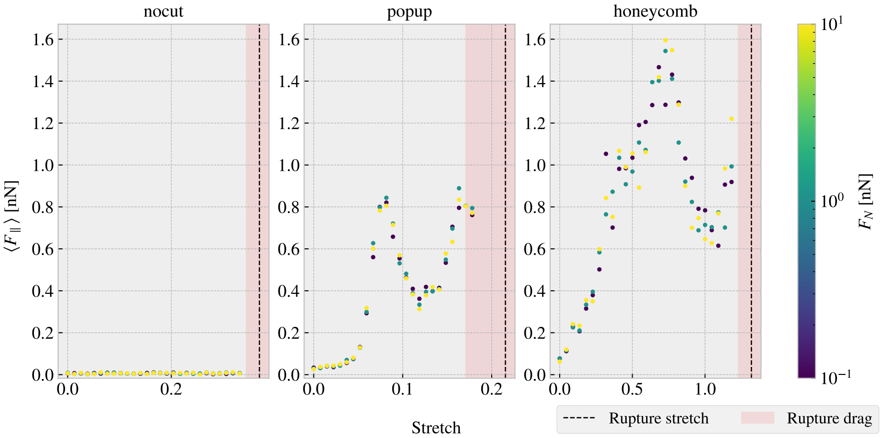

Figure: Mean friction force $F_{\parallel}$ parallel to drag direction as a function of stretch of the sheet for different cut configurations.

(Stage 4 - Nanomachine applications)

Negative friction coefficient

$$\left.\begin{aligned} \text{Normal force}: F_f &= k \cdot F_N \\ \text{Stretch}: F_f &\sim s \cdot \text{stretch} \\ \text{Nanomachine}: \text{stretch} &= \pm R \cdot F_n \end{aligned}\right\} \implies F_f \propto \underbrace{(k \pm sR)}_{\mu} \cdot F_n$$

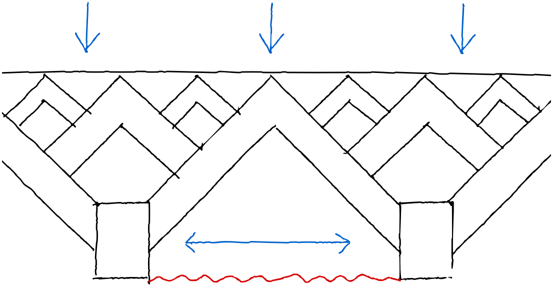

Figure: Sketch for nanomachine coupling normal force and stretch. Black represents nanomachine components and red the sheet.

Stage 3 - Inverse design

Inverse design

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

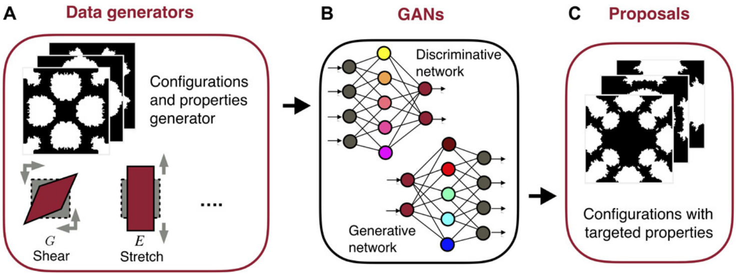

Figure: (A) Data generators to generate datasets of configurations and properties of architectured materials. (B) GANs trained by the datasets. (C) New designs of architectured materials with the targeted properties proposed by the GANs.

Interpretation of PhD project

Topic and methods

- Alpine mass movements and cascading processes
- Multi-phase material point method (MPM)

Tasks

- Writing high performance code for solvers and data analysis
- Benchmarking different implementations
  - Melting block of ice
  - Sliding on 3D-printed topography
  - Avalanches on test sites
  - Previous disasters

Development expectations

- Gain knowledge of snow and granular mechanics
- Gain knowledge of MPM method
- Build strong academic and social connections
- Experience the lifestyle of an alpine environment