

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

Designs for a negative friction coefficient

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- Motivation

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- Negative friction coefficient

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⑤ Summary and outlook

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
- Designs: Macroscale → nanoscale

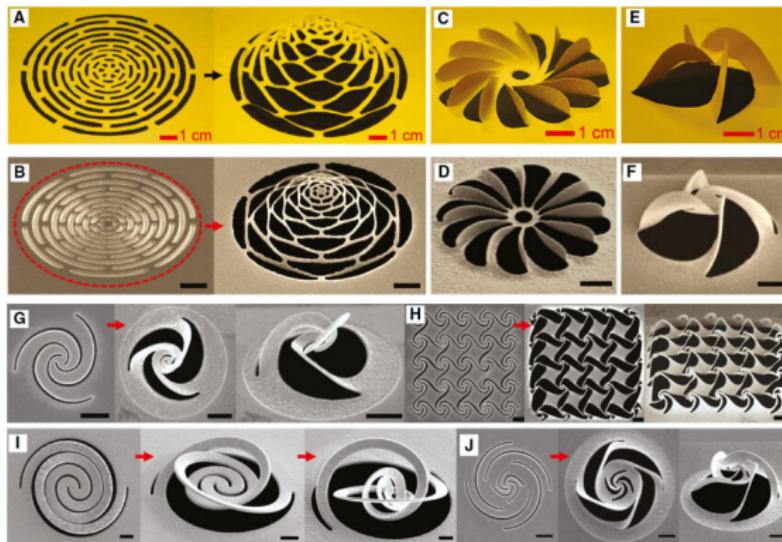
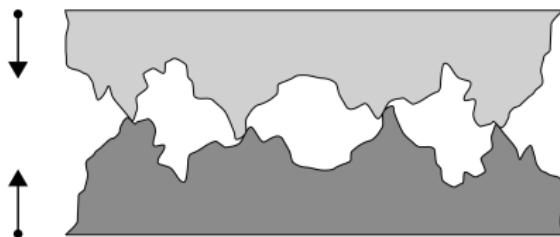


Figure: Example of macroscale Kirigami designs implemented on a nanoscale using a focused ion beam (FIB). Black scale bars: $1 \mu\text{m}$. Reproduced from [1].

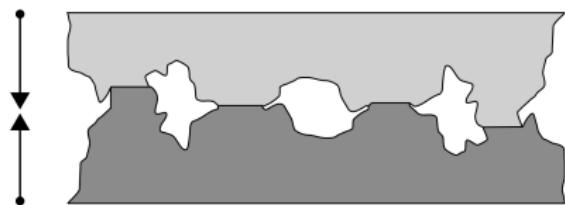
Motivation

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.

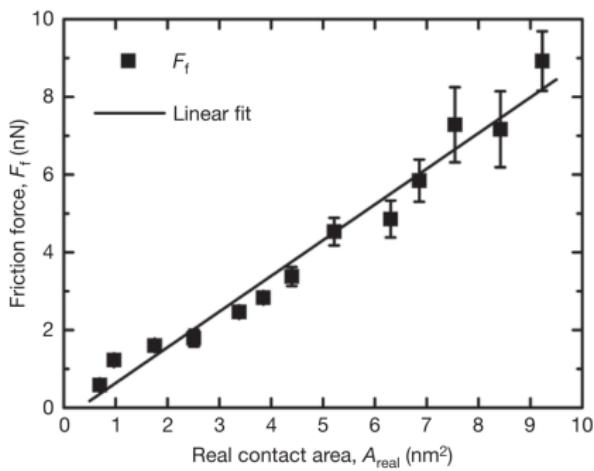


(b) High load.

