Title

Subtitle

by

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Title

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Abstract

Abstract.

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

The study of friction, wear and lubrication between two surfaces in relative motion is called tribology. [2].

We will limit ourself to the elementary processes of dry, wearless surface sliding. In general we can divide friction in to two scales: Macroscopic and microscopic, for which the properties turns out to differ quite substantially.

Make an explicit distinction between macroscale and microscale. Get some numbers on it!

Sliding friction that takes place between two surfaces in the absence of lubricant is termed "dry" friction even if the process occurs in an ambient environment. (Nanotriology and Nanomechanics, p. 329)

The differences between the conventional or macrotribology and micro/nanotribology are contrasted in Figure 1.3.1. In macrotribology, tests are conducted on components with relatively large mass under heavily loaded conditions. In these tests, wear is inevitable and the bulk prop- erties of mating components dominate the tribological performance. In micro/nanotribology, measurements are made on components, at least one of the mating components, with relatively small mass under lightly loaded conditions. In this situation, negligible wear occurs and the surface properties dominate the tribological performance. [3][p. 5]

1.1.1 Friction on a macroscopic scale - macroscale theories

1.1.1.1 Amontons' law.

The first well known studies of friction concerns itself is based on a macroscopic level. That is, the scale of visible everyday objects. The work of Leonardo da Vinci (1452–1519), Guillaume Amontons (1663-705) and Charles de Coulomb (1736-1806) all contributed to 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. Instead it relies only on the normal force F_N 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 a stationary and a sliding contact surface 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 $\mu_s \geq \mu_k$ [2][p. 6]. Allthough this models is a common base for understanding friction is has it limitations. For instance 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 [4]. For kinetic friction the independency of sliding velocity also dissapears for low velocities as thermal effects becomes important and for high velocities due to intertial effetcs. [2][pp. 5-6].

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

1.1.3 Surface roughness

Sources in general: [5]

Since the formulation of Amontons' law it has been discovered that most surfaces is actually rough on a smaller scale. In reality the surface consist of a large number of smaller contacts, so-called asperities, each with contact area A_{asp}. This true contact area $\sum A_{\text{asp}}$ is found to be much smaller than the macroscopic area A_{macro} and has been shown to be proportional to the friction force as

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

where $\vec{\tau}$ is an effective shear strength of the contacting bodies. However, this is still compatible with Amontons' law if the true contact area depends linearly on the applied normal force. Thus many studies have focused individual asperities to reveal the relationship between the contact area and the normal force (Copy sources 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 (copy source 17 from [5]), which predicted $A_{\text{asp}} F_N^{2/3}$. Later adhesion effects were included in a number of subsequent models, including Maugis-Dugdale theory (copy source 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.

A model for non-adhesive contact between homogenous, isotropic, linear elastic spheres, was first developed by Hertz17, who showed that Aasp!L2=3. Adhesion effects were included in a number of subsequent models, among which Maugis-Dugdale theory18 has been frequently used because of its high degree of flexibility. The common feature of all the single-asperity theories is that Aasp is a sublinear function of L. In addition, several scanning force microscopy (SFM) studies have reported that Ff tAasp, with t being an interfacial shear strength13,19. In this case, Ff will be a sublinear function of load20.

[5].

I

However, practical single- and multiplecontact conditions are characterized by complex interaction profiles plus nontrivial internal dynamics. As a result, the interplay of thermal drifts, contact ageing, contact-contact interactions, and macroscopic elastic deformations introduce significant complications, and make the depinning transition from static to kinetic friction an active field of research. [6][p. 2].

1.1.3.1 Stick slip

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].

1.1.3.2 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/)

1.1.3.3 Tomlinson model

1.1.3.4 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)

1.1.4 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)

- 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

Method

1.7 Free floating bullet points to remember

- Describe two different approaches:
  Nanomachine setup (sheet as the inner layer of nanomachine influencing the stretch)
  Graphene skin setup (sheet on the outside probed with tip, stretched and fixed on object)

1.8 Setting up the system

- Substrate material (crystalline or amorphous)
- Intra- and intermolecular potentials
- Ensembles: NVE, NVT
- Choice of dt, relax time etc.

1.9 Measuring properties

- Out-of-plane buckling
- Contact area
- Friction (static, dynamic)

1.10 Making cuts in graphene

- Indexing the sheet
- Manual patterns as a starting point(Pop-up pattern and half octans)
- Cut rules and problems with dangling fringes
- Different variations of manual patterns
- Random walks

1.11 Simulation procedures

- Relaxing
- Stretching
- Friction
- Different combinations of stretch and applied normal force

1.12 Working title: tweeking simulation settings

- Substrate structure
- Drag speed
- Spring stifness
- ...

