PhD Interview Presentation

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University of Oslo

Interview regarding the PhD position
at Karlsruhe Institute of Technology
January 26, 2023

Academic Background

Education

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

Scientiffic interests

- Numerical methods
- Optimization problems
- Machine learning
- Materials science and statistical mechanics
- Design and innovation

Programming experience

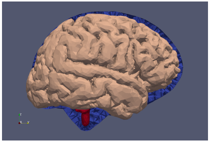
High level languages

Python

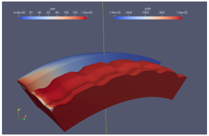
- Workhorse for most of my work
- Object oriented code
- Machine learning through PyTorch and TensorFlow

Julia

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



(a)



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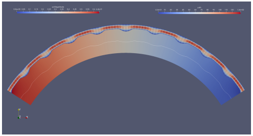

(c)

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 as a teaching assistant

C

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

LAMMPS
Large-scale Atomic/Molecular Massively Parallel Simulator

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

PyTorch (TensorFlow)

- Basic ML concepts:
  - Optimizers
  - 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 techniques for AI prediction explanations
  - Shapley values
  - Gradient linearization methods

Master's thesis

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
    - Nonlinear friction coefficients (even negative)

Kirigami: Variation of origami with cuts permitted.

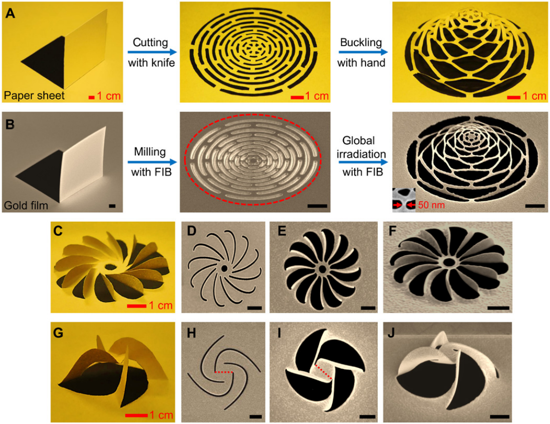

Figure: Example of transistion from macro- to nano-kirigami using a focused ion-beam (FIB) (Nano-kirigami with giant optical chirality, ZHIGUANG LIU, 2018).

Master's thesis

Choosing a cut pattern

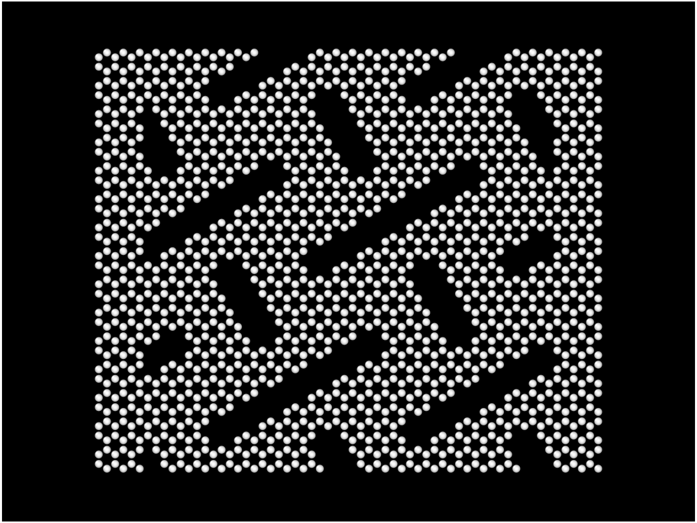

Figure: Kirigami sheet stretch in vaccuum.

Master's thesis

Investigating 3D buckling

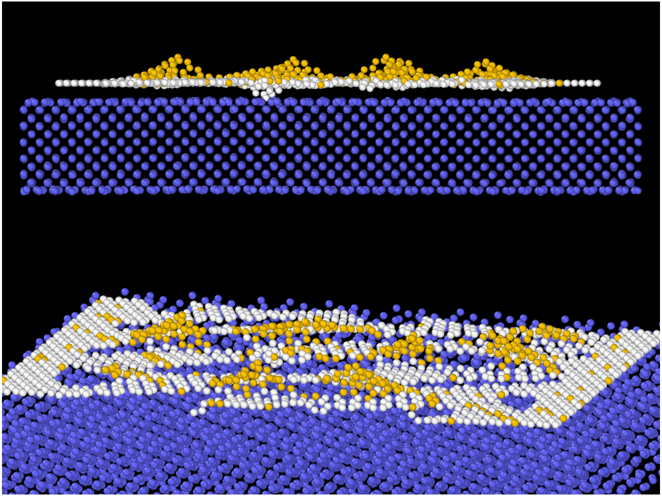

Figure: Kirigami stretch in contact with Si-substrate.