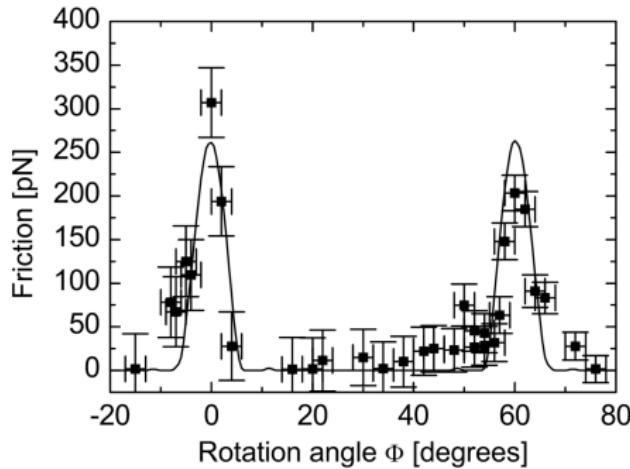
Figure: Reproduced from [4].

Motivation

Contact area and commensurability



(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

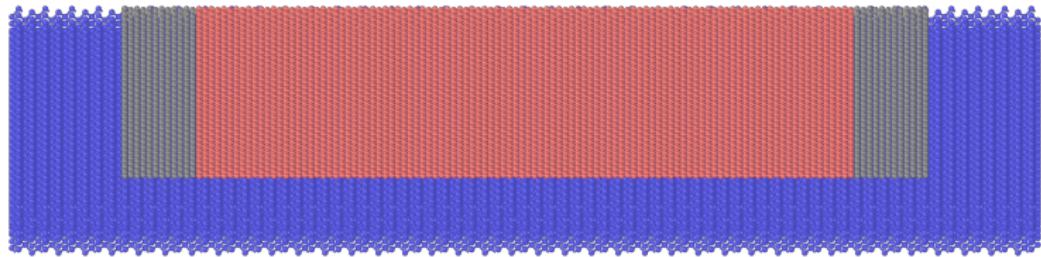


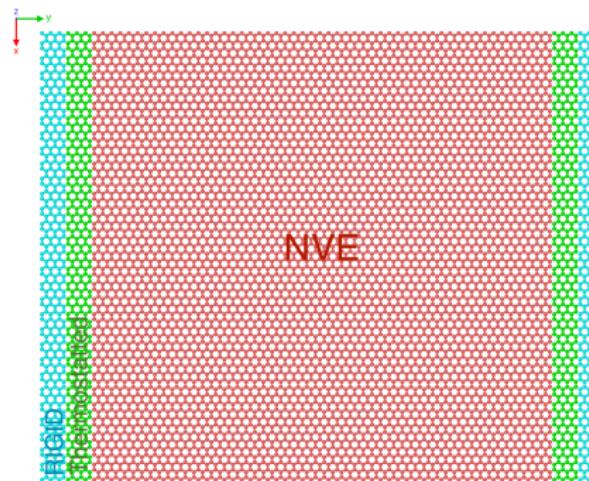
Figure: Graphene sheet on a silicon substrate. Blue: Substrate, Red: Inner sheet, Grey: Pull blocks.

Creating a graphene Kirigami system

System setup



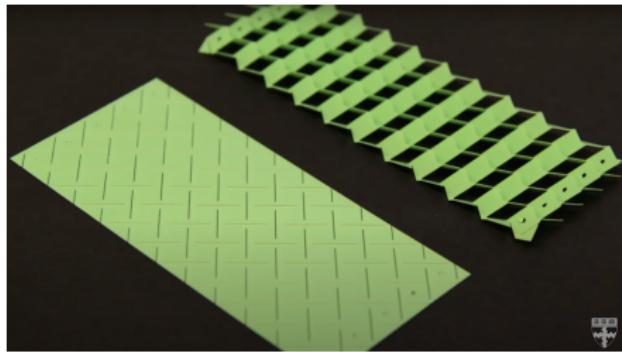
(a) Side view.



(b) Top view.

Creating a graphene Kirigami system

Sheet Kirigami



(a)



(b)

Figure: Macroscale kirigami cut patterns used as inspiration for the nanoscale implementation. (a) Tetrahedron: Alternating perpendicular cuts producing a tetrahedron-shaped surface buckling when stretched. Reproduced from [8]. (b) Honeycomb: Scotch™ Cushion Lock™ [9] producing a honeycomb-shaped surface buckling when stretched. Reproduced from [9].

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).
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- [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).