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

Friction is a fundamental physcial concept that takes part in almost all thinkable interactions with matter. Even though the everyday person might not be quite familiar with the content of the term "friction" we would undoubtly notice its disappearing. Without friction it would not be possible to cross a flat surface by foot, lean against the wall without sliding to the floor or even using nails and screws to secure stuff. On the other hand we are not suprised when a moving object comes to a stop when not supplied with yet another push and we know intuitively that sliding down a snow covered hill is much more exiting that its grassy counterpart. It is probably safe to say that the concept of friction is well integrated in out everyday life to such an extent that we seem to take it for granted. We also do not question the fact that solid materials repeal other solid materials or similar. However, recognitizing the fundamentality and impact of friction we know surprisingly about the mechanisms behind it (source and or quote here). As a qonsequence we also have limited knowdelegde of how to affect friction or whether it is even possible to do so. In an investigation of the potential influence improvement in friction reduction it was reported

> "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." [1].

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

The good thing about the process of inverse design is that the uncertainty and missing information from the network (black box) is not important if we are able to locate a working design. Thus we can test the suggested design and remove the doubt of whether this is a good design or not. Thus we do not have to trust the network prediction at all. However, if the predictions is not accurate enough we will most liekely never get any usefull designs from the ML process, but at least we will be informed whether the designs are good or bad in the end with respect to the simulations. However the question is rather if we can trust the simulation results. In the ned we should test the designs in real life to be completely sure and thus the certainity of the quality of any proposed designs is determined by the simulation quality.

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: [2].

- 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. [3][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 [4]. 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. [3][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. [5].

Sources in general: [6], [5]

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 [6]). 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 [6]), 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 [6]), which also predicts a sublinear relatinship between A_{asp} and f_N leading to a similar sublinear relationship for F_f and F_N.
[6].

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 [6]) 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. [7][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

1.1.5 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

1.1.6 Molecular Dynamics

1.1.6.1 Potentials

1.1.6.2 LAMMPS

1.1.6.3 Intregration

1.1.6.4 Thermostats

1.1.7 Defining the system

Include figure of system to point out thermo layers and freeze layers.

1.1.8 Creating sheets

We are going to create a 2D sheet graphene sheet.

1.1.8.1 Graphene

Graphene is a single layer of carbon atom, graphite is the bulk, arranged in a hexagonallattice structure. We can describe the 2D crystal structure in terms of its primitive lattice vector and a basis. That is we populate each lattice site by the given basis and translate it to fill the whole plane by any linear combination of the lattice vectors

$$\vec{T}_{mn} = m\vec{a_1} + n\vec{a_2}, \qquad m, n \in \mathbb{N}.$$

For graphene we have the primitive lattice vectors

$$\vec{a_1} = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right), \qquad \vec{a_2} = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \qquad |\vec{a_1}| = |\vec{a_2} = 2.46 \text{ Å}.$$

Notice that we deliberately excluded the third coordinate as we only consider a single graphene layer on not the bulk graphite consisting of multiple layers stacked on top of each other. The basis is

$$\left\{\Big(0,0\Big), \frac{a}{2}\Big(\frac{1}{\sqrt{3}}, 1\Big)\right\}$$

It turns out that the spacing between atoms is equal for all paris with an interatomic distance

$$\left|\frac{a}{2}\Big(\frac{1}{\sqrt{3}}, 1\Big)\right| \approx 1.42 \text{ Å}.$$

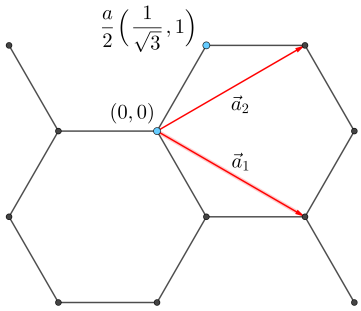

Figure 1.1: Graphene crystal structure with basis.

1.1.8.2 Indexing

In order to define the cut patterns applied to the graphene sheet we must define an indexing system. We must ensure that this gives an unique description of the atoms as we eventually want to pass a binary matrix, containg 0 for removed atom and 1 for present atom, that uniquely describes the sheet. We do this by letting the x-coordinate point to zigzag chains and the y-coordinate to the position along that chain. This is illustrated in figure 1.2. Other solutions might naturally invole the lattice vectors, but as these only can be used to translate to similar basis atoms a unfortunate duality is introduced as ones need to include the basis atom of choice into the indexing system. With the current system we notice that locallity is somewhat preserved. That is, atom (i, j) is in the proximity of $\{(i+1, j), (i-1, j), (i, j+1), (i, j-1)\}$, but only three of them is categorized as nearest neighbours due to the hexgonal structure of the lattice. While $(i, j \pm 1)$ is always nearest neighbours the neighbour in the x-direction flip sides with incrementing y-coordinate. That is the nearest neighbours (NN) is decided as

$$j \text{ is even} \rightarrow \text{NN} = \{(i+1, j), (i, j+1), (i, j-1)\},$$
$$j \text{ is odd} \rightarrow \text{NN} = \{(i-1, j), (i, j+1), (i, j-1)\}.$$

