Title

Subtitle

by

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THESIS

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Abstract

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Acknowledgments

Acknowledgments.

Contents

List of symbols?

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

Introduction

0.1 Some headline for the introtext

0.2 Introduction to friction and motivation

friction a part of the (wider) field tribology.

- Where is friction important (motivation)
- The economical interest in tribology (quote)
- The missing knowdelegde about friction.
- What possibilities do we have if we could control friction (friction coefficient).

0.3 Introduction to MD simulations and machine learning approaches

0.4 Defining the goal of the thesis and restrictions

Make bullet point objectives for the thesis and state which is completed, which is perhaps not conslusive and which I did not answer at all / do at all. Perhaps also make a list of problems/questions to answer (also state which one I actually answer here).

0.5 Contributions

0.6 Thesis structure

Introduction. A citation to avoid error for now: [1].

- Nanotribology
- Quantitative Structure-Property Relationship
- Forward simulation using ML
- Inverse designs

Practically, systems achieving low values of dry sliding friction are of great technological interest to significantly reduce dissipation and wear in mechanical devices functioning at various scales. (Current trends in the physics of nanoscale friction)

These experiments have demonstrated that the relationship between friction and surface roughness is not always simple or obvious. (Introduction to Tribology, p. 527).

"In other words, it's not just the material itself" that determines how it slides, but also its boundary condition — including whether it is loose and wrinkled or flat and stretched tight, he says. (https://news.mit.edu/2016/sliding-flexible-graphene-surfaces-1123).¡– Talking about quality of contact for friciton.

Chapter 1

Background Theory and Method

Small introtext to motivate this chapter. What am I going to go over here.

1.1 Tribology - friction

1.1.1 Friction on a macroscopic scale - macroscale theories

1.1.1.1 Amontons' law.

The work of Leonardo da Vinci (1452–1519), Guillaume Amontons (1663-705) and Charles de Coulomb (1736-1806) all contributed to what is commonly known as Amontons' law describing the frictional force accuring when starting and keeping a solid block sliding against a solid surface. This emperical law states that the frictional force tangential to the sliding direction is entirely independent of contact area and sliding velocity (at ordinary sliding velocities). Instead it relies only on the normal force F_N acting from the surface on the block and the material specific friction coefficient μ as

$$F_f = \mu F_N.$$

Further it distinguish between *static* and *kinetic* friction as the cases of stationary and sliding contact resepectively. Each type of friction comes with its own friction coefficient, μ_s for static and μ_k for kinetic friction, usually with values lower than one and $\mu_s \geq \mu_k$ in all cases. [2][p. 6].

This simple law is a natural starting point for the

Allthough this model is a common base for understanding friction on a macroscopic level is has its limitations. It turns out that static friction is not constant, but depends on the so-called contact history with increasing friction as the logarithm of time of stationary contact [3]. For the kinetic friction the independency of sliding velocity dissapears at low velocities as thermal effects becomes important and for high velocities due to intertial effetcs. [2][pp. 5-6].

It fails to explain the mechanisms behind fritction.

In order to understand what is causing friction between moving objects and how this might result in a linear relationship between friction and normal force we must take the study to a smaller scale... Having an emperical law that seems to predict the friction in many cases leads to the next natural desire for deriving these from fundamental atomic or molecular principles.

1.1.2 Friction on a microscopic scale - Nanotribology

It is generally accepted that friction is caused by two mechanism: mechanical friction and chemical friction. The mechanical friction is the plowing of the surface by hard particles or asperities. The chemical mechanism is adhesion between contacting surfaces. [4].

