

Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

Designs for a negative friction coefficient.

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Abstract

Abstract.

Acknowledgments

Acknowledgments.

List of Symbols

F_N Normal force (normal load)

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Chapter 1

Introduction

1.1 Motivation

Friction is the force that prevents the relative motion of objects in contact. Even though the everyday person might not be familiar with the term *friction* we recognize it as the inherent resistance to sliding motion. Some surfaces appear slippery and some rough, and we know intuitively that sliding down a snow-covered hill is much more exciting than its grassy counterpart. Without friction, it would not be possible to walk across a flat surface, lean against the wall without falling over or secure an object by the use of nails or screws [p. 5] [1]. It is probably safe to say that the concept of friction is integrated into our everyday life to such an extent that most people take it for granted. However, the efforts to control friction date back to the early civilization (3500 B.C.) with the use of the wheel and lubricants to reduce friction in translational motion [2]. Today, friction is considered a part of the wider field *tribology* derived from the Greek word *Tribos* meaning “rubbing” and includes the science of friction, wear and lubrication [2]. The most compelling motivation to study tribology is ultimately to gain full control of friction and wear for various technical applications. Especially, reducing friction is of great interest as this has tremendous advantages for energy efficiency. It has been reported that tribological problems have a significant potential for economic and environmental improvements [3]:

“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.” [4].

On the other hand, the reduction of friction is not the only sensible application for tribological studies. Controlling frictional properties, besides minimization, might be of interest in the development of a grasping robot where finetuned object handling is required. While achieving a certain “constant” friction response is readily obtained through appropriate material choices, we are yet to unlock the full capabilities to alter friction dynamically on the go. One example from nature inspiring us to think along these lines are the gecko feet. More precisely, the Tokay gecko has received a lot of attention in scientific studies aiming to unravel the underlying mechanism of its “togglable” adhesion properties. Although geckos can produce large adhesive forces, they retain the ability to remove their feet from an attachment surface at will [5]. This makes the gecko able to achieve a high adhesion on the feet when climbing a vertical surface while lifting them for the next step remains relatively effortless. For a grasping robot, we might consider an analog frictional concept of a surface material that can change from slippery to rough on demand depending on specific tasks; Slippery and smooth when interacting with people and rough and firmly gripping when moving heavy objects.

In recent years an increasing amount of interest has gone into the studies of the microscopic origin of friction, due to the increased possibilities in surface preparation and the development of nanoscale experimental methods. Nano-friction is also of great concern for the field of nano-machining where the frictional properties between the tool and the workpiece dictate machining characteristics [3]. With concurrent progress in computational capacity and development of Molecular Dynamics (MD), numerical investigations serve as an invaluable tool for getting insight into the nanoscale mechanics associated with friction. This simulation-based approach can be considered as a “numerical experiment” enabling us to create and probe a variety of high-complexity systems which are still out of reach for modern experimental methods.

In materials science such MD-based numerical studies have been used to explore the concept of so-called *metamaterials* where material compositions are designed meticulously to enhance certain physical properties [6–

11]. This is often achieved either by intertwining different material types or removing certain regions completely. In recent papers by Hanakata et al. [6, 7] numerical studies have showcased that the mechanical properties of a graphene sheet, yield stress and yield strain, can be altered through the introduction of so-called *kirigami* inspired cuts into the sheet. Kirigami is a variation of origami where the paper is cut additionally to being folded. While these methods originate as an art form, aiming to produce various artistic objects, they have proven to be applicable in a wide range of fields such as optics, physics, biology, chemistry and engineering [12]. Various forms of stimuli enable direct 2D to 3D transformations through folding, bending, and twisting of microstructures. While original human designs have contributed to specific scientific applications in the past, the future of this field is highly driven by the question of how to generate new designs optimized for certain physical properties. However, the complexity of such systems and the associated design space make for seemingly intractable problems ruling out analytic solutions.

Earlier architecture design approaches such as bioinspiration, looking at gecko feet for instance, and Edisonian, based on trial and error, generally rely on prior knowledge and an experienced designer [9]. While the Edisonian approach is certainly more feasible through numerical studies than real-world experiments, the number of combinations in the design space rather quickly becomes too large for a systematic search, even when considering the computation time on modern-day hardware. However, this computational time constraint can be relaxed by the use of machine learning (ML) which has proven successful in the establishment of a mapping from the design space to physical properties of interest. This gives rise to two new styles of design approaches: One, by utilizing the prediction from a trained network we can skip the MD simulations altogether resulting in an *accelerated search* of designs. This can be further improved by guiding the search accordingly to the most promising candidates, for instance, as done with the *genetic algorithm* based on mutation and crossing of the best candidates so far. Another more sophisticated approach is through generative methods such as *Generative Adversarial Networks* (GAN) or diffusion models with the latter being used in state-of-the-art AI systems such as OpenAI's DALL-E2 or Midjourney **SOURCE?**. By working with a so-called *encoder-decoder* network structure, one can build a model that reverses the prediction process. That is, the model predicts a design from a set of physical target properties. In the papers by Hanakata et al both the *accelerated search* and the *inverse design* approach was proven successful to create novel metamaterial kirigami designs with the graphene sheet.

Hanakata et al attribute the variety in yield properties to the non-linear effects arising from the out-of-plane buckling of the sheet. Since it is generally accepted that the surface roughness is of great importance for frictional properties it can be hypothesized that Kirigami-induced out-of-plane buckling can also be exploited for the design of frictional metamaterials. For certain designs, we might hope to find a relationship between the stretching of the sheet and frictional properties. If significant, this could give rise to an adjustable friction behavior beyond the point of manufacturing. For instance, the grasping robot might apply such a material as artificial skin for which stretching or relaxing of the surface could result in a changeable friction strength.

In addition, the Kirigami graphene properties can be explored through a potential coupling between the stretch and the normal load, through a nanomachine design, with the aim of altering the friction coefficient. This invites the idea of non-linear friction coefficients which might in theory also take on negative values. The latter would constitute a rarely found property which is mainly found for the unloading phase of adhesive surfaces [13] or for the loading phase of particular heterojunction materials [14, 15]

To the best of our knowledge, Kirigami has not yet been implemented to alter the frictional properties of a nanoscale system. However, in a recent paper by Lieferrink et al. [16] it is reported that macroscale kirigami can be used to dynamically control the macroscale roughness of a surface through stretching. They reported that the roughness change led to a changeable frictional coefficient by more than one order of magnitude. This supports the idea that Kirigami designs can be used to alter friction, but we believe that taking this concept to the nanoscale regime would involve a different set of underlying mechanisms and thus contribute to new insight in this field.

