PhD Interview - DTU Sustain

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Master's thesis presentation
and PhD project interpretation

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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. Inverse design: Predict cut patterns based on frictional properties and optimize for desired properties using machine learning
    - Low/high friction coefficient
    - Coupling between stretch and friction
    - Negative friction coefficients

Motivation

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

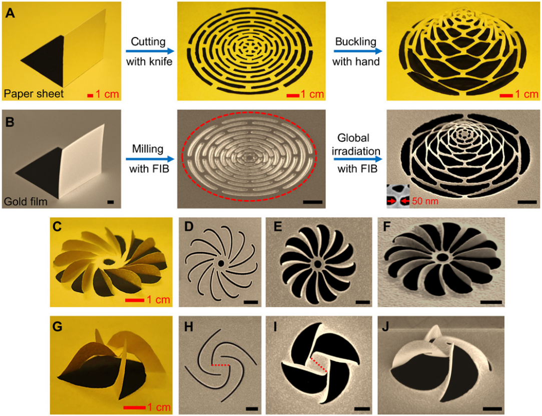

Figure: Example of transistion from macro- to nano-kirigami using a focused ion-beam (FIB) (Nano-kirigami with giant optical chirality, ZHIGUANG LIU, 2018).

Stage 1 - Sheet Kirigami

Choosing a cut pattern

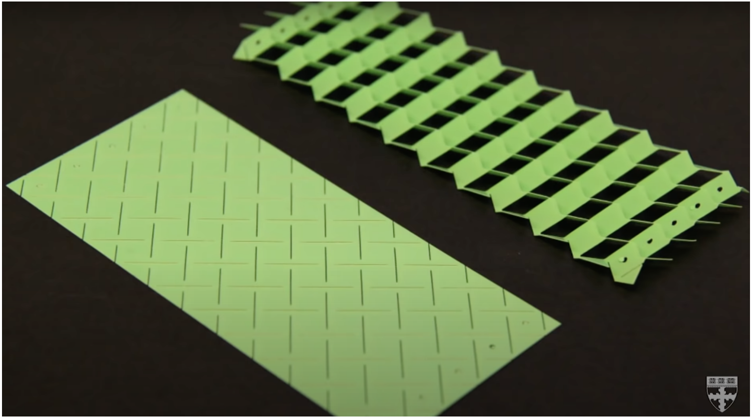

Figure: New pop-up strategy inspired by cuts, not folds - Leah Burrows, Harvard John A. Paulson School of Engineering and Applied Sciences.

Stage 1 - Sheet Kirigami

Choosing a cut pattern

Figure: Scotch Cushion Lock Protective Wrap.

The Atomic Simulation Environment (ASE)

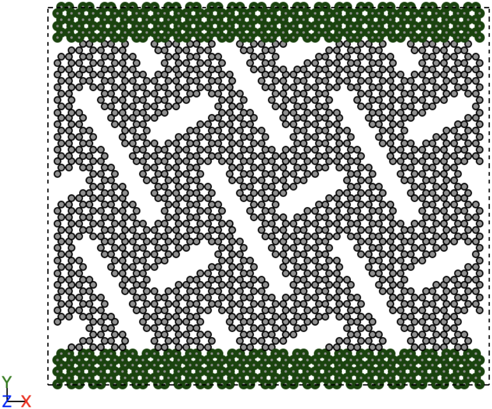

Figure: Example of “popup” cut pattern. Grey color marks the cuttable sheet while green marks added blocks for stretching and dragging the sheet.

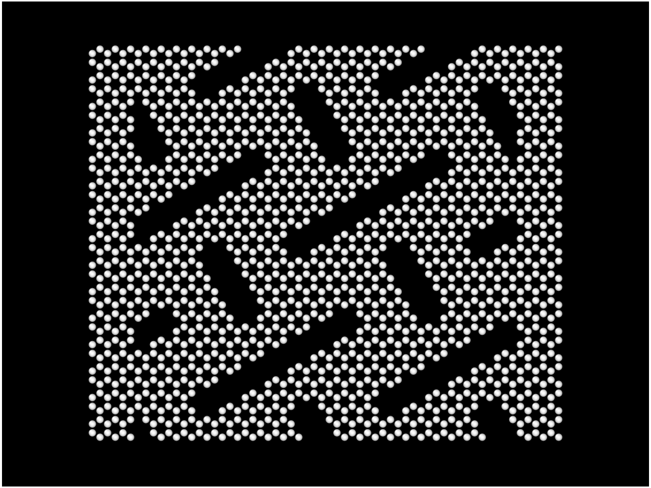

Figure: Kirigami sheet stretch in vaccuum.

