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

Designs for a negative friction coefficient

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Outline

Overview

Three main parts

1. **Sheet kirigami**: Alter a graphene sheet using atomic scale cuts and stretching
2. **Forward simulation**: Calculate the frictional properties of the sheet using MD simulations
3. **Accelerated search**: Use machine learning to replace the MD simulations and perform an accelerated search for new designs

Can we control the frictional properties of a graphene sheet using this technique?

Motivation

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

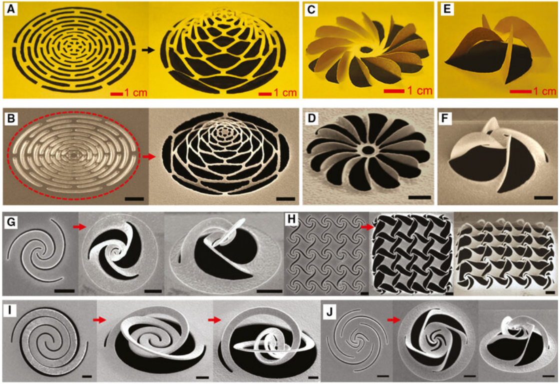
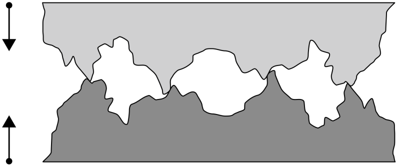


Figure: Example of macroscale Kirigami designs implemented on a nanoscale using a focused ion beam (FIB). Black scale bars: $1\ \mu\mathrm{m}$. Reproduced from [1].

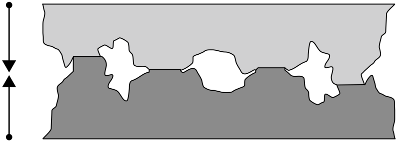
Motivation

Out-of-plane buckling

- Hanakata et al. [2, 3] found out-of-plane buckling with Kirigami designs
- Surface properties are predicted to be important for friction properties
  - Asperity theory: Contact area
  - Frenkel–Kontorova models: Commensurability

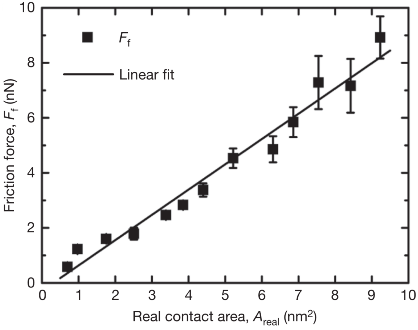


(a) Small load.

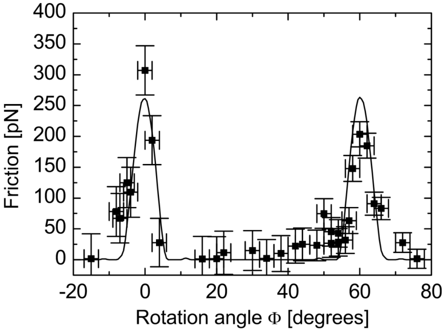


(b) High load.

Figure: Reproduced from [4].



(a) Numerical MD results using an amorphous carbon tip and a diamond sample. Reproduced from [5] with permission from the Springer Nature.



(b) Experimental results of a graphene sheet sliding on graphite. Adapted from [6], reproduced from [7] with permission from the American Physical Society.

Creating a graphene Kirigami system

System setup

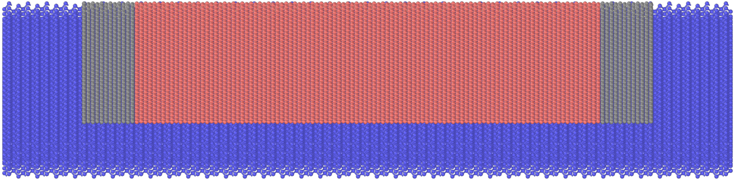
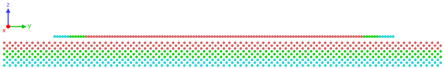
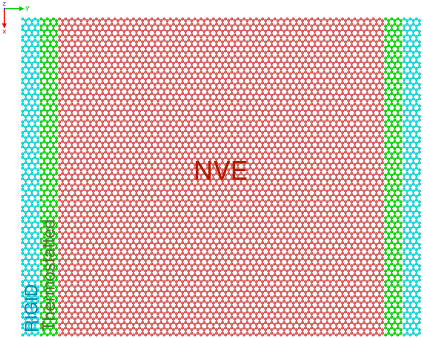


Figure: Graphene sheet on a silicon substrate. Blue: Substrate, Red: Inner sheet, Grey: Pull blocks.