1.2 Goals

In this thesis, we investigate the possibility to alter the frictional properties of a graphene sheet through the application of Kirigami-inspired cuts and stretching of the sheet. With the use of molecular dynamics (MD) simulations, we evaluate the frictional properties of various Kirigami designs under different physical conditions. With the use of machine learning (ML), we perform an accelerated search of designs to explore new designs. The main goals of this thesis can be summarized as follows.

1. Design an MD simulation procedure to evaluate the frictional properties of a Kirigami graphene sheet under specified physical conditions.
2. Develop a numerical framework for creating various Kirigami designs, both by seeking inspiration from macroscale designs and by the use of a random walk based algorithm.
3. Investigate the frictional behavior under varying load and stretch for different Kirigami designs.
4. Develop and train an ML model to predict the MD simulation result and perform an accelerated search of new designs for the scope of optimizing certain frictional properties.

1.3 Contributions

What did I actually achieve Include Github link

1.4 Thesis structure

In ?? : Background Theory, we cover the theoretical background related to Friction (??), Molecular Dynamics (??) and Machine Learning (??).

In ?? : Friction, we introduce the most relevant theoretical concepts of friction through a division by scale: Macroscale (??), Microscale (??) and nanoscale (??). We emphasize the nanoscale since this is of the most importance for our study. This is followed by a summary of relevant experimental and numerical results ?? and a more formal specification of our research questions (??).

In ?? : Molecular Dynamics, we introduce the main concepts related to the simulations used in this thesis. The main parts involve a description of the potentials used (??), the numerical solutions (??) and the modeling of temperature (??).

In ?? : Machine Learning, we introduce the basics of machine learning through a general presentation of the neural network ?? followed by the convolutional network (??) which we will use in our study. Additionally, we discuss a strategy for choosing model hypertuning (??) and a simple approach for model prediction explanations (). Finally, we introduce a version of the genetic algorithm applicable for accelerated search based on a machine learning model (??).

In ?? : Simulations, we define our numerical procedure and present and discuss the main findings of this thesis.

In ?? : System, we ...

In ?? : Pilot study, we ...

In ?? : XXX ...

In ?? : XXX, ...

The thesis is summarized in ??

Additional figures are shown in ??, ?? and ??. get appendix with only letter A., B. and C.

Part I

Background Theory

Part II

Simulations

Chapter 2

Pilot study

Having defined our system, we carry out an initial study of the frictional properties. First, we evaluate the numerical results for a non-cut sheet in order to define suitable metrics for a numerical evaluation of friction and justify some of the default parameter choices. This provides a basis for the following study where we consider the Tetrahedron and Honeycomb Kirigami patterns as well. We conduct a more systematic investigation of the friction dependencies to temperature, sliding speed, spring constant and timestep. Finally, we consider the mean friction of all three configurations when stretched. This includes an analysis of the dependence to contact area and the friction-load curves.

2.1 Friction simulation parameters

The MD simulations we will carry out to measure friction are governed by a small set of parameters. For the purpose of creating a machine learning we need to standardize these parameters. This we keep most of them constant with only a small subset of parameters being varied: sheet configuration, strain and load. Instead of starting with the parameter selection process, we first state the final choice in ?? . Due to the great number of parameters, we do not make an exhaustive search of all parameters before deciding on the final settings. Instead, we take a basis in parameters used in similar friction simulations [17–21] and adjust accordingly to the aim of getting stable measurements and reducing computation time where possible. Parameters such as initial relaxation time, pauses and strain speed are chosen mainly from the results of initial stability tests. The sheet and pull block sizes are chosen with a consideration of the balance between Kirigami design options and computational resources. The scan direction is chosen to be parallel to the connection line between the pull blocks. This is mainly chosen in order to avoid unnessecary complexity in the motion since it can be hypethesized that the center of the sheet can drag behind for other scan directions. The remaining parameters: Temperature T , sliding speed v_{slide} , spring constant K , normal load F_N , timestep dt and sliding distance have been chosen because the friction output remains relatively stable with moderate perturbations around these default values. We will explain this in more detail later in the chapter. Note that the default values in ?? will be used when nothing else is stated explicitly.

Table 2.1: Parameters involved for the numerical MD simulation for measuring friction. The default values correspond to the final choice used for the dataset. The shaded cells denote the parameters varied in the ML dataset.

Parameter	Default value	Description
T	300 K	Temperature of the system.
v_{slide}	20 m/s	Sliding speed for the sheet translation.
K	∞	Spring constant for the coupling between the virtuel atom and the sheet pull blocks.
Scan direction	$(x, y) = (0, 1)$ (zigzag direction)	The direction for which we translate the sheet.
Sheet configuration	Contiguous	Binary mapping describing which atoms are removed (0) and which is still present (1) in the graphene sheet.
Strain amount	[0, rupture]	The ratio of change in length to the original length.
F_N	[0.1, 10] nN	Applied normal force to the pull blocks.
dt	1 fs	MD integration timestep.
Initial relaxation time	15 ps	Initial relaxation time before straining.
Pauses	5 ps	Relaxation pauses after strain, and during the normal load phase (before translating the sheet).
Strain Speed	0.01 ps^{-1}	The rate of straining for the sheet.
Slide distance	400 Å	How far the sheet is translated.
Sheet size	$130.029 \times 163.219 \text{ Å}$	Spatial 2D size of the sheet.
Pull block size	$2 \times 130.029 \times 15.183 \text{ Å}$	Spatial 2D size of the pull blocks.

2.2 Force traces

We begin by assessing the friction force traces, i.e. force vs. time curves, for a single friction simulation using the default parameters shown in ?? for a non-cut sheet with no stretch applied and a normal load of 1 nN.

2.2.1 Force oscillations

We evaluate the friction force as the force acting on the sheet from the substrate. We consider initially the force component F_{\parallel} parallel to the drag direction as plotted in ?. We use a sample rate of $10 \text{ ps}^{-1} = 100 \text{ timesteps}^{-1}$ for which each sample is the mean value of the preceding 100 timesteps. We observe immediately that the data carries oscillations on different time scales which match our general expectations for sliding involving periodic surfaces. By applying a Savgol filter to the data with a polynomial order of 5 and a window length of 150 timesteps (corresponding to a sliding distance of 3 Å or a time window of 15 ps) we can qualitatively point out at least two different frequencies of oscillation. During the first 10 Å of sliding, seen in ?, we see roughly three waves on the Savgol filter corresponding to a relatively high frequency, while for the duration of 100 Å of sliding, seen in ?, the same Savgol filter reveals a lower frequency on top, creating the visual pattern of a wavepacket. The data does not indicate clear signs of stick-slip behavior as otherwise found in other studies, e.g. by Zhu and Li [20] for graphene on gold, who saw a more typical saw tooth shape in the force trace. Besides the difference in the substrate material, using gold instead of silicon, they used a lower sliding speed of 10 m/s and a soft spring of $K = 10 \text{ N/m}$. By adopting these parameters we get a slightly different force trace behavior as shown in ? and ?. This change breaks the symmetry in the force oscillations but still does not produce any significant discontinuities in the trace. By keeping the spring constant $K = 10 \text{ N/m}$ and lowering the sliding speed further down to 1 m/s we are able to demonstrate a proper stick-slip behavior as shown in ? and ?. Considering all three simulations we might classify the results from the default settings, $K = \infty, v = 20 \text{ m/s}$, as smooth sliding, $K = 10 \text{ N/m}, v = 10 \text{ m/s}$, as a transition phase with possible occasional slipping, and $K = 10 \text{ N/m}, v = 1 \text{ m/s}$ as certain stick-slip behaviour. This confirms the qualitative observation the stick-slip behavior is suppressed

