PhD interview presentation

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Master's thesis midway presentation
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Academic Background

Summary and interest?

Education

- Bachelor in physcis
- Master in Computational Science: Materials Science

Interest

- Computational approach
- Design and creation
- Optimization problems
- Machine learning

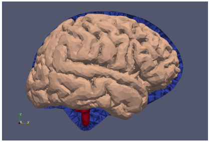
Programming experience
High level languages

Python

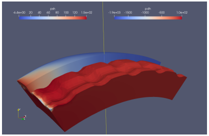
- Workhorse of all my work.
- Object oriented code.
- Machine learning through PyTorch and TensorFlow.

Julia

- Alternative to Python
- Finite element analysis using Gridap
- Mesh geometris using Gmsh



(a)



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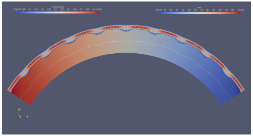

(c)

Programming experience
Lower level languages

C++

- Object oriented code.
- Project work in computational physics.
  - Eigenvalue problems and matrix operations.
  - Ordinary and partial differential equations
  - Integration
  - Simulation of stochastic systems.
- Two years teaching assistant.

C

- High performance computing
  - General code optimization.
  - Data traffic and cache managenemt.
  - Parallel programming (MPI and OpenMP).
  - Modern data architecture.

Programming experience

Molecular dynamics

LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator

- Statistical mechanics and thermodynamics
- Structure recognition
- Porous systems
- Contact forces
- Friction properties

Programming experience

Machine learning (ML)

Pytorch (/ TensorFlow)

- Basic ML concepts:
  - Optimizers
  - Loss / cost functions
  - General learning strategies (learning rates, drop out, normalization etc.)
- Data handling and augmentation.
- Fundamental architecture types
  - Feed Forward Networks
  - CNN
  - RNN
  - GAN
- Network performance analysis
- Basic basic techniques for AI predictions explainations
  - Shapley values
  - Gradient linearization methods

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Scope

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.

Kirigami: Variation of origami with cuts permitted.

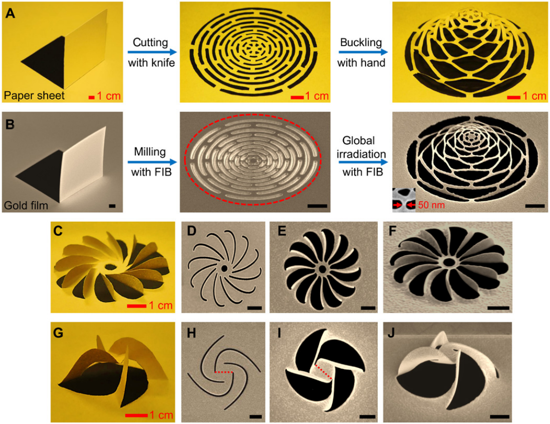

Figure: Example of transistion from macro- to nano-kirigami using a focused ion-beam (FIB) (Nano-kirigami with giant optical chirality, ZHIGUANG LIU, 2018).

- Kirigami design on macroscale.

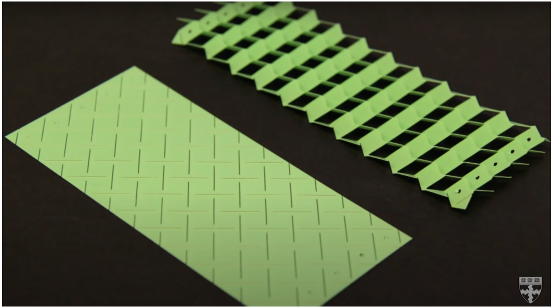

Figure: New pop-up strategy inspired by cuts, not folds - Leah Burrows, Harvard John A. Paulson School of Engineering and Applied Sciences.

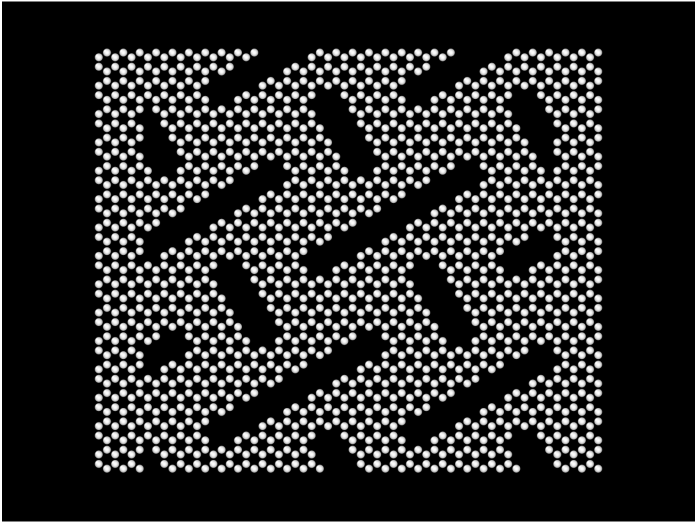

Figure: Kirigami sheet stretch in vaccuum.