1.13 Sampling data

- Different drag angles

1.14 Machine learning

- Input: atom position matrix
- Target properties: friction coefficient (low/high), maybe load curve for nonlinear relations
- Output: Cut pattern, stretch amount (%)
- Architecture and network types
- Loss function and evaluation

Big lines

- Make indexing system/ description of the sheet
- Collect data
  - pop-up pattern
  - RN walk
  - RN straight cuts?
  - RN single atoms removes
  - Rules for patterns
- Train mahcine learning algorithm to predict properties
  - Static/Dynamic friction coefficient from atom matrix.

Possible subjects

- Indexing the graphene sheet
- Creating a pop-up pattern
- Potentials and materials
- Creating substrate
  - quenching
- Creating data sets
  - random walk?

Things to remember

- Word: Nanotribology

Choosing material and potentials

Looking at https://aip.scitation.org/doi/pdf/10.1063/1.481208.

The main material of study is the graphene sheet. Graphene is simply a single layer of graphite. For the friction study we need a substrate and a tip which pushes down into the sheet. For the tip and substrate we have considered both diamond and silicon. Here we look at tersoff, REBO and Airebo as possible potentials candiates for intramolecular potentials. For the intermolecular potential we can use a typical 12-6 Lennard-Jones (LJ) potential. Could also choose exp-6 potential which is slightly more complex I think. The repulsive wall is known to be quite hard. Above article is talking about a LJ switch to overcome the hard repulsive wall.

The LJ potential is taking from https://pubs.rsc.org/en/content/articlehtml/2015/nr/c4nr07445a refering to https://journals.aps.org/prb/pdf/10.1103/PhysRevB.81.155408.

Work in progress simulation setup

Silicon substrate (crystalline or amorphous) with a single graphene sheet resting on top. A Si tip apex described as a rigid body connected to a moving support (with no atomic interaction) via a harmonic spring to drag the tip apex across the sheet.

Step 1: Load the tip with a normal force such that the tip begin to interact with the sheet. Step 2: Drag the tip in the horizontal direction and measure either static or dynamic friction.

- Which way to drag? Different angles (zigzag direction, armchair direction or something inbetween). The optimial cut-pattern for friction properties will depend on the "scan" angle (see https://pubs.rsc.org/en/content/articlehtml/2015/nr

Find right timestep

From article (Nanoscrathing of multi-layer graphene): The equations of particles motion were solved using the Verlet algorithm, and the simulation time step is 1 fs, which is adequate for system relaxation by examining the stability through the root mean square deviations of the atoms.

Results and Discussion

Frictional properties of the intact graphene sheet

The friction measurment simulation is governed by the following parameters, which is divided into three sub categories for the purpose of this thesis as shown in table 1.1.

Table 1.1: Parameters of the numerical procedure for measuring friction.

Category	Parameter name: description	Category purpose
Physical	- T: Temperature for the Langevin thermostat. - v_{drag}: Drag speed for the sheet translation.	Parameters that we expect to have an inevitably effect on the system friction properties, for which the choice will be a baseline for our studies.
Measurement	- dt: Integration timestep. - t_R: Relaxtion time before strething. - Pauses between stretch and adding normal force and between dragging the sheet. - Stretch Speed: How fast to stretch the sheet. - K: Spring constant for the spring responsible of translating the sheet. An infinte spring constant is achieved by moving the end blocks as a rigid body (Lammps: fix move). - Drag Length: How far to translate the sheet. - Sheet size: Spatial size of the 2D sheet.	Paramters that effects the simulation dynamics and the 'experimental procedure' that we a mimicking. We aim to choose to these paramters such that the friction properties is stable for small perturbations.
ML input	- Sheet configuration: A binary matrix containing information of which atoms is removed (0) and which is still present (1) in the graphene structure. - Scan angle: The direction for which we translate the sheet. - Stretch amount: The relative sheet stretch in percentage. - F_N: Applied normal force to the end blocks.	The ramaining paramters that serve as the governing variables in the optimization process for certain friction properties and is thus the input variables for the ML part.

We should try to set the physcis and measurement parameters in such a way that we reduce computation speed where it is doesn't infer with the frictional properties study.

We need to define some ranges for the ML input paramters. F_N, stretch ranges where it is not prone to ruptures. The configuration it self does not have clear rules but is also being regulated by the no rupture requirement.

Observations

- stretch = 0 % and $F_N = 188$ eV/Å yielded a very small amount of wear (two atoms visually out of place), for which the sheet dug into the substrate when passing by the second time. For the same normal force but 0.25 % this problem did not occour. We need to stay out of the friction wear regime. Amorphic substrate is even more prone to this problem of wear.

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