with stiff springs [22] springs and high sliding velocity [19]. Having a low sliding speed comes with a high computational cost which is the reason that we choose a relatively high sliding speed of 20 m/s. The choice of an infinite spring constant is related to the stability of the measurements and is discussed later in this chapter **make sure it is, maybe make a reference.**

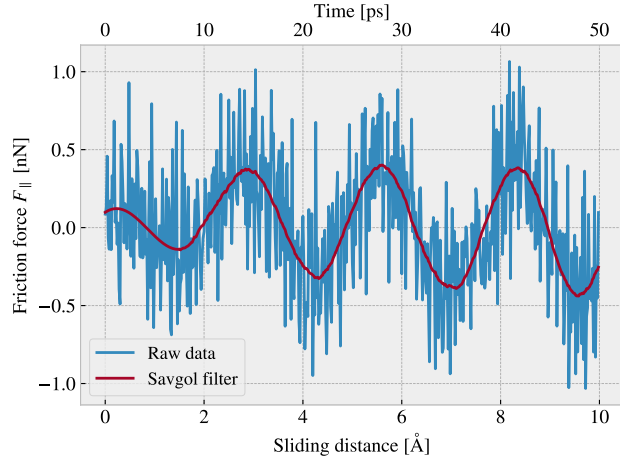
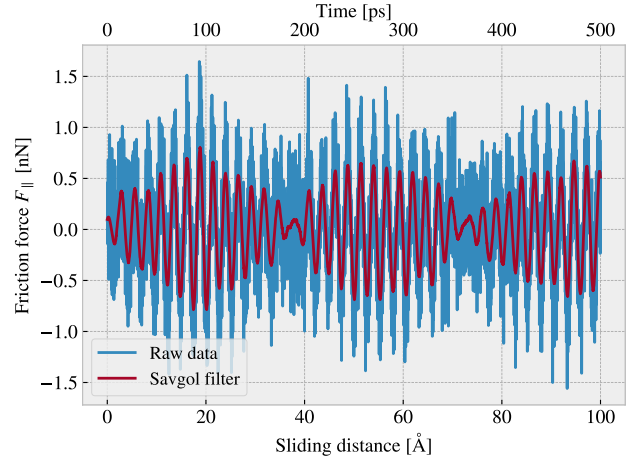
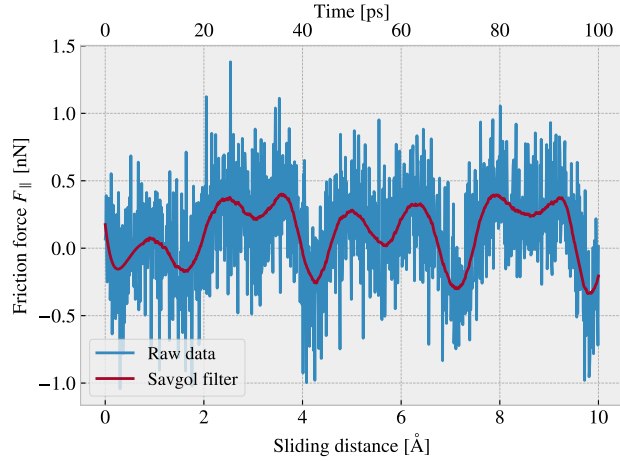
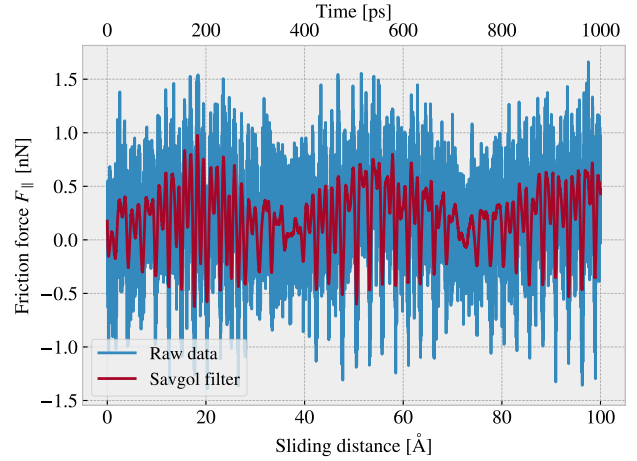
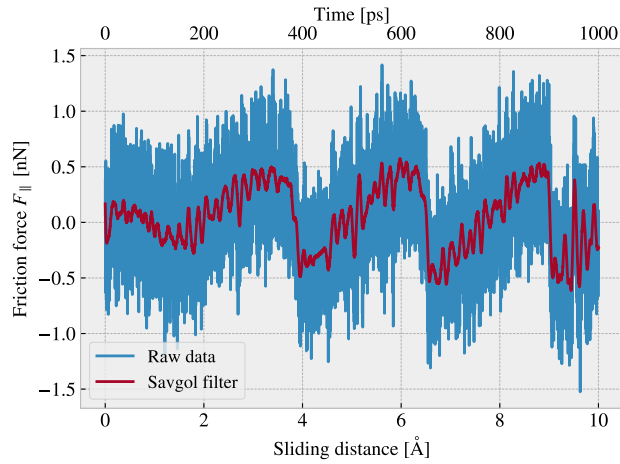
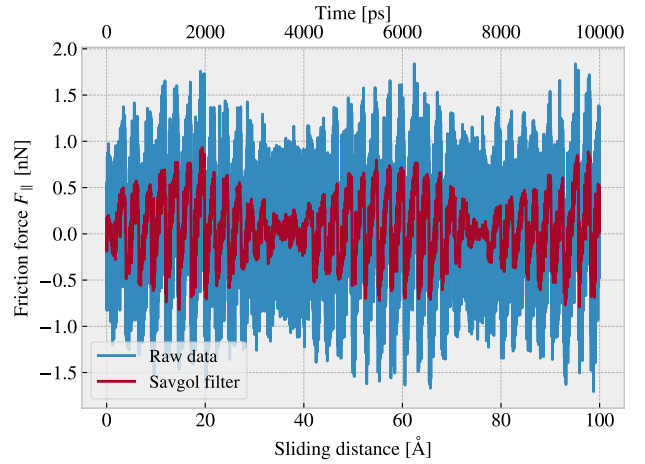
(a) $K = \text{inf}$, $v = 20 \frac{\text{m}}{\text{s}}$ (10 Å sliding).(b) $K = \text{inf}$, $v = 20 \frac{\text{m}}{\text{s}}$ (100 Å sliding).(c) $K = 10 \frac{\text{N}}{\text{m}}$, $v = 10 \frac{\text{m}}{\text{s}}$ (10 Å sliding).(d) $K = 10 \frac{\text{N}}{\text{m}}$, $v = 10 \frac{\text{m}}{\text{s}}$ (100 Å sliding).(e) $K = 10 \frac{\text{N}}{\text{m}}$, $v = 1 \frac{\text{m}}{\text{s}}$ (10 Å sliding).(f) $K = 10 \frac{\text{N}}{\text{m}}$, $v = 1 \frac{\text{m}}{\text{s}}$ (100 Å sliding).