Sources in general: [5], [4]

1.1.2.1 Surface roughness - Asperity theories

Going beyond a macroscopic perspective we realise that most surfaces is in fact rough. The contact between two surfaces consist of numerous smaller contact point, so-called asperities, each with a contact area of A_{asp}. The true contact area $\sum A_{\text{asp}}$ is found to be much smaller than the apperent macroscopic area A_{macro}. The friction force is shown to be proportional (extra source on this) to this true contact area as

$$F_f = \vec{\tau} \sum A_{\text{asp}},$$

where $\vec{\tau}$ is an effective shear strength of the contacting bodies. This is still compatible with Amontons' law as long as we differenciate between the macroscopic macroscopic and true area and by having the true contact area dependt linearly on applied normal force.

Thus many studies have focused individual asperities to reveal the relationship between the contact area and normal force (13-15 from [5]). By assuming perfectly smooth asperities with radii of curvature from nanometers to micrometres in size continuum mechanics can be used to predict the deformation of asperities as normal force is applied. A model for non-adhesive contact between homogenous, isotropic, linear elastic spheres was first developed by Hertz (17 [5]), which predicted $A_{\text{asp}} \propto F_N^{2/3}$. Later adhesion effects were included in a number of subsequent models, including Maugis-Dugdale theory (18 from [5]), which also predicts a sublinear relatinship between A_{asp} and f_N leading to a similar sublinear relationship for F_f and F_N.
[5].

1.1.2.2 Atomic level friction

On the smallest possible scale, atomic scale, the surfaces does not have structural asperities. Instead atomic level friction is being model as a consequencse of the rough potential of the atomic landscape.

1.1.2.3 Frenkel-Kontorova-Tomlinson (FKT)

Describes atomic scale friction (not fully accurately though) and gives insight in stick slip motion.

1.1.2.4 Commensurate and incommensurate

1.1.2.5 Stick slip

At nanoscales things get a bit more unclear. SFM (explain) experiments have reported (copy sources 5, 6, 21 from [5]) where $F_f \propto F_N$ or even with these quantities being nearly independent of each other.
In several works by J. Fineberg's group [2–4] the transition from sticking to sliding is characterized by slip fronts propagating along the interface. [6][p. 2].

1.1.2.6 Commensurate and incommensurate

As expected, high levels of friction were present in the commensurate positions and extremely low friction was found when the surfaces were incommensurate. (https://physicsworld.com/a/friction-at-the-nano-scale/)

1.1.2.7 Superlubricity?

Superlubricity, now a pervasive concept of modern tribology, dates back to the math- ematical framework of the Frenkel Kontorova model for incommensurate interfaces [40]. When two contacting crystalline workpieces are out of registry, by lattice mismatch or angular misalignment, the minimal force required to achieve sliding, i.e. the static friction, tends to zero in the thermodynamic limit – that is, it can at most grow as a power less than one of the area – provided the two substrates are stiff enough. (Current trends in the physics of nanoscale friction)
Superlubricity is experimentally rare. Until recently, it has been demonstrated or im- plied in a relatively small number of cases [29, 42–46]. There are now more evidences of superlubric behavior in cluster nanomanipulation [32, 33, 47], sliding colloidal layers [48–50], and inertially driven rare-gas adsorbates [51, 52]. (Current trends in the physics of nanoscale friction)

A breakdown of structural lubricity may occur at the heterogeneous interface of graphene and h-BN. Because of lattice mismatch (1.8%), this interface is intrinsically incommen- surate, and superlubricity should persist regardless of the flake-substrate orientation, and become more and more evident as the flake size increases [57]. However, vertical cor- rugations and planar strains may occur at the interface even in the presence of weak van der Waals interactions and, since the lattice mismatch is small, the system can de- velop locally commensurate and incommensurate domains as a function of the misfit angle [58, 59]. Nonetheless, spontaneous rotation of large graphene flakes on h-BN is observed after thermal annealing at elevated temperatures, indicative of very low friction due to incommensurate sliding [60, 61]. (Current trends in the physics of nanoscale friction)

Indeed, we know from theory and simulation [74–76] that even in clean wearless friction experiments with perfect atomic structures, superlubricity at large scales may, for example, surrender due to the soft elastic strain deformations of contacting systems. (Current trends in the physics of nanoscale friction)

1.1.3 Temperature dependence

Thus, it is commonly expected that the friction of a dry nanocontact should classically decrease with increasing temperature provided no other surface or material parameters are altered by the temperature changes [77, 80–83]. (Current trends in the physics of nanoscale friction)

1.1.4 Summary of expected frictional properties

1. Friction should decrease by increasing temperature.
2. We expect stick slip motion
3. What about dependence on normal force?
4. Dependence on contact area?
5. Dependense on speed?