System size = ???



(a) Side view.



(b) Top view.

Primitive lattice vectors

$$\mathbf{a_1} = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \qquad \mathbf{a_2} = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \qquad |\mathbf{a_1}| = |\mathbf{a_2}| = a = 2.46\,\text{Å}.$$

Basis

$$\left\{\left(0, 0\right), \frac{a}{2}\left(\frac{1}{\sqrt{3}}, 1\right)\right\}.$$

Interatomic distance

$$\left|\left|\frac{a}{2}\left(\frac{1}{\sqrt{3}}, 1\right)\right|\right| \approx 1.42\,\text{Å}.$$

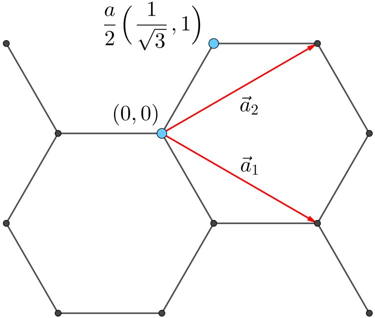


Figure: Graphene crystal structure.

Creating a graphene Kirigami system

Sheet Kirigami

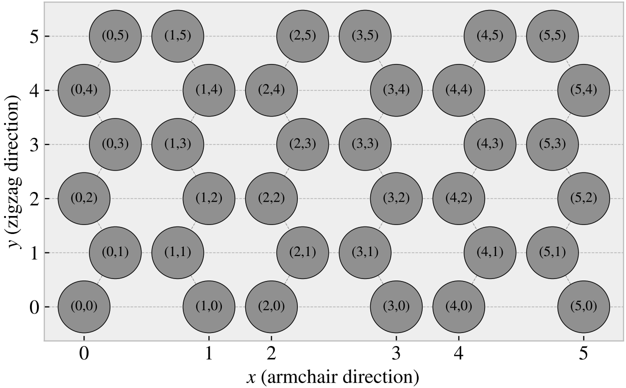


Figure: Graphene atom site indexing.

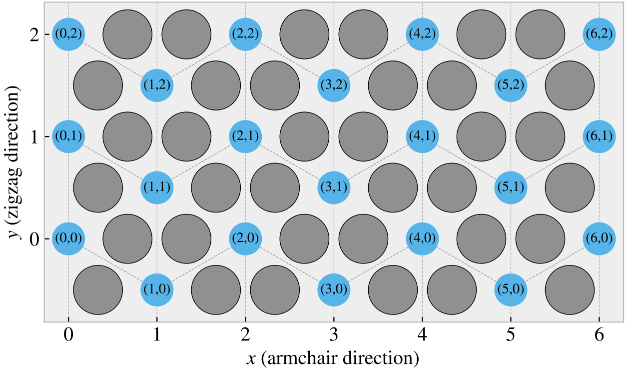
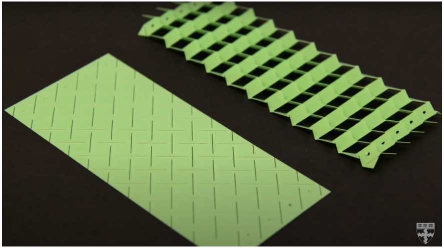


Figure: Graphene center element indexing.

Creating a graphene Kirigami system
Sheet Kirigami



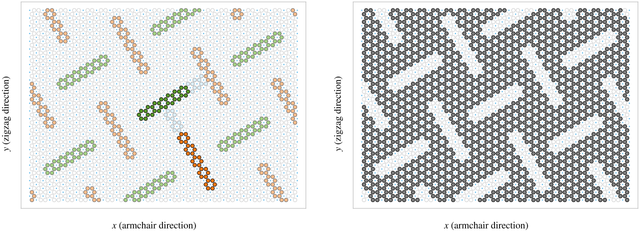
(a) Tetrahedron: Alternating perpendicular cuts producing a tetrahedron-shaped surface buckling when stretched. Reproduced from [8].

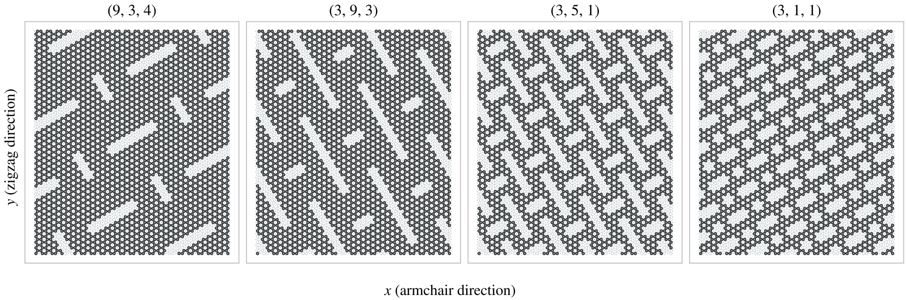
(b) Honeycomb: Scotch^{TM} Cushion Lock^{TM} [9] producing a honeycomb-shaped surface buckling when stretched. Reproduced from [9].

