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

Designing a Negative Friction Coefficient

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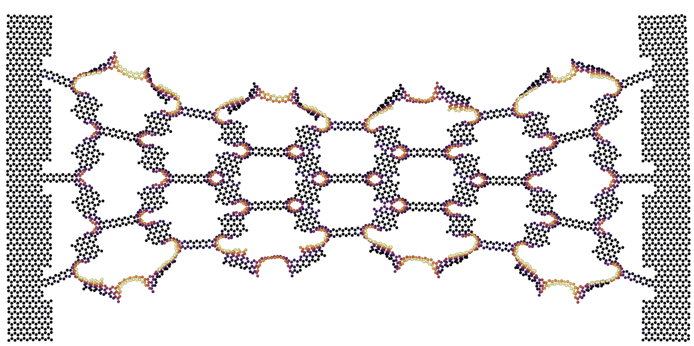

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Abstract

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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. 2

ML Machine learning. 2

Chapter 1

Introduction

Structure of Motivation section:

1. Introduce and motivate friction broadly.
2. Motives for friction control using a grasping robot as example.
3. Analog to gecko feet where adhesive properties are turned on and off.
4. Interest in origin of friction through nanoscale studies which further motivates the use of MD.
5. Intro to metamaterials and the use of kirigami (/origami) design
6. How to optimize kirigami designs with reference to Hanakata and motivating the use of ML.
7. Out-of-plane buckling motivates the use of kirigami for frictional properties.

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 without falling over or secure an object by the use of nails or screws [p. 5] [1]. 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 in general 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 besides minimization might be of interest in the development of a grasping robot where a finetuned object handling is required. While achieving a certain "constant" friction response is readily obtained through appropiate material choices 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 are the gecko feet. More precisely, the Tokay gecko has recieved a lot of attention in scientific studies aiming to unravel the underlying mechanism of its "togglable" adhesion properties. Although geckos are able to produce large adhesive forces, they retain the ability to remove their feet from an attachment surface at will [5]. This makes the gecko able to achieve a high adhesion on the feet when climbing a vertical surface while lifting it for the next step remains reletively effortless. For a grasping robot we might consider an analog frictional concept of a surface material that can change from slippery to rough on demand depending on specific tasks.

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 devolopment of Molecular Dynamics (MD), numerical investigations serve as an extremely useful tool for getting insight into the nanoscale mechanics associated with friction. This simulation based approach can be considered as a "numerical experiment" enabling us to create and probe a variety of high complexity system which are still out of reach for modern experimental approaches.

In materials science such MD-based numerical studies have been used to explore the concept of so-called *metamaterials* where material compositions are designed meticulously to enhance certain physical properties [6][7][8][9][10][11]. This is often achieved either by intertwining different material types or removing certain regions completely. In recent papers by Hanakata et al. [6](2018) [7](2020) numerical studies have 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 resistance to rupturing under tension. Kirigami is a variation of origami where the paper is cut additionally to being folded. While these originate as an art form aiming to produce various artistic objects, they have proven to be applicable in a wide range of fields such as optics, physics, biology, chemistry and engineering [12]. Various forms of stimuli enable direct 2D to 3D transformations through folding, bending, and twisting of microstructures. While orginal human designs may have contributed to specific scientiffic applications, the use of kirigami and origami driven designs are highly driven by the question of how to generate new designs with optimize certain physical properties.

Earlier architecture design approaches such as bioinspiration, looking at gecko feet for instance, and Edisonian, based on trial and error, generally rely on prioir knowdelegde and an experienced designer [9]. While the Edisonian approach is certainly more feasible through numerical studies real world experiments, the number of combinations in the design space rather quickly becomes too large to search systematically, even when considering the simmulation time of modern hardware. The complexity of metamaterials like the kirigami graphene sheet additionally makes for a seemingly intractable problem meaning that analytic solutions are of the table. However, such problems can be mittigated by the use of machine learning (ML) which have proven successful in the establishment of a connection between kirigami designs and physical properties (Cite again?). The recent advancements in the field of ML makes it possible to capture ever more complex patterns in data which can be used to learn a mapping from the design space to physcial properties of interest. This gives rise to two different design approaches: One, by utilizing the prediction from a trained network we can skip the MD simulations all together resulting in an accelerated search of designs. This can be further improved by guiding the search as for instance through a genetic algorithm where one creates new designs based on the best candidates so far. Optinally, one could perform MD simulations on the top candidates at regularly intervales to expand the dataset and improve the ML model which constritute a so-called *active learing* search loop as used in [6]. Secondly, an even more sophisticated approach is 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, the network predict a corresponding 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 of the sheet. 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 applied by Hanakata et al. can also be exploited for the design of fricitonal metamaterials. For certain designs we might hope to find a relationship between stretching of the sheet and frictional properties which give rise to a contrable friction after the point of manufacturing. For instance, the grasping robot might apply such a material as artifical skin for which stretching or relaxing of 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 as well given the right sign of the effect from stretching. The latter would constitute an extremely rare property. This has been reported indirectly for bulk graphite by Deng et al. [13] where the friction kept increasing during the unloading phase. Check for other cases.

To the best of our knowledge, kirigami has not yet been implemented to alter the frictional properties on a nanoscale. In a recent paper by Liefferink et al. [14](2021) it is reported that macroscale kirigami can be used to dynamically control the macroscale roughness of a surface by stretching which was 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 the nanoscale would envolve a different set of underlying mechanisms and thus contribute to new insight in this field.

1.2 Approach

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

Appendices

Appendix A

Appendix B

Appendix C

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