Title

Subtitle

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Title

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Abstract

Abstract.

Acknowledgments

Acknowledgments.

Contents

Introduction

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

- Nanotribology

- Quantitative Structure-Property Relationship

- Forward simulation using ML

- Inverse designs

Theory

0.1   Friction

Check out: Fundamentals of Friction: Macroscopic and Microscopic Processes or search for other background information.

0.1.1   Macroscopic scale

Dry friction

(from wikipedia so far: https://en.wikipedia.org/wiki/Friction)

- Amontons' First Law: The force of friction is directly proportional to the applied load.

- Amontons' Second Law: The force of friction is independent of the apparent area of contact.

- Coulomb's Law of Friction: Kinetic friction is independent of the sliding velocity.

Columbd friction

$$F_f \leq \mu F_n$$

Static and dynamic/kinetic friction

0.1.2   Microscopic scale

- Different friction models on macro-and microscopic scale

0.2   Graphene

- General properties and crystal structure

0.3   MD simulations

- Basics and MD simulations: Integration and stuff

0.4   Real life experimental procedures

- 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)

0.5   Machine Learning (ML)

- Feed forward fully connected

- CNN

- GAN (encoder + decoder)

- Genetic algorithm

Method

Setting up the system

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

Measuring properties

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

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

Simulation procedures

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

Working title: tweeking simulation settings

- Substrate structure

- Drag speed

- Spring stifness

- ...

Sampling data

- Different drag angles

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.

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*, .