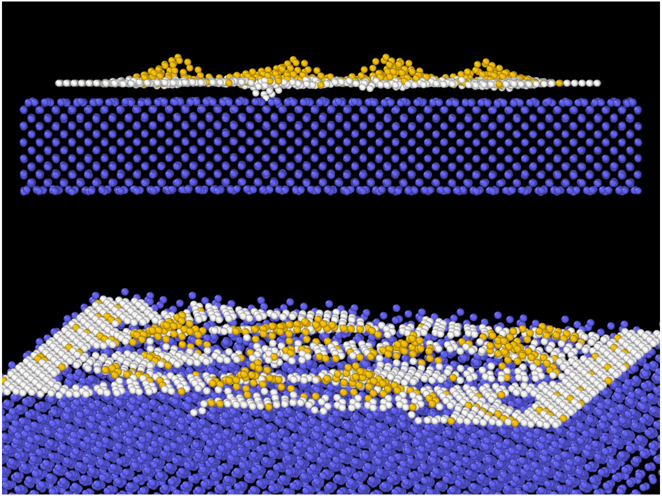

Figure: Kirigami stretch in contact with Si-substrate.

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Investigating 3D buckling

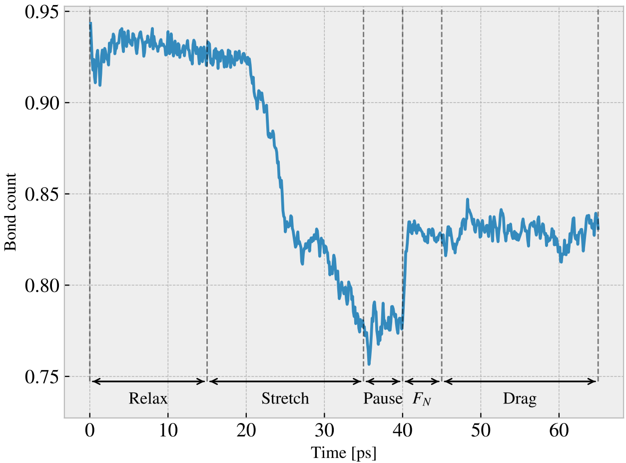

Figure: Contact area approximation: Number of C-Si bonds within a threshold distance of 110% the LJ interaction equilibrium distance.

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Friction stretch dependency

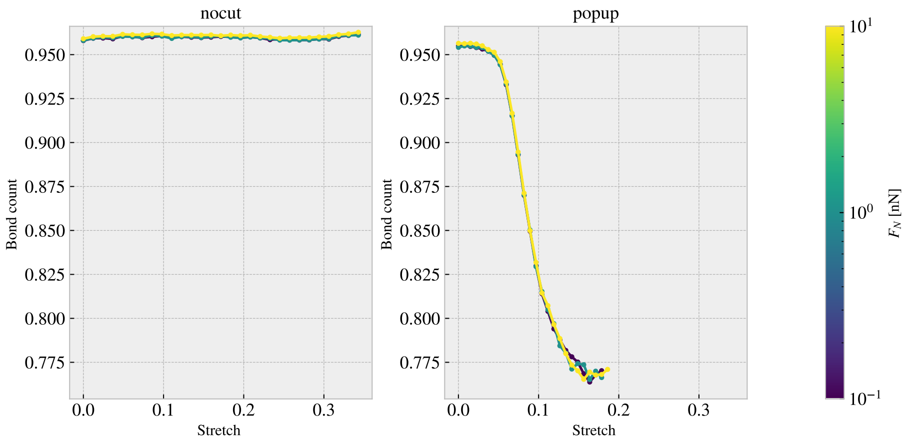

Figure: Relative number of bonds between sheet and substrate as a function of stretch of the sheet with and without cuts.

