Master project topics

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April 16, 2020

Contents

Simulating the contact mechanics of hydrogels

This project is concerned with the contact mechanics of hydrogels at the micrometer length scale. Hydrogels are random networks of long hydrophillic polymer chains surrounded by a water. They have many applications, especially in medicine. They are for example used in wound dressing, tissue engineering, and drug delivery.

The goal of the project is to simulate the contact mechanics of hydrogels. To this end, you will start from the existing molecular-dynamics code written in C++ by a previous student and external collaborator Martin Müser. The code needs to be extended to include additional physics that is crucial for viscoelastic behaviour of gels. You will then use this program to perform indentation and sliding simulations. You will study how the polymer network deforms and how the polymer concentration changes under strain. The simulations can be used to test theories how shear and normal stresses depend on crucial parameters, in particular, on the cross-link density of the polymer network.

Required background

A basic programming course and an interest in modelling or programming.

Supervisor

Astrid S. de Wijn (MTP) <astrid.dewijn@ntnu.no>
Alex Hansen (Physics) <alex.hansen@ntnu.no>
(Who will be the main supervisor depends on the department of the student.)

Research environment: `http://syonax.net/science/research.html`.

Collaborator

Martin Müser, Saarland University

Work load

This project is intended for a combined specialization project thesis and master thesis, i.e. 45 ECTS in total.

Simulating noise generation by friction

Car brakes sometimes produce an annoying loud squealing noise. There are many other cases where noise is generated by rubbing objects together, for example in a violin. In a previous project, we have developed a simple model for studying the interplay between the dynamics at the sliding interface, and the generation of noise in a resonator such as a brake system. The goal of this project will be to further investigate this model, and study how the noise can be controlled.

The project will use a simple computational setup. As part of the project you can either use existing numerical simulations of the model or write your own. You will then expand on the old simulations. If necessary, you will run simulations on high-performance computing facilities.

This project will entail a lot of programming, and it helps if you have good understanding of mechanics. Since we already know what the model should look like, it is a fairly well-defined project.

Required background

A basic programming course and an interest in modelling or programming. Tribology, basic statistical mechanics, or classical mechanics.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>
Bjørn Haugen <bjorn.haugen@ntnu.no>

Research environment: `http://syonax.net/science/research.html`.

Work load

This project is intended for a combined specialization project thesis and master thesis, i.e. 45 ECTS in total.

Modelling extremely low friction of quasicrystals

In this project, you will focus on a particular class of crystalline materials that have an unusual structure: quasicrystals. The discovery of quasicrystals was awarded the Nobel Prize in chemistry in 2011. The project is concerned with how the quasi-crystal structure will affect the friction of these surfaces, through structural superlubricity. This is a dramatic effect by which friction is reduced enormously due to structural incompatibility between two surfaces at the atomic level. You will write a simple numerical simulation to compute interactions of contacts with quasi-crystalline surfaces, and whenever possible do analytical calculations to accompany them.

Required background

Tribology or classical mechanics. A basic programming course and an interest in modelling or programming.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

Research environment: `http://syonax.net/science/research.html`.

Work load

This project is intended for a combined specialization project thesis and master thesis, i.e. 45 ECTS in total.

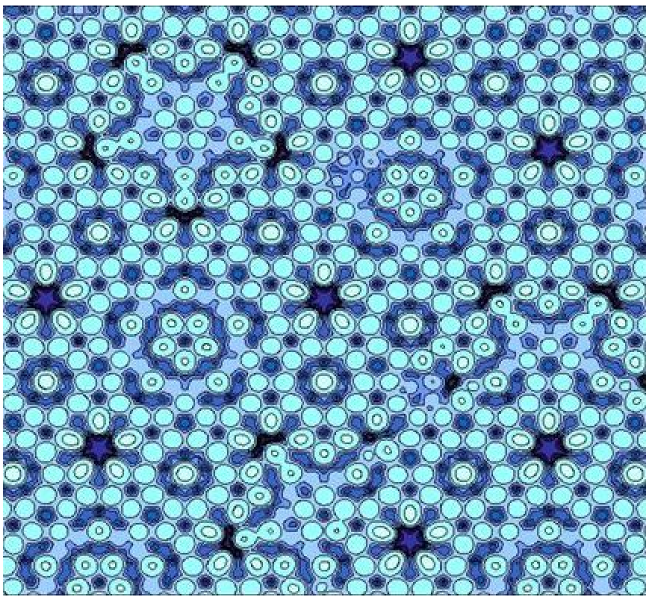

Figure 1: Example of a quasicrystal surface, atomic model of fivefold icosahedral-Al-Pd-Mn. (Picture from Wikimedia Commons.)

Simulating mechanical properties of 2d materials

In this project, we will investigate the mechanisms of solid lubrication using Molecular-Dynamics simulations. In lubrication with a solid powder, small, nm-thin flakes of the solid slide easily past eachother. While we have some understanding of the behaviour of single sliding flakes, we are only beginning to explore the effects of having multiple flakes that can act collectively, or how multiple layers interact with each other [1].

This project will focus on possible effects of tearing of layers, as well as the interactions between layers. Another possible line of inquiry is the interactions between flakes. You will employ the existing openly available molecular dynamics code LAMMPS in combination with python scripting to create the models and to analyze the results.