Master's thesis

Investigating 3D buckling

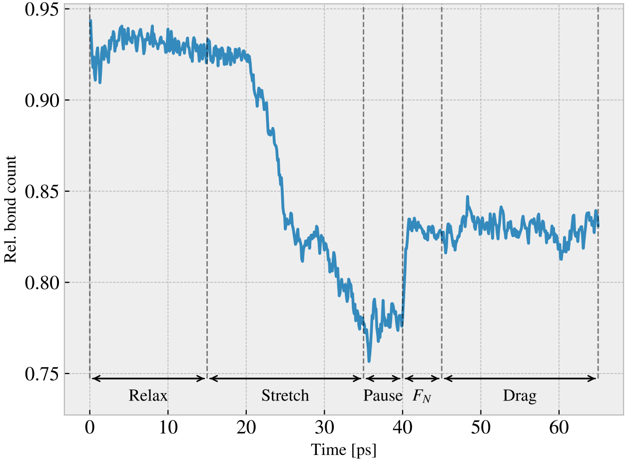

Figure: Contact area approximation: Number of C-Si bonds within a threshold distance of 110% the LJ interaction equilibrium distance.

Master's thesis

Contact stretch dependency

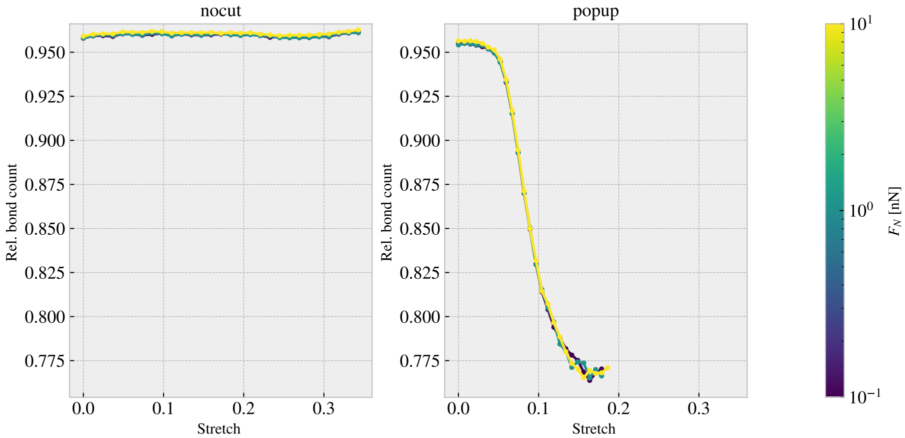

Figure: Relative number of bonds between sheet and substrate as a function of stretch of the sheet with and without cuts.

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Mean friction stretch dependency

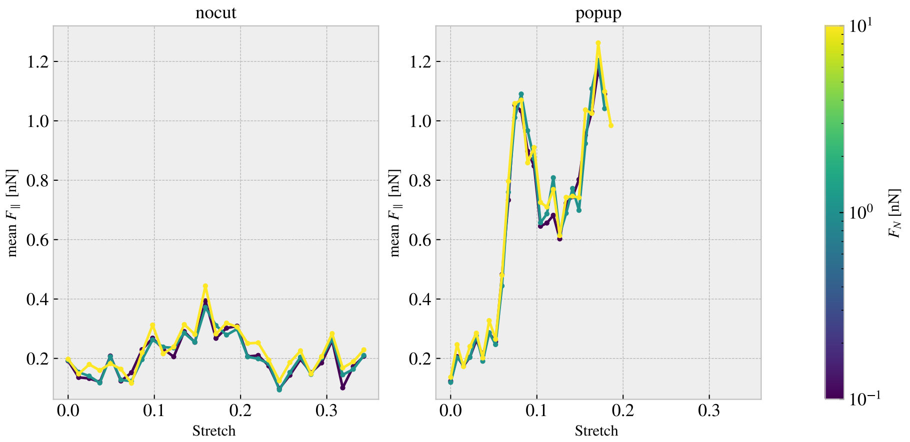

Figure: Mean friction force $F_{\parallel}$ parallel to drag direction as a function of stretch of the sheet with and without cuts.

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

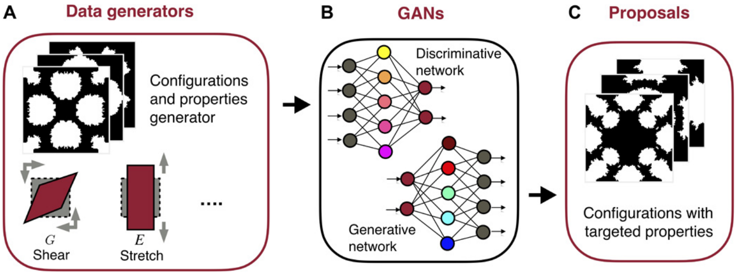

Figure: (A) Data generators to generate datasets of configurations and properties of architectured materials. (B) GANs trained by the datasets. (C) New designs of architectured materials with the targeted properties proposed by the GANs.

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Possible application: Nanomachine for negative friction coefficient

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

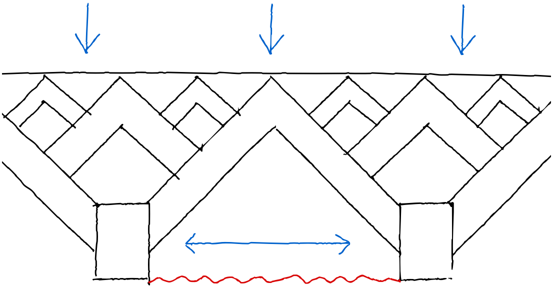

Figure: Sketch for nanomachine coupling normal force and stretch. Black represents nanomachine components and red the sheet.