- Different friction models on macro-and microscopic scale

1.2 Graphene

Because of this frictional reduction, many studies indicate graphene as the thinnest solid-state lubricant and anti-wear coating [104–106]. (Current trends in the physics of nanoscale friction)

Accurate FFM measurements on few-layer graphene systems show that friction decreases by increasing graphene thickness from a single layer up to 4-5 layers, and then it approaches graphite values [97, 99, 101, 107, 108]. (Current trends in the physics of nanoscale friction)

- General properties and crystal structure

1.3 Molecular Dynamics

1.3.1 Potentials

1.3.2 LAMMPS

1.3.3 Intregration

1.3.4 Thermostats

1.3.5 Graphene

- MD simulation (classical or ab initio)
- Basics of classical MD simulations: Integration and stuff
- Ab initio simulation (quantum mechanics, solving schrödinger)

1.4 Real life experimental procedures

From Introduction to Tribology, Second Edition, p. 526:

The surface force apparatus (SFA), the scanning tunneling microscopes (STM), and atomic force and friction force microscopes (AFM and FFM) are widely used in nanotribological and nanomechanics studies.

- Real life procedures to mimic in computation, for instance Atomic Force Microscoopy (AFM) for friction measurements.
- Available technology for test of my findings if successful (possibilities for making the nano machine)

1.5 Machine Learning (ML)

- Feed forward fully connected
- CNN
- GAN (encoder + decoder)
- Genetic algorithm
- Using machine learning for inverse designs partly eliminate the black box problem. When a design is produced we can test it, and if it works we not rely on machine learning connections to verify it's relevance.
- However, using explanaitons techniques such as maybe t-SNE, Deep dream, LRP, Shapley values and linearizations, we can try to understand why the AI chose as it did. This can lead to an increased understanding of each design feature. Again this is not dependent on the complex network of the network as this can be tested and veriied independently of the network.

1.5.1 Feed forward network / Neural networks

1.5.2 CNN for image recognition

1.5.3 GAN (encoder + deoder)

1.5.4 Inverse desing using machine learning

1.5.5 Prediction explanation

1.5.5.1 Shapley

1.5.5.2 Lineariations

1.5.5.3 LRP

1.5.5.4 t-SNE

1.6 Generating cuts in the graphene sheet

1.6.1 Defining the sheet configuration

1.6.1.1 Indexing

1.6.1.2 Removing atoms

1.6.1.3 Pull blocks

1.6.2 Kirigami inspired cut out patterns

1.6.2.1 Pop-up pattern

1.6.2.2 Honeycomb

1.6.2.3 Random walk

Bibliography

[1] S. Li, Q. Li, R. W. Carpick, P. Gumbsch, X. Z. Liu, X. Ding et al., *The evolving quality of frictional contact with graphene*, .

[2] E. Gnecco and E. Meyer, *Elements of Friction Theory and Nanotribology*. Cambridge University Press, 2015, 10.1017/CBO9780511795039.

[3] J. H. Dieterich, *Time-dependent friction in rocks*, *Journal of Geophysical Research (1896-1977)* **77** (1972) 3690–3697, [https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/JB077i020p03690].

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

[5] Y. Mo, K. T. Turner and I. Szlufarska, *Friction laws at the nanoscale*, .

[6] N. Manini, G. Mistura, G. Paolicelli, E. Tosatti and A. Vanossi, *Current trends in the physics of nanoscale friction*, *Advances in Physics: X* **2** (may, 2017) 569–590.