[1] *Understanding the friction of atomically thin layered materials*, David Andersson and Astrid S. de Wijn, Nature Communications **11**, 420 (2020).

Required background

A basic programming course and an interest in modelling or programming. Tribology, basic statistical mechanics, or classical mechanics.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

Research environment: `http://syonax.net/science/research.html`.

Resources

The project will make use of high-performance computing resources that are already available through NTNU IT's HPC facilities and Sigma2.

Work load

This project is intended for a combined specialization project thesis and master thesis, i.e. 45 ECTS in total.

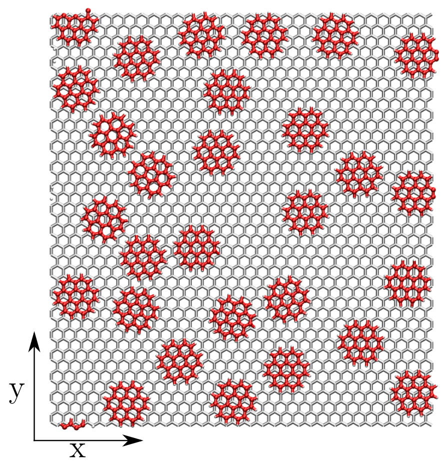

Figure 2: A top view of a simulation of a single layer of graphene flakes acting as a solid lubricant.

Modelling of strengthening mechanisms in Aluminum alloys

Norway is a major producer of aluminum alloys and has several producers of aluminum products for the car industry. In this project you will investigate the nano-scale details concerning plasticity and strengthening of aluminum alloys. To increase the strength in aluminum, alloying elements are added. In addition is the material is heat treated after production. The heat treatment will result in the formation of small ordered particles coherent with the aluminum lattice. Theses particles can be as small as a few nanometer, but are still detrimental for the strength of the final aluminum product. During plastic deformation, dislocations travel through the aluminum lattice and will meet these particles. Depending on the size, the dislocations may either loop or shear the particle.

In this project you will study the energetics of different possible pathways for a dislocation shearing a particle in an 6xxx aluminum alloy (Al, Mg, Si) using molecular dynamics and transition state theory. You will employ the existing openly available molecular dynamics code LAMMPS in combination with python scripting to create the models and to analyze the results.

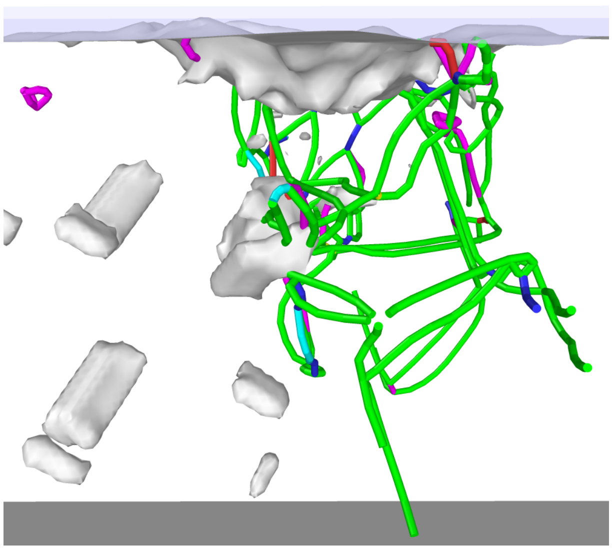

Figure 3: Molecular dynamics simulation of a nanoindentation of aluminium including particles. The lines visualizes the dislocations and the blobs are Mg-Si particles.

Required background

Basic material science. A basic programming course and an interest in modelling.

Supervisors

Astrid S. de Wijn <astrid.dewijn@ntnu.no>
Inga Ringdalen <inga.ringdalen@sintef.no>
Randi Holmestad <randi.holmestad@ntnu.no>

Research environment:
`http://syonax.net/science/research.html`
`https://www.ntnu.edu/web/casa/casa`

Resources

The project will make use of high-performance computing resources that are already available through NTNU IT's HPC facilities and Sigma2.

Work load

This project is intended for a combined specialization project thesis and master thesis, i.e. 45 ECTS in total.

Modelling spreading phenomena in social networks

Large networks of interacting components are more common than you might think. Examples are human social interaction, communication networks, power grids, and ecological networks of species. When the components fail (people get sick, communication hubs break down, species go extict), this weakens the network and the other components. Once a few components have failed a cascade of failures can start, spreading rapidly through the network. The spread of a disease through social interaction, such as is happening right now, is an obvious example. Some large power blackouts affect hundreds of thousands of people and can last hours or even days. The purpose of this project is to study how the size of these failures is related to the interaction between the components. We have designed a simple general model for these types systems, and it will be your task to simulate this model and study the results.

This project will involve a lot of programming to simulate the model, and statistical analysis of the simulations of the model. It may be necessary to study very large networks, which means that your code will need to be efficient. If necessary, you will run simulations on high-performance computing facilities.

Required background

A basic programming course and an interest in modelling or programming.

Supervisor

Astrid S. de Wijn <astrid.dewijn@ntnu.no>

External people involved

Baruch Barzel (Bar Ilan University, Israel)

Work load

This project is intended for a combined specialization project thesis and master thesis, i.e. 45 ECTS in total.