Stage 2 - Forward Simulation

Contact vs. Stretch

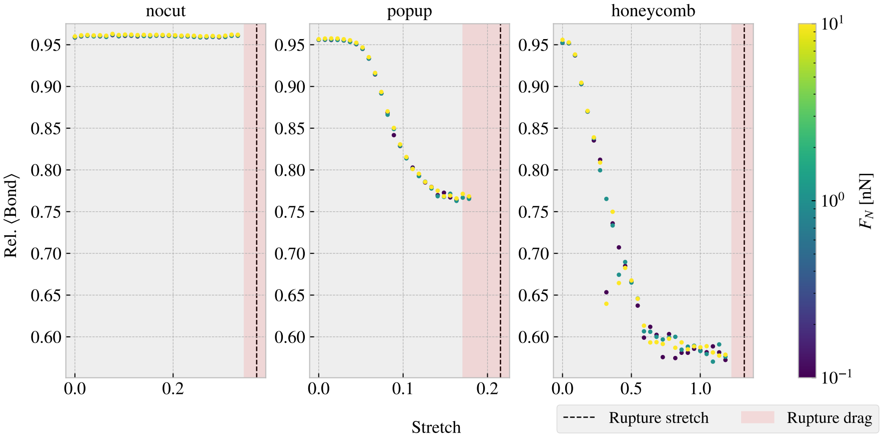

Figure: Average relative amount of bonds between sheet and substrate as a function of stretch for different cut configurations.

Stage 2 - Forward Simulation

Friction vs. Stretch

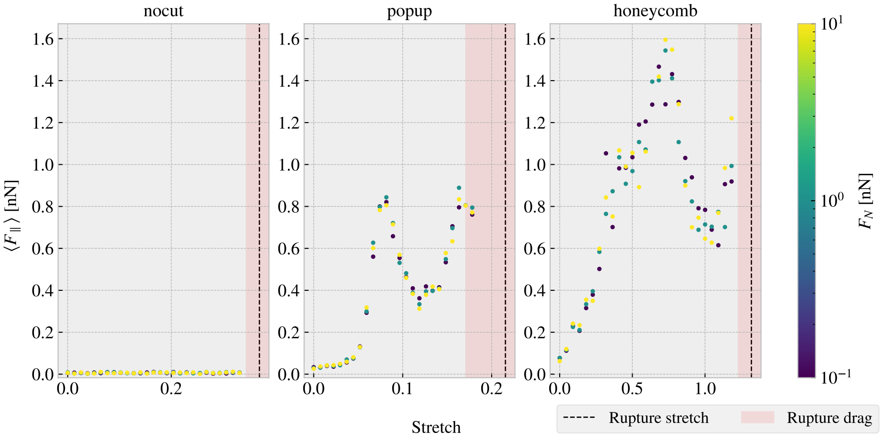

Figure: Mean friction force $F_\parallel$ parallel to drag direction as a function of stretch of the sheet for different cut configurations.

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

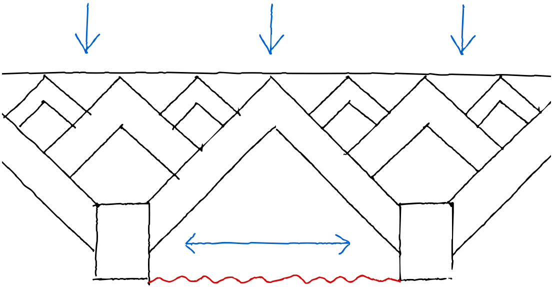

Figure: Sketch for nanomachine coupling normal force and stretch. Black represents nanomachine components and red the sheet.

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

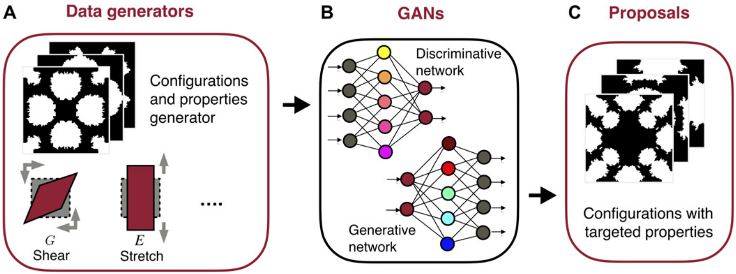

Figure: (A) Data generators to generate datasets of configurations and properties of architectured materials. (B) GANs trained by the datasets. (C) New designs of architectured materials with the targeted properties proposed by the GANs.

Interpretation of PhD project

Next generation environmental simulation models

- **Data** driven ML + **Theory** driven numerical modelling
  - Parametrization of numerical models
  - Adding physical constrains in ML models
  - Highlight feature dependency and discover anomalies
- Exploiting recently emerged ML techniques
  - CNN for image data
  - RNN (width LSTM) for time series
  - Transfer learning in case of sparse data
  - GAN or Diffusion models for proposals
  - Model interpretation techniques

Goals

- Better assessments across environmental domains
  - Multi scale
  - Generalized
- Speed: Implementation in web- and mobile environments
- Increasingly data based rather than idealized assumptions