Figure: Macroscale kirigami cut patterns used as inspiration for the nanoscale implementation.

Creating a graphene Kirigami system

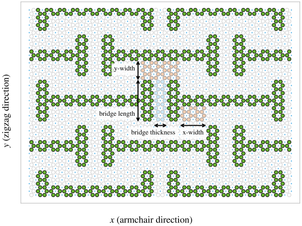
Sheet Kirigami

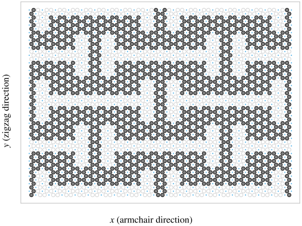


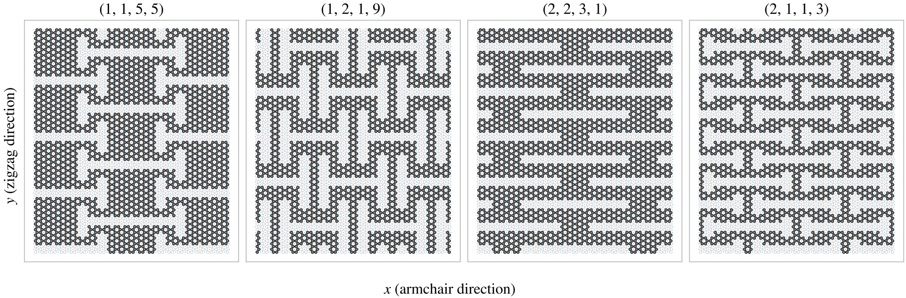


Creating a graphene Kirigami system

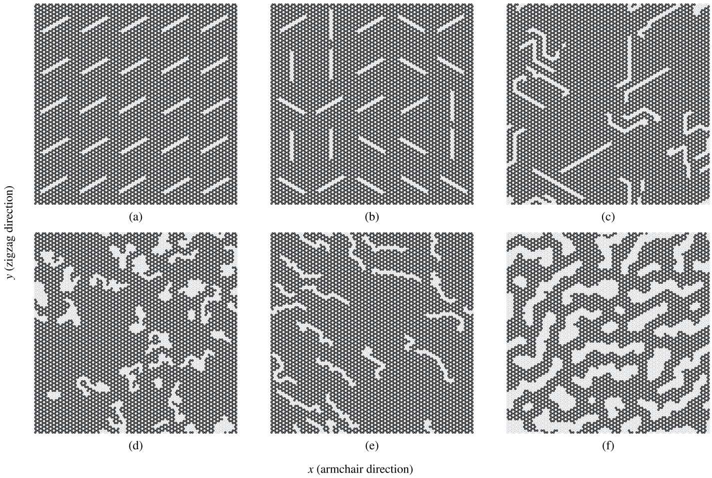
Sheet Kirigami







Random walk



References

[1] J. Li and L. Zhiguang, “Focused-ion-beam-based nano-kirigami: from art to photonics”, Nanophotonics **7**, 10.1515/nanoph-2018-0117 (2018).

[2] P. Z. Hanakata, E. D. Cubuk, D. K. Campbell, and H. S. Park, “Accelerated search and design of stretchable graphene kirigami using machine learning”, Phys. Rev. Lett. **121**, 255304 (2018).

[3] P. Z. Hanakata, E. D. Cubuk, D. K. Campbell, and H. S. Park, “Forward and inverse design of kirigami via supervised autoencoder”, Phys. Rev. Res. **2**, 042006 (2020).

[4] W. Commons, *File:asperities.svg — wikimedia commons, the free media repository*, (2023) https://commons.wikimedia.org/w/index.php?title=File:Asperities.svg&oldid=659167170 (visited on 02/03/2023).

[5] Y. Mo, K. T. Turner, and I. Szlufarska, “Friction laws at the nanoscale”, Nature **457**, 1116–1119 (2009).

[6] M. Dienwiebel, N. Pradeep, G. S. Verhoeven, H. W. Zandbergen, and J. W. Frenken, “Model experiments of superlubricity of graphite”, Surface Science **576**, 197–211 (2005).