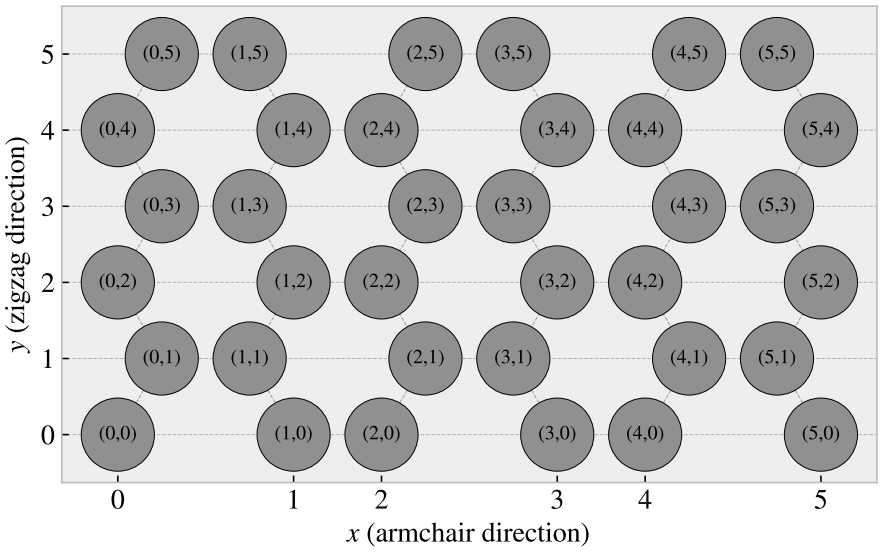

Figure 1.2: Graphene atom indexing

1.1.8.3 Removing atoms

As a mean to ease the formulation of cut patterns we introduce pseudo center element in each gap of the hexagonal honeycombs, see figure 1.3.

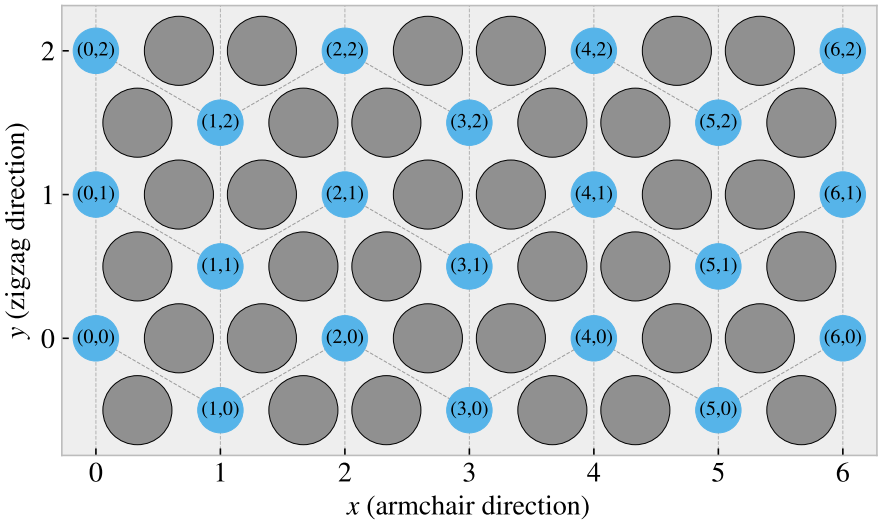

Figure 1.3: Graphene center indexing

Similar to the case of the indexing for the carbon atoms themself the nearest neighbour center elements alternate with position, this time along the x-coordinate. Each center element has six nearest neighbours, in clock wise direction we can denote them: “up”, “upper right”, “lower right”, “down”, “lower left”, “upper left”. The “up” and “down” is always accesed as $(i, j \pm 1)$, but for even i the $(i + 1, j)$ index corresponds to the “lower right” neighbour while for odd i this corresponds to the “upper right” neighbour. This shifting applies for all left or right neighbours and the full neighbour list is illustrated in figure 1.4.