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Friction stretch dependency

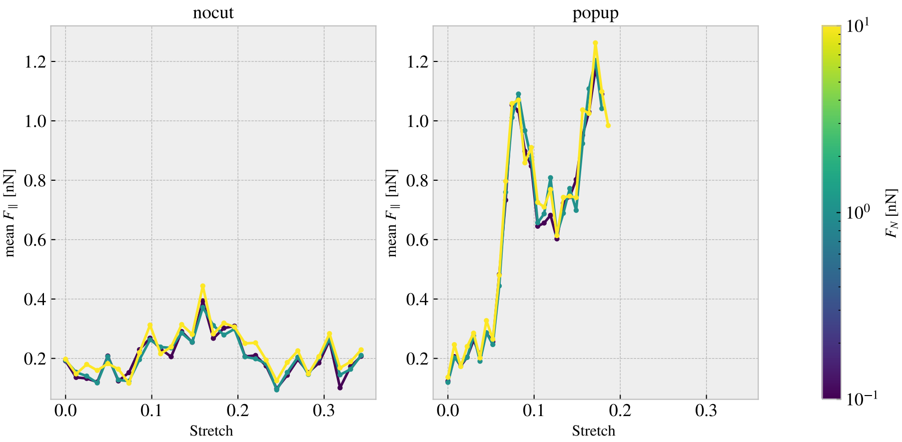

Figure: Mean friction force $F_{\parallel}$ parallel to drag direction as a function of stretch of the sheet with and without cuts.

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Friction stretch dependency

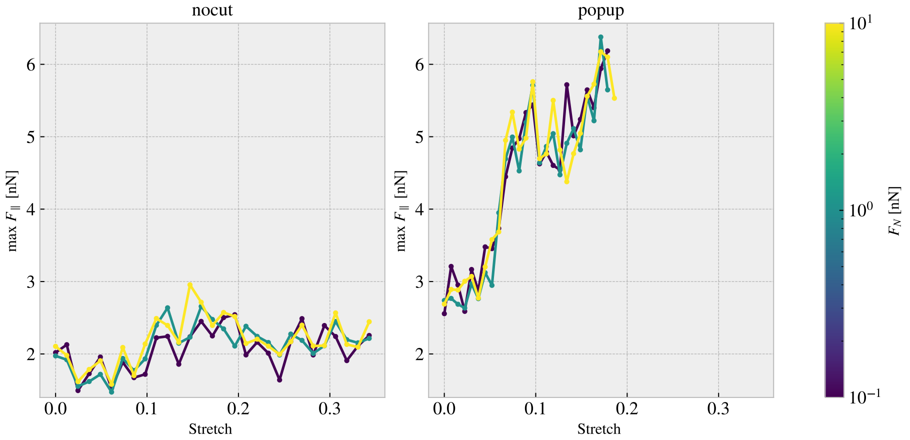

Figure: Max friction force $F_{\parallel}$ parallel to drag direction as a function of stretch of the sheet with and without cuts.

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

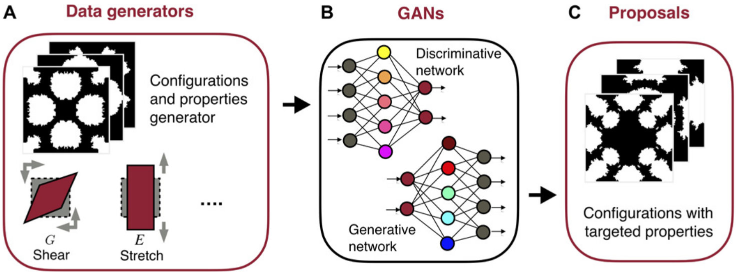

Figure: (A) Data generators to generate datasets of configurations and properties of architectured materials. (B) GANs trained by the datasets. (C) New designs of architectured materials with the targeted properties proposed by the GANs.

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Possible application: Nanomachine for negative friction coefficient

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

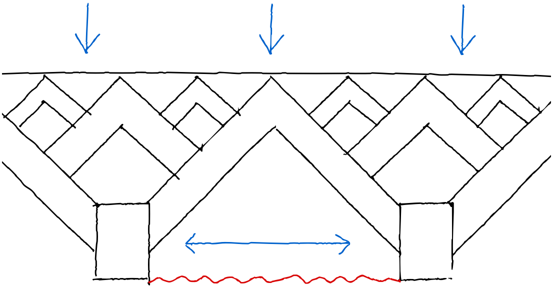

Figure: Sketch for nanomachine coupling normal force and stretch. Black represents nanomachine components and red the sheet.