Tuning Frictional Properties of Kirigami Altered Graphene Sheets using Molecular Dynamics and Machine Learning

Designing a Negative Friction Coefficient

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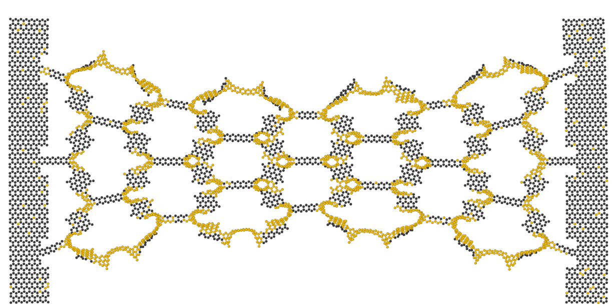

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Abstract

Abstract.

Acknowledgments

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Contents

List of Symbols

The next list describes several symbols that will be later used within the body of the document

F_N Normal load as a test

Acronyms

MD Molecular dynamics. 1

ML Machine learning. 2

Chapter 1

Introduction

1.1 Motivation

Friction is a fundamental force that takes part in almost all interactions with physical matter. Even though the everyday person might not be familiar with the term "friction" we would undoubtedly notice its disappearing. Without friction, it would not be possible to walk across a flat surface, lean against the wall or secure an object by the use of nails or screws [p. 5] [1]. Similarly, we expect a moving object to eventually come to a stop if not supplied with new energy, and we know intuitively that sliding down a snow covered hill is much more exciting than its grassy counterpart. It is probably safe to say that the concept of friction is well integrated in our everyday life to such an extent that most people take it for granted. However, the efforts to control friction dates back to the early civilization (3500 B.C.) with the use of the wheel and lubricants to reduce friction in translational motion [2].

Friction is a part of the wider field tribology derived from the Greek word *Tribos* meaning rubbing and includes the science of friction, wear and lubrication [2]. To this day, one of the most important motivations to study tribology is ultimately to gain full control of friction and wear for various technical applications. Especially, reducing friction is of great interest as this has tremendous advantages regarding energy effeciency. It has been reported that that monetary value of tribological problems has significant potential for economic and environmental improvements [3]:

> "On global scale, these savings would amount to 1.4% of the GDP annually and 8.7% of the total energy consumption in the long term." [4].

On the other side, the reduction of friction is not the only sensible application for tribological studies. Increasing friction by demand might be of interest in the development of grasping robots where a finetuned object handling is required. In the recent years an increasing amount of interest has gone into the understanding of the microscopic origin of friction, due to the increased possibilities in surface preperation and the development of nanoscale experimental methods. Nano-friction is also of great concern for the field of nano-machining where the frictional properties between the tool and the workpiece dictates machining charascteristics [3]. With the progress in computational power and devolpment of Molecular Dynamics (MD) a numerical approach gives new insight in the nanoscale behaviour of friction.

In recent papers by Hanakata et al. [5](2018), [6](2020) numerical investigations has showcased that the mehcanical properties of a graphene sheet, yield stress and yield strain, can be altered through the introduction of so-called kirigami inspired cuts into the sheet. By the use of machine learning through accelerated search [5] and inverse design [6], they are able to extract cut pattern proposals which optimizes the mechanical properties in certain ways, e.g. stretchability or resistance to yield. This kind of study shows how numerical modelling and machine learning can extremely usefull for the designing of metamaterials, i.e. materials with properties not found in naturally occurring materials. Hanakate et al. assert the complexity of the mehcanical properties of the kirigami cut sheet to the out of plane buckling accouring when the sheet is stretched.

Since it is generally accepted that the surface roughness is of great importance for fritional properties it can be hypothesized that the cut and stretch procedure can be exploited for the design of fricitonal metamaterials as well. If successfull, the link between stretch and friction properties might also rise to a metamaterial with tunable friction properties after the point of manufacturing. That is, a material which fricitonal properties will change during stretch and relaxtion. For such a material, coupling the normal load and stretch of the sheet through a nanomachine design would allow for an altered friction coefficient which in theory might take negative values in certain ranges of normal load. To the best of our knowledge kirigami has not yet been implemented to alter the frictional properties on a nanoscale. However, in a recent paper by Liefferink et al. [7](2021) it is reported that macroscale kirigami can be used to dynamically control the macroscale roughness of a surface by stretching which can be used to change the frictional coeffcient by more than one order of magnitude.

Something about machine learning and inverse design.

1.2 Approach

Explain my specific approach in more detail one this is settled in completely.

What if I use the acronym ML on this page as well?

1.3 Objective of the study

1. Design a MD simulation to evaluate the frictional properties of the grapehene sheet under different variations of cut patterns, stretching and loading, among other physical variables.
2. Find suitable kirigami patterns which exhibit out of plane buckling under tensile load.
3. Create a procedure for generating variaiton of the selected kirigami patterns along with random walk based cut patterns in order to create a dataset for ML training.
4. Train a neural network to replace the MD simulation completely.
5. (Variation 1) Do an accelerated search using the ML network for exotic frictional properties such as low and friction coeffcients and a strong coupling between stretch and friction.
6. (Variation 2) Make a GAN network using the forward network in order to extract cut configuration proposals for above frictional properties.
7. Make a nanomachine or artifical numerical setup which couples normal load and stretch with the intention of making a proof of concept for negative friction coefficients.

1.4 Contributions

What did I actually achieve

1.5 Thesis structure

How is the thesis structured.

Part I

Background Theory

Part II

Simulations

Summary

1.6 Summary and conclusion

1.7 Outlook / Perspective

- What did we not cover?
- What kind of further investigations does this study invite?

Things to include here

- Could be valuable to spend more time on the validation of the MD simulations. How does material choice and potential effects the results. How realistic is the simmulations?
- Are there any interesting approaches for compressed kirigami structures?
- How does these results scale? I imagaind that the nanomachine systems should be applied in small units to avoid scaling problems, but in general I could spend way more time on the scaling investigation.
- Since the normal force is applied at the pull blocks the normal force distribution changes from the sides more towards and even distirbution as the sheet is put under tension (stretched). If we imagined a sheet for which the center part was either a different material or had some kind of pre-placed asperity on it, could we then exploit this force distirbution to get exotic properties as well? By studying this we might get a clearer understanding of what is the cause of my results.
- Possibility to study hysteresis effects. Maybe the frictional behvaiours change significantly through repeated cycles of stretch and relax.

Appendices

Appendix A

Appendix B

Appendix C

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