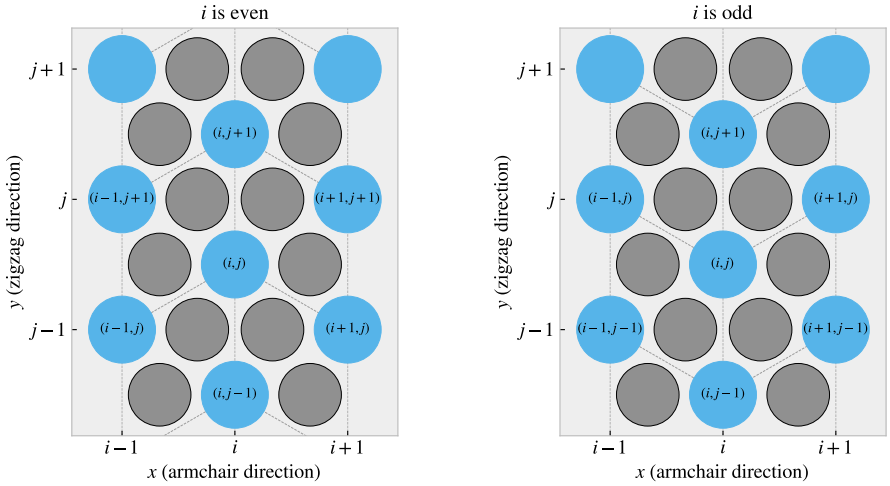

Figure 1.4: Graphene center elements directions

We define a cut pattern by connecting center elements into connected paths. As we walk element to element we remove atoms according to one of two rules

1. Remove intersection atoms: We remove the pair of atoms placed directly in the path we are walking. That is, when jumnping to the "up" center element we remove the two upper atoms located in the local hexagon of atoms. This method is sensitive to the order of the center elements in the path.

2. Remove all surrounding atoms: We simply remove all atoms in the local hexagon surrounding each center element. This method is indepdent of the ordering of center elements in the path.

We notice that removing atoms using either of these rules will not garuantee an unique cut pattern. Rule 1 is the more sensitive to paths but we realize that, for an even i, we will remove the same five atoms following either of the following paths.

$$(i,j) \rightarrow \underbrace{(i+1,j+1)}_{\text{upper right}} \rightarrow \underbrace{(i,j+1)}_{\text{up}} \rightarrow \underbrace{(i+1,j+2)}_{\text{upperright + up}} \rightarrow \underbrace{(i+1,j+1)}_{\text{upper right}}$$

$$(i,j) \rightarrow \underbrace{(i+1,j+1)}_{\text{upper right}} \rightarrow \underbrace{(i+1,j+2)}_{\text{upperright + up}} \rightarrow \underbrace{(i,j+1)}_{\text{up}}$$

For rule 2 it is even more abovious that different paths can result in the same atoms being removed. This is the reason that we needed to define and indexing system for the atom position itself even though that all cuts generated manually will use the center element path as reference.

Illustrate some delete path?

1.1.8.4 Pull blocks

1.1.9 Kirigami inspired cut out patterns

1.1.9.1 Pop-up pattern

1.1.9.2 Honeycomb

1.1.9.3 Random walk

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

1.1.10 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)

1.1.11 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.

1.1.12 Feed forward network / Neural networks

1.1.13 CNN for image recognition

1.1.14 GAN (encoder + deoder)

1.1.15 Inverse desing using machine learning

1.1.16 Prediction explanation

1.1.16.1 Shapley

1.1.16.2 Lineariations

1.1.16.3 LRP

1.1.16.4 t-SNE

Method

1.2 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)

1.3 Setting up the system

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

1.4 Measuring properties

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

1.5 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

1.6 Simulation procedures

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

1.7 Working title: tweeking simulation settings

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

1.8 Handling ruptures

Considered the following parameters to define rupture events.

- Stress (in stretch direction) drop
- Max velocity peak (peak in cummax divided by std)
- peak in value MSD (com ave)
- Drop in coordination number
- Number of clusters (should be constant 1). This is the most secure one

Ideally one would store the nearest neighbours for each atom and check that thoose neighbours satays in proximity during the simulation. This would capture even the smallest rupture, but this is not availble at runtime in Lammps which made it non ideal. In addiditon this calculation would also be computational heavy because of the algorithm needed to make this investigation but also considering the fact that we cannot due early stopping and thus need to run a lot of ruptured sheet to the end of the simulation time.

1.9 Sampling data

- Different drag angles

1.10 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.

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.

Simulations

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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