Figure 2.1: Force traces of the friction force F_{\parallel} with respect to the drag direction acting from the substrate on the full sheet. The force traces are plotted against the sliding distance (lower x-axis) and the corresponding sliding time (upper x-axis). The sliding distance is measured by the displacement of the virtual atom tethering the sheet. The red line represents a Savgol filter with polynomial order 5 and a window length of 150 timesteps (corresponding to a sliding distance of 3 Å or a time window of 15 ps). Each row, (a,b), (c,d), (e,f), represents a different choice of the spring constant K and sliding speed v , while the columns show the same result for two different time scales. The default settings are represented in figure (a) and (b).

By performing a Fourier Transform on the data, using the default parameters, we can quantify the leading frequencies observed in figure ?? and ?. The Fourier transform is shown in ??, and by plotting the two most dominant frequencies $f_1 = 0.0074 \text{ ps}^{-1}$ and $f_2 = 0.0079 \text{ ps}^{-1}$ as a sine sum, $\sin(2\pi f_1) + \sin(2\pi f_2)$, we find a qualitatively convincing fit to the observed wavepacket shape as seen in ?. We can convert the frequencies according to that of a wavepacket. By using the trigonometric identity

$$\begin{aligned}\sin(a+b) &= \sin(a)\cos(b) + \cos(a)\sin(b), \\ \sin(a-b) &= \sin(a)\cos(b) - \cos(a)\sin(b),\end{aligned}$$

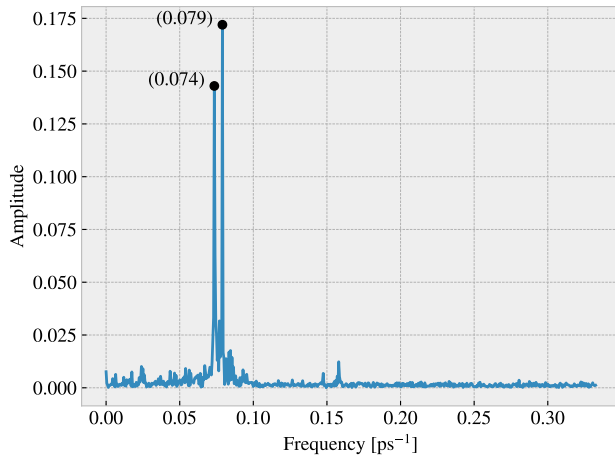
and decomposing the frequencies as $f_1 = a - b$, $f_2 = a + b$, we can rewrite the sine sum as the sinusoidal product

$$\begin{aligned}\sin(2\pi f_1) + \sin(2\pi f_2) &= \sin(2\pi(a-b)) + \sin(2\pi(a+b)) \\ &= \sin(2\pi a)\cos(2\pi b) + \cos(2\pi a)\sin(2\pi b) + \sin(2\pi a)\cos(2\pi b) - \cos(2\pi a)\sin(2\pi b) \\ &= 2\sin(2\pi a)\cos(2\pi b),\end{aligned}$$

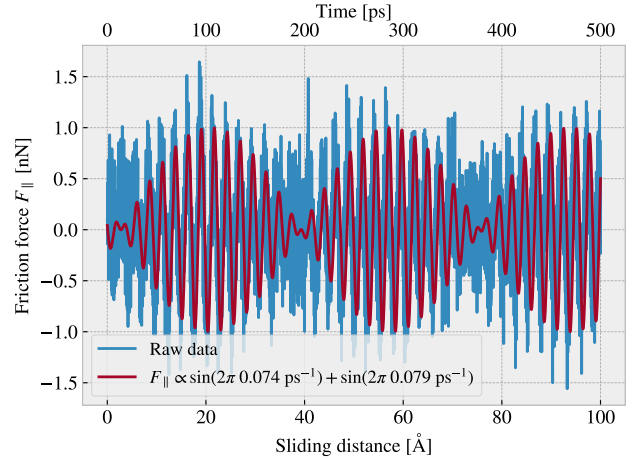
with

$$\begin{aligned}a &= \frac{f_1 + f_2}{2} = 0.0763 \pm 0.0005 \text{ ps}^{-1}, & b &= \frac{f_2 - f_1}{2} = 0.0028 \pm 0.0005 \text{ ps}^{-1}, \\ &= 0.381 \pm 0.003 \text{ \AA}^{-1}, & &= 0.014 \pm 0.003 \text{ \AA}^{-1}.\end{aligned}$$

In the latter transition, we have denoted the frequency with respect to the sliding distance by considering the default sliding speed of $20 \text{ m/s} = 0.2 \text{ \AA/ps}$. This makes us recognize the high oscillation frequency as a and the low frequency as b . The faster one has a period of $T_a = 2.62 \pm 0.02 \text{ \AA}^{-1}$ which corresponds well with the magnitude of the lattice spacing and especially that of graphene at 2.46 \AA as expected theoretically. The longer period $T_b = 71 \pm 15 \text{ \AA}$ is not obviously explained. We notice a similarly long period oscillation for all three cases ??, ?? and ??, and thus we have no reason to believe that this is dependent on the stick-slip behavior. The initial build-up in friction force is reminiscent of friction strengthening, which is often reported [17, 23], but the periodicity goes against this idea. Instead, we might attribute it to some phonon resonance which could be a physical phenomenon or simply a feature of our MD modeling.



(a) FT result shown for a reduced frequency range.



(b) Two most dominant frequencies applied to the data from ?.

Figure 2.2: Fourier transform analysis of the full friction force data (all 400 \AA sliding distance) shown in ?. (a) shows the two most dominant frequency peaks. Note that no significant peaks were found in a higher frequency than included here. (b) shows a comparison between the raw data and the wavefunction corresponding to the two peaks in figure (a).

