Project description for Mikkel Metzsch Jensen

Friction, the force resisting relative motion between two solid surfaces in contact, is an important problem in fundamental and applied physics. Being able to design surfaces with particular frictional properties can enhance applications like object grasping robots or other systems that require a fine-tuned and predictable frictional force.

The earliest systematic formulation of the laws of friction was by Leonardo da Vinci, who found that the friction force only depended on the materials in contact, and the normal load on the interface, not on the apparent area of contact. Amontons later added a formulation that incorporated the common observation that it is easier to keep something sliding than to make it slide. That is, before sliding, a threshold $F_N\mu_s$ needs to be overcome to start sliding, whereas after sliding has begun, the frictional resistance is reduced to $F_N\mu_k$. μ_k is called the coefficient of dynamic friction, and μ_s is called the coefficient of static friction. This simple picture was extended by Coulomb, who added a velocity term to the friction law, so that the relative speeds of the interfaces influenced the friction force, as did the amount of time the surfaces have been in contact. Upon detailed investigation of frictional interfaces, it has been shown that this simple behavior can be traced back to the evolution of the real contact area between two rough surfaces: A typical distribution of micro-asperities on an elastic and randomly rough surface results in a linear relationship between the applied normal load and the real area of contact. This real area of contact is again proportional to the static friction.

The simple theory by Amontons and Coulomb fails for surfaces that so not have a typical surface roughness. It also does not incorporate a notion of the propagation of rupture fronts at the onset of frictional sliding, leading to phenomena like precursors [1, 2] and slow fronts [3, 4]. This friction law also breaks down on the nanoscale [5, 6]. Thus friction is a richer phenomenon than one might get the impression of from the Amontons–Coulomb friction law. This complicates the study of friction, but it also allows for the design of materials and surfaces with exotic frictional properties.

Kirigami frictional surfaces

Graphene is a 2-dimensional material that is both strong and light. It can also be manipulated on the nanoscale, for example to make nanoscale kirigami [7]. By making various cuts in a graphene sheet, one can alter the elastic resonse of a graphene sheet, and also how it bends and buckles into the 3rd dimension. However, the number of possible cut configurations is enormous. It is on the order of 2^N where N is the number of atoms in the graphene sheet. Even if restricting to cutting along *one* of the coordinate diretions on a grid of 10×10 cells, the number of possible cut configurations is 2^{100}, which makes it intractable to explore all the configurations in experiments or even with molecular dynamics simulations. We therefore need to have clever ways of choosing what configurations we want to sample. One way that has been shown to work previously is to run forward physics simulations of a subset of the configuration space and then let a machine learning algorithm

interpolate the rest. By applying such a method in an iterative manner, one may for example optimize for cuts leading to a high stretchability of a graphene sheet [8]. The latter study used a deep neural network to explore the configuration space exhaustively. Another approach is for example to use generative machine learning algorithms to produce structures [9].

In this project we use molecular dynamics simulations to study the frictional properties of graphene sheets (or similar materials like MoS_2) when performing a series of kirigami-inspired cuts before stretching the sheet. Kirigami cut-patterns in a 2D sheet can result in 3D structures when the sheet is stretched, and thus we aim to introduce differently shaped and placed asperities. By the combined use of machine learning and MD simulations we aim to investigate different designs of cutting patterns and how this might contribute to the properties of friction when the sheet is stretched. In addition this gives rise to an investigation of how such properties depends on the amount and direction of stretching in order to search for multiproperty materials or exotic behavior.

The project consists of the following parts (brief timeline):

- Set up a simulation pipeline for evaluating the structural and frictional properties of a graphene sheet with a given configuration of cuts. (August–september 2022)
- Train a machine learning algorithm to predict the physics simulation outcomes just from an input image of the kirigami cuts. (October–December 2022)
- Create a procedure that generates structures aiming at optimizing for a given frictional property such as a very high or very low coefficient of friction. (January–march 2023)
- Finish thesis (April–may 2023)

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