Title

Subtitle

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THESIS

for the degree of

MASTER OF SCIENCE

Faculty of Mathematics and Natural Sciences
University of Oslo

Autumn 2022

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

Printed: Reprosentralen, University of Oslo

Abstract

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Acknowledgments

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Contents

Structure

Introduction

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

Theory

Friction

- Different friction models on macro-and microscopic scale

Graphene

- General properties and crystal structure

MD simulations

- Basics and MD simulations: Integration and stuff

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)

Machine Learning (ML)

- Feed forward fully connected
- CNN
- GAN (encoder + decoder)
- ...

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

Sampling data

- ...

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

Introduction

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

Method

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/20

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.