¹The uncertainty Δy is calculated as $\Delta y = \left| \frac{\partial y}{\partial x} \Delta x \right|$ for uncertainty Δx and $y(x)$

2.2.2 Decompositions

In the previous analysis, we looked only at the friction force for the full sheet, including the rigid pull blocks, and with respect to the drag direction. We found this way of measuring the friction force to be the most intuitive and reliable, but we will present the underlying arguments for this choice in the following.

Since we are only applying cuts to the inner sheet, and not the pull blocks, it might appear more natural to only consider the friction inner sheet. If the desired frictional properties can be achieved by altering the inner sheet one can argue that any opposing effects from the pull blocks can be mitigated by simply scaling the relative size between the inner sheet and the pull blocks. However, when looking at the force traces decomposed with respect to the inner sheet and pull block regions respectively in ??, we observe that the friction force arising from those parts is seemingly antisymmetric. That is, the distribution of the frictional pull from the substrate on the sheet is oscillating between the inner sheet and the pull blocks. Keeping in mind that normal force is only applied to the pull blocks we might take this as an intrinsic feature of the system that does not necessarily disappear with a scaling of the spatial ratio between the inner sheet and pull blocks. Any interesting friction properties might depend on this internal distribution of forces. Hence, we hedge our bets and use the full sheet friction force as a holistic approach to avoid excluding relevant information in the measurement data.

Similarly, we might question the decision of only considering the frictional force projected onto the sliding direction as we are then neglecting the “side shift” induced during sliding. In ?? we show the decomposition in terms of the force components parallel F_{\parallel} and perpendicular F_{\perp} to the sliding direction respectively. We notice that the most dominant trend appears for the parallel component. If we want to include the perpendicular component as well we would have to evaluate friction as the length of the force vector instead. However, this would remove the sign of the force direction and shift the mean friction force up as we see both negative and positive contributions in the parallel force trace. One option to accommodate this issue is by using the vector length for the magnitude but keeping the sign from the parallel component. However, we omit such compromises as this might make the measurement interpretation unnecessarily complex, and we use only the parallel component going forward.

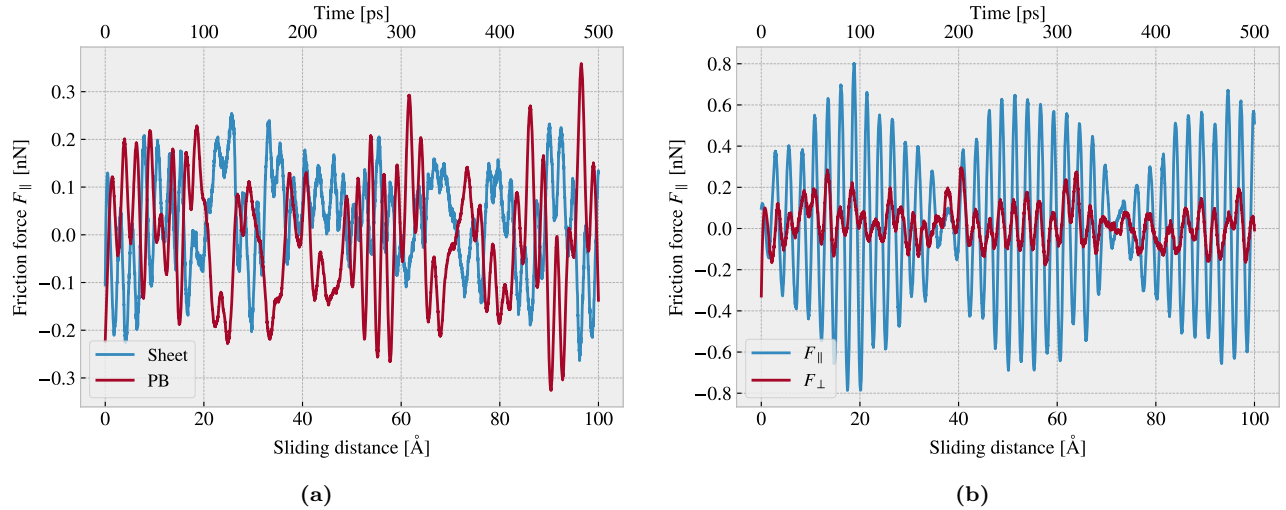


Figure 2.3: Friction force decomposition on the default parameter force trace shown in ?? showing only the applied Savgol filters. (a) Decomposition into group inner sheet (sheet) and pull blocks (PB). (b) Decomposition into parallel (F_{\parallel}) and perpendicular (F_{\perp}) to drag sliding direction.

2.2.3 Center of mass path

From the previous observations of the force traces in ?? we found both smooth sliding and stick-slip behavior depending on the sliding speed and spring constant. Considering the force decomposition in ?? we know that a frictional force in the perpendicular direction to sliding is also present. By looking at the x, y -position for the sheet Center of Mass (CM) we find a qualitatively different behavior when reconsidering the spring constants and sliding speeds investigated in ??. These results are shown in ??. The default case in ?? shows a rather straight path forward with only a small side motion in comparison to the cases in ?? and ??. However, the CM accelerates

and deaccelerates with a high frequency, much too high to be associated with the lattice spacing on the order of 2.46 \AA . One possible explanation is that the sheet and substrate constitute an incommensurable contact for which traveling kink excitations make the atoms move in such a way that the sheet CM is incremented in small “burst”. When looking at the $K = 10 \frac{\text{N}}{\text{m}}$, $v = 10 \frac{\text{m}}{\text{s}}$ case in ?? we see a completely different CM path where the rapid movements aligns visually better with the force oscillations shown earlier in ?. The CM accelerates forward and then deaccelerates in combination with a side motion that leads to the CM path making a loop as it slows down. Finally we have the $K = 10 \frac{\text{N}}{\text{m}}$, $v = 10 \frac{\text{m}}{\text{s}}$ in ?? which is confirmed to have stick-slip behavior in ?. Here the CM path shows a more chaotic movement between acceleration, but with the rapid parts aligning which also visually well with the timing of the slips seen in ?. The chaotic motion is not connected to the stick-slip motion, but we might associate it with the thermal contributions being dominant in this regime.

