Title

Subtitle

by

Mikkel Metzsch Jensen

THESIS

for the degree of

MASTER OF SCIENCE

Faculty of Mathematics and Natural Sciences
University of Oslo

Spring 2023

Title

Subtitle

Mikkel Metzsch Jensen

Title

http://www.duo.uio.no/

Abstract

Abstract.

Acknowledgments

Acknowledgments.

iv

Contents

List of symbols?

Maybe add list of symbols and where they are used like Trømborg.

Introduction

0.1   Motivation

0.1.1   Friction

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. 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 [1]. 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 [1].

The most important motivation to study tribology is ultimately to gain full control of frictional and wear for vairous 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 [2]:

> "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." [3].

The reduction of friction is not the only sensible application as a controlled increase in friction might be of interest in the development of grasping robots or perhaps breaking system (get some sourced examples maybe...).

0.1.2   Thesis

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. Kirigami is a variation of origami where the paper is cut additionally to being folded. Hanakata et al. [4] 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.

0.2   Approach

In the study by Hanakata et al. [4] they used a machine learning (ML) approach to overcome the complexity of the nonlinear effects arrising from the out-of-plane buckling which made them succesfully map the cutting patterns to the mechanical properties of yield and stress. The dataset used for the ML training was generated by molecular dynamics (MD) simulations for a limited set of cut configuration. By training the network the MD simiulaitons could effectively be skipped all together making for an accelerated search through new cut configurations for certain mechanical properties. By setting up a MD simulation that qunatifies the frictional

properties of the graphene sheet we aim to make an analog study regarding the search for certain frictional properties.

We will take this on step further by creating a GAN network that utilises the latter network for creating an inverse design framework. That is, a network that takes frictional properties as input and return the corresponding cut configuration. By having such a tool we can execute a targeted search for exotic frictional properties. Particularly, we are interested in nonlinear and possibly even negative friction coefficients. Friction is essentially observed to increase with increasing load on the frictional surface, and we often describe this as having a positive friction coefficient. However, if we are able to couple the stretching of the sheet with friction we might be able to break this barrier for the coefficient. By imagining some nanomachine which translates downward pressure into either compression of expansion of the altered graphene, we could have a coupling between downward pressure and stretch of the sheet. In that case, a friction force depending on stretch could effectively be made to decrease with increasing load which would correspond to a negative friciton coeffcient following this definition (formulate such that we do not imply free acceleration from nothing).

One of the features from inverse design, seperating it from the general class of ML approaches, is that we do not depend on trusting the ML predictions. While a standard neural network might be extremely efficient on a certain prediciton task we have usually no information on how these predictions are based. We say that the internal workings of the network is a black box beyond our capacaity of interpretation. However, for the inverse design problem we are prompted with a few promising design propsals which can immediately be tested in the MD simulations which we will regard as the most reliable predictor in this setting. Hence, if arriving at a successful design in alignment our search prompt, we can disregard any uncertainty in the network. In that case the remaining gap to bridge is that of the MD simulation and real life implementations.

0.3   Objective of the study

1. Design a MD simulation to evaluate the frictional properties of the grpahene sheet under different variations of cut patterns, stretching and loading, among other physical variables.

2. Train a network to replace the MD simulation completely.

3. (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.

4. (Variation 2) Make a GAN network using the first network and predict cut configurations for some of the above mentiond frictional properties.

5. (If I have time) Make a nanomachine that couples load and stretch (perhaps just artificially without any molecular mechanism) to test the hypothesize of a negativ friction coefficient.

0.4   Contributions

What did I actually achieve

0.5   Thesis structure

How is the thesis structured.

Bibliography

[1] Bhusnan, *Introduction*, ch. 1, pp. 1–8. John Wiley & Sons, Ltd, 2013.
https://onlinelibrary.wiley.com/doi/pdf/10.1002/9781118403259.ch1.
https://doi.org/10.1002/9781118403259.ch1.

[2] H.-J. Kim and D.-E. Kim, *Nano-scale friction: A review*, .

[3] K. Holmberg and A. Erdemir, *Influence of tribology on global energy consumption, costs and emissions*, .

[4] 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** (Oct, 2020) 042006.