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

Designing a Negative Friction Coefficient

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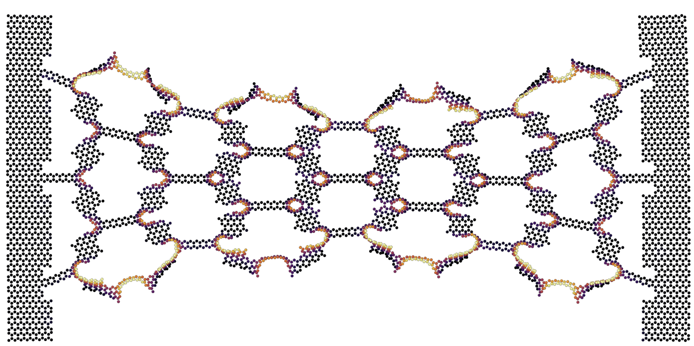

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Abstract

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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, 2

ML Machine learning. 2

Chapter 1

Introduction

1.1 Motivation

Friction is a fundamental force that takes part in most of all interactions with physical matter. Even though the everyday person might not be familiar with the term *friction* we recognize it as the inherent resistance to sliding motion. Some surfaces appear slippery and some rough, and we know intuitively that sliding down a snow covered hill is much more exciting than its grassy counterpart. Without friction, it would not be possible to walk across a flat surface, lean against the wall with falling over or secure an object by the use of nails or screws [p. 5] [1]. Handling objects, hitting the breakes in the car and getting around in general would be a completely different story in a frictionless world. It is probably safe to say that the concept of friction is 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].

Today, friction is considered 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]. The most compelling motivation 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 for energy effeciency. It has been reported that tribological problems have a 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 hand, the reduction of friction is not the only sensible application for tribological studies. Controlling frictional properties in ranges apart from minimization might be of interest in the development of grasping robots where a finetuned object handling is required. While achieving a certain baseline friction is rather easily obtained through appropiate material during manufacturing, we are yet to unlock the capabilities to alter friction dynamically on the go. One example from nature inspiring us to think along theese lines is the Gekko foot. More precisely, the Tokay gecko have recieved a lot of attention in scientific studies trying to unravel the underlying mechanism of its extrodinary properties. The Gekko is able to produce an adhesive force on the order of 20 nN between the feet and a wide range of smooth and rough surfaces, but it retains the ability to remove its feet from an attachment surface at will [5]. This makes the Gekko able to achieve a high adhesion and friction force on the feet when climbing up a vertical surface while lifting it for the next step remains reletively effortless. For a grasping robot we might consider an analog concept of a skin material that can change from slippery to rough on demand depending on the specific task of the robot; Slippery and smooth when in contact with people and rough and firmly gripping when moving heavy objects.

In the recent years an increasing amount of interest has gone into the studies 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 concurrent progress in computational power and devolpment of Molecular Dynamics (MD), numerical investigations now serves as an extremely useful way of achieving a greater insight into the nanoscale mechanics associated with friction. By proposing a variation of system with approximating physical properties we can evaluate and refine our physical models through a simulation based approach. These “numerical experiments” enable us to probe systems of high complexity which is still out of reach for experimental approaches.

Recent numerical studies in material science have explored the concept of creating so-called *metamaterials* where materials compositions are designed to enhance certain physical properties [6][7][8][9][10][11]. This is often achieved by either intertwining different material types or removing material in certain configuration. In recent papers by Hanakata et al. [6](2018) and [7](2020) numerical investigations has showcased that mechanical properties of a graphene sheet, in this case yield stress and yield strain, can be altered through the introduction of so-called *Kirigami* inspired cuts into the sheet. That is, by removing atoms at certain locations on the sheet it is possible to alter the stretchability and resitance to tearing apart under tension. Having found such a design space with prospects of changing a set of physical properties a new questoin emerges: How do we optimize the design for certain properties?

Earlier architecture design approaches such as bioinspiration, looking at Gekko feet for instance, and Edisonian, also known as trial and error, generally rely on prioir knowdelegde of an experienced designer [9]. While the Edisonian approach is certainly more feasible through numerical studies in comparison to real world experiments, the number of possible kirigami configurations are still overwhelming in combination with a realistic simmulation time on modern hardware. The complexity of metamaterials like the graphene sheet studied by Hanakata et al. makes for a seemingly intractable problem making analytic solutions impossible. However, such problems can be mittigated by the use of machine learning ML which have proved successful in the establishment of a connection between kirigami configurations and physical properties. The recent advancements in this field makes it possible to capture ever more complex patterns in data yielding reletively accurate predictions of physical properties for a given design. This give rise to two different main design frameworks. One, by utilizing the prediction from a trained network we can skip the MD simulations all together resulting in an accelerated search of configurations. This can be further improved by targeting the search dynamically as for instance done through a genetic algorithm where on creates new design configurations based on the best attempts so far. This can be used to further expand the dataset which the ML network was trained upon which constritute a so-called *active learing* search loop [6]. An even more sophisticated approach is the through generative methods such as Generative Adversarial Networks (GAN). By working with a so-called *encoder-decoder* network structure one can build a network that reverses the prediction process. That is, we predict a design given a set of physical target properties. In the papers by Hanakata et al. both the *accelerated search* and the *inverse design* was proven successful to create novel metamaterial designs.

Hanakata et al. attributes the variety in yield properties to the non-linear effects arrising from the out-of-plane buckling. 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, any connection between stretch and friction properties might give rise to a metamaterial with dynamic friction properties after the point of manufacturing. For instance, the grasping robot might apply such a material as skin for which stretching or relaxing the surface could result in a changeable friction; Slippery and smooth in contact with people and rough and firmly gripping when moving heavy objects. In addition, a possible coupling between stretch and the normal load through a nanomachine design would allow for an altered friction coefficient. This invites the idea of non-linear friction coeffcients which might in theory take on negative values for certain ranges. 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. [12](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. This support the idea that kirigami designs can in fact be used to alter friction, but we believe that taking this concept to a nanoscale would maximize the probabilities for the discovering of excotic frictional properties, not to mention the contribution to the understanding of the underlying mechanics associated to friction.

1.2 Approach

In this thesis we investigate the possibility to control the frictional properties of a graphene sheet by applying strategically positioned cuts to the sheet inspired by kirigami patterns. Kirigami is a variation of origami where the paper is cut additionally to being folded. Hanakata et al. [7] has shown that kirigami inspired cuts on a graphene sheet can be used to alter the yield strain and yield stress of the sheet. They observed that the stretching of the cutted sheet induced a out-of-plane buckling which serves as a key observation for the motivation of this thesis. It is currently well established/believed that the friction between two surfaces is proportional to the real microscopic contact area (source here?). Hence, one can hypothesize that the buckling of the sheet will affect the contact area and consequently the frictional properties.

1.3 Objective of the study

Generally we want to contribute to the understadning of nanoscale friction while finding kirigami designs associated with excotic friction properties. This also serves as a proof of concept for the future work in this direction, perhaps with some more clear defined applications in mind.

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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