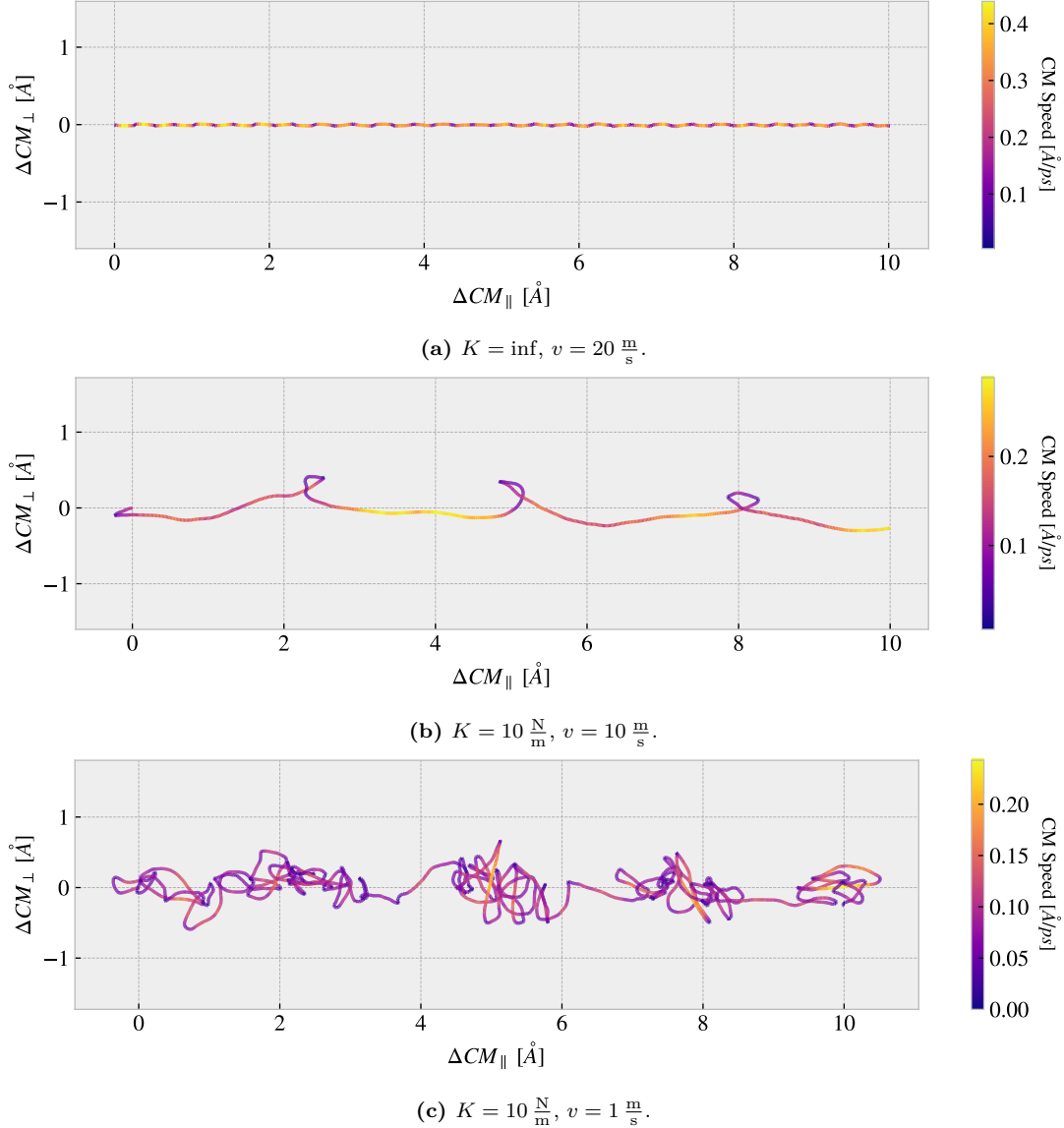


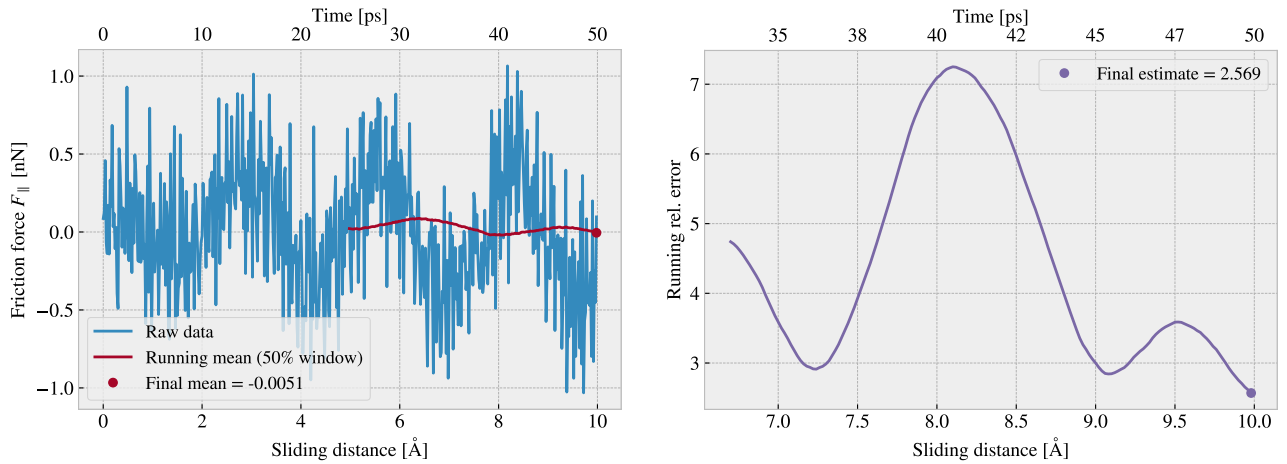
Figure 2.4: Center of Mass (CM) position relative to the start of the sliding phase in terms of the direction parallel to the sliding direction ΔCOM_{\parallel} and the axis perpendicular to the sliding direction ΔCOM_{\perp} . The colorbar denotes the absolute speed of the CM motion. Figure a-c shows different parameters used for the spring constant K and sliding speed v similar to that used in ?. (a) Default: $K = \text{inf}$, $v = 20 \frac{\text{m}}{\text{s}}$. (b) $K = 10 \frac{\text{N}}{\text{m}}$, $v = 10 \frac{\text{m}}{\text{s}}$. (c) $K = 10 \frac{\text{N}}{\text{m}}$, $v = 1 \frac{\text{m}}{\text{s}}$.

2.3 Defining metrics for friction

In order to evaluate the frictional properties of the sheet we aim to reduce the force trace results, addressed in section ??, into single metrics describing the kinetic and static friction respectively.

2.3.1 Kinetic friction

We measure kinetic friction as the mean of the friction force trace. More precisely, we take the mean value of the last half of the dataset in order to ensure that we are sampling from a stable system. For a full sliding simulation of 400 Å our mean value will be founded on the last 200 Å (1000 ps) of sliding. In ?? we have shown the force trace for the first 10 Å of sliding together with a 50% running mean window. The choice of such a short sliding distance is merely to illustrate the sampling procedure, and we see that the final mean estimate (marked with a dot) takes a negative value due to the specific cut-off of the few oscillations captured here. Nonetheless, one approach to quantify the uncertainty of the final mean estimate is to consider the variation of the running mean preceding the final mean value. The more the running mean fluctuates the more uncertainty associated with the final estimate. Only the running mean “close” to the ending should be considered, since the first part will rely on data from the beginning of the simulation. From the Fourier analyze in section ?? we found the longest significant oscillation period to be ~ 71 Å. Hence, we find it reasonable to use the standard deviation (std) for the last ~ 71 Å of the running mean window to evaluate the fluctuations. When including the full sliding length this corresponds to the last $\sim 35\%$ of the running mean window. We consider the std as an estimate of the absolute error and calculate the relative error by a division of the final mean value. In ?? we showcase a running relative error based on the std, with a window of length 35% the mean window, in a continuation of the illustrative case of a 10 Å sliding from ??. In this case, we get an extremely high relative error of $\sim 257\%$, but this is consistent with the fact that the short sampling period leads to an unphysical negative value which should be associated with high uncertainty.



(a) Running mean with window length 5 Å (50% the data length). (b) Running std with window length 1.75 Å (35% the mean window length.)

Figure 2.5: Running mean (a) and running relative error (std) (b) on the friction force data from a reduced sliding distance of 10 Å. The running mean window is 50% the data length while the running std window is 35% the running mean window length. The values are plotted at the end of their respective windows such that window precedes the actual point on the graph.

When including the full dataset of 400 Å of sliding, such that the std window actually matches with the longest period of oscillations expected, we get a final relative error of $\sim 12\%$ as shown in fig ??. This is arguable just at the limit of an acceptable error, but as we shall see later on in ?? this high relative error is mainly associated with the cases of low friction. When investigating different configurations under variation of load and strain we see a considerably lower relative error as the mean friction evaluates to higher values. One interpretation of this finding is simply that the oscillations in the running mean are to some degree independent of the magnitude of

the friction. In that case, the relative error will spike for the low friction cases, and the absolute error might be the more reliable measure, i.e. using simply the std without dividing by the final mean value.

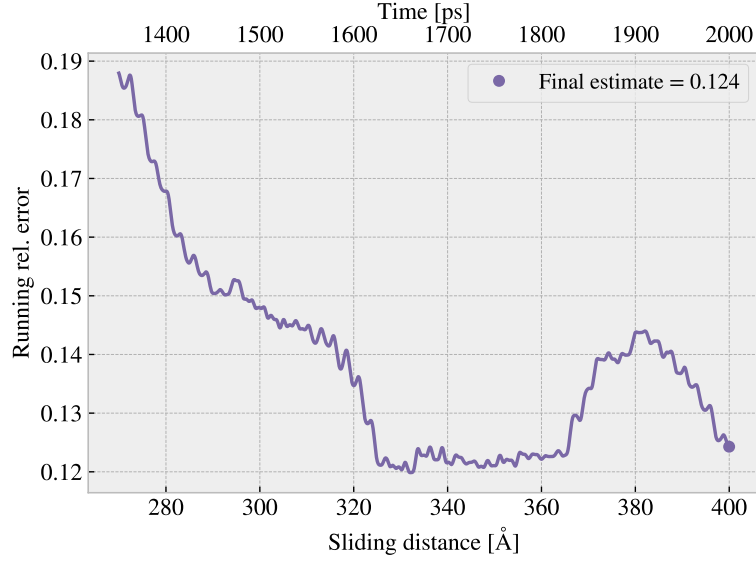


Figure 2.6: Running standard deviation (std) for a full 400 Å sliding simulation. The running std window is 70 Å (35% the running mean window of 50% the data length).

2.3.2 Static friction

The maximum value is one of the common choices for addressing static friction, even though the definition of static friction is a bit vague. When considering the force traces in ?? we observe that the force oscillations increase in magnitude toward a global peak at ~ 20 Å. Thus, one could be inclined to identify this peak as the maximum value associated with the static friction force. However, as we have already clarified, this steady increase in friction is part of a slower oscillation that repeats by a period of ~ 71 Å. By plotting the top three max values recorded during a full 400 Å simulation, for 30 logarithmically spaced load values in the range $[0.1, 100]$ nN, we observe that the global max rarely falls within this first oscillation period as shown in ?. Only 2 out of 30 global maxima and 4 out of 90 top three maxima can be associated with the start of the sliding by this definition. Thus, this result suggests that our default system does not yield a static friction response in the sense of an initial increase in friction due to a depinning of the sheet from the static state. Some parameter changes that might increase the likelihood of seeing a significant static friction response are either extending the relaxation period since static friction is theorized to increase logarithmically with time [24], or increasing the sliding force more slowly through a soft spring tethering. As an attempt to test the latter part of this hypothesis we run a series of simulations with varying spring constant, $K \in [5, 200]$ nN including also $K = \infty$, but keeping the relaxation time and sliding speed at the default values. The result is shown in ? and do not show any support for the hypothesis that a softening of the spring constant will eventually lead to the friction maximum occurring in the first period of sliding. We note that this might be suppressed by having a too short relaxation period or a too high sliding speed (related to the initial force increase), but due to the ambiguousness in the assessment of the static friction we will mainly concern ourselves with the kinetic friction in the remaining of this thesis.

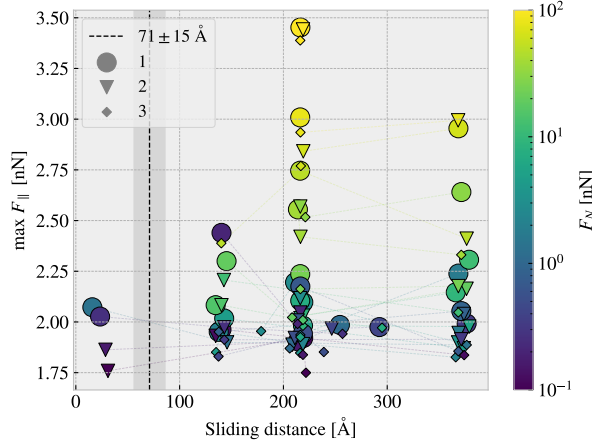


Figure 2.7: Distribution of top three max friction force peaks for 30 uniformly sampled normal forces $F_N \in [0.1, 10]$ nN. The dotted line and the grey area mark the slowest significant oscillation period found in the data and thus marking a dividing line for whether a peak falls within the “beginning” of the sliding simulation.

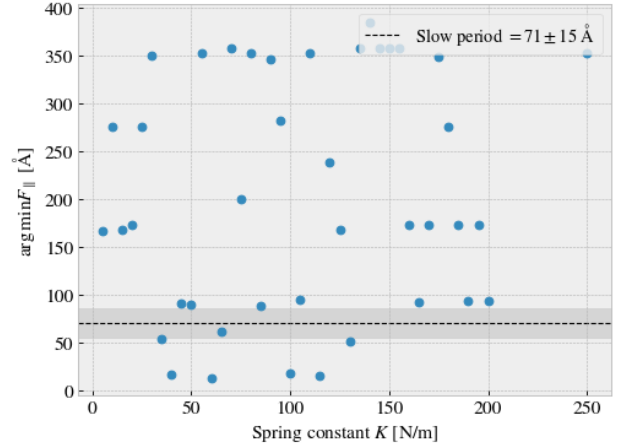


Figure 2.8: Sliding displacement for the max friction peak to appear as a function of spring constant. **Fixmove is tmp mapped to $K = 200$ here without any discontinuous lines.**

2.4 Out-of-plane buckling

The out-of-plane buckling is one of the motivations for investigating the application of Kirigami cuts in the context of friction properties. Therefore, we perform a stretch simulation, at low temperature ($T = 5$ K) without any substrate, in order to verify that we can reproduce an out-of-plane buckling with the Tetrahedron and Honeycomb patterns intended for our study (see ??). For this investigation we consider the Tetrahedron (7, 5, 1) and the Honeycomb (2, 2, 1, 5) pattern in comparison to the non-cut sheet. We quantify the out-of-plane buckling by assessing the distribution of atoms along the z-direction (perpendicular to the plane) during stretching. We calculate the minimum and maximum z-value as well as the atom count quartiles 1%, 10%, 25%, 50% (median), 75%, 90% and 99% as shown in ??. The results show significant buckling for the Tetrahedron and Honeycomb patterns in comparison to the non-cut sheet which only exhibits minor buckling of ~ 2 Å which is on the same order as the lattice spacing. Moreover, we notice that the Tetrahedron pattern buckles more in consideration to the min. and max. peaks while the remaining quartiles seem to be more closely spaced than for the Honeycomb. By addressing the simulation results visually, using the *Open Visualization Tool OVITO*, we find that this can be attributed to fringes on the edge “flapping around” and thus increasing the min. and max. values.

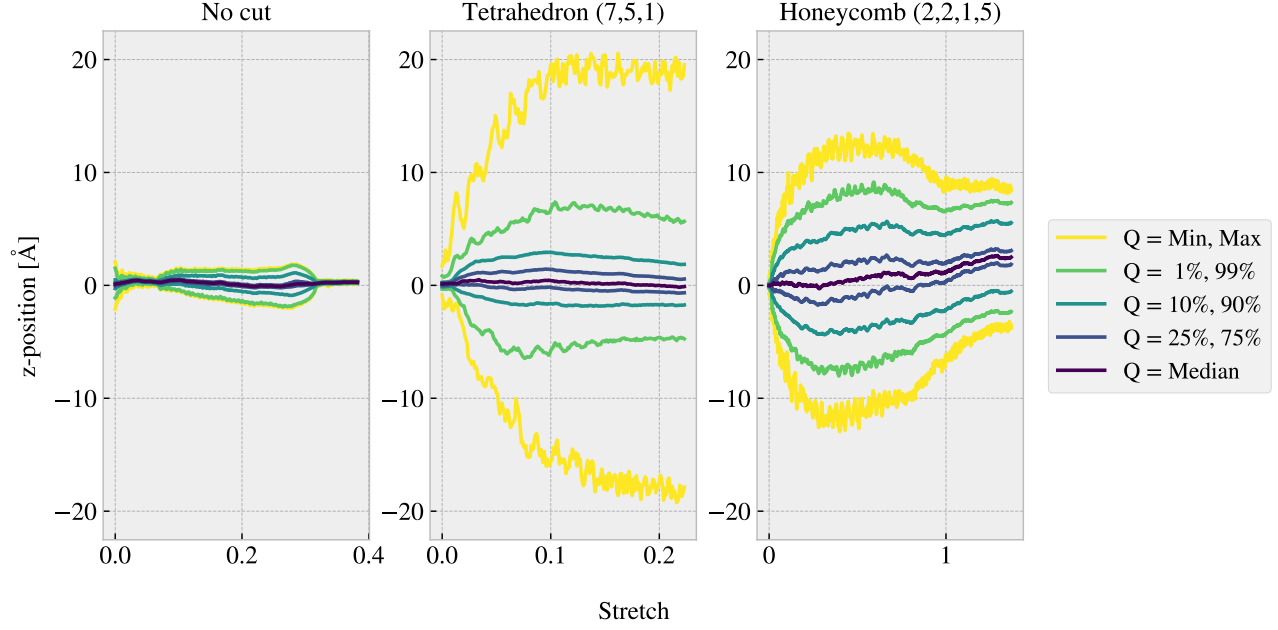


Figure 2.9: Out-of-plane buckling during stretching of the No cut, Tetrahedron (7, 5, 1) and Honeycomb (2, 2, 1, 5) sheet respectively in vacuum at low temperature $T = 5$ K. The buckling is measured by the distribution of the atom z-position (perpendicular to the sheet plane), for which the colors indicates selected quantiles. The yield strain were, reading from left to right, 0.38, 0.22 and 1.37.

Given the confirmation of out-of-plane buckling in a vacuum, as seen in ??, we reintroduce the substrate in order to investigate whether this effect carries over to a changing contact area. For this simulation we raise the temperature to the default value of $T = 300$ K. We keep the normal force off and let the sheet stick purely by the adhesion forces between the sheet and substrate. We quantify the contact area through the relative amount of atoms in the sheet within chemical range of the substrate. The cut-off for this interaction is set to 4 Å, inspired by [17], corresponding to $\sim 120\%$ the LJ equilibrium distance. Usually, the contact area is calculated as the number of contacting atoms multiplied by an associated area for each atom. However, since we are not interested in the absolute value of the area, but rather the relative change, we omit the multiplication factor. That is, we consider the relative number of atoms within the contact range, which is proportional to the contact area, as our metric of choice. The relative contact for the three configurations (No cut, Tetrahedron (7, 5, 1) and Honeycomb (2, 2, 1, 5)) during stretching are shown in figure ??. The figure reveals a significant drop in contact as the sheets are stretched, which agrees qualitatively with the buckling observed in ?? without the substrate. The Honeycomb pattern turns out to be both the most stretchable, with a rupture strain of 1.27, and the one with the biggest decrease in relative contact with a minimum of approximately 43%. Notice, that the relative contact is never actual 1.0 but instead reaches a maximum of 96% with no stretching. This is attributed to the temperature fluctuations and the choice of cut-off. Thus we might

Selected frames from the simulation result are shown in ?? which reveals a bit more information on how the buckling occurs. The Tetrahedron pattern deforms rather quickly and smoothly into small tetrahedron spikes, as the name suggests. In the Honeycomb pattern, on the other hand, the deformations initiate from one side first. As the sheet stretches more rows of the pattern are activated, producing the honeycomb-looking shape when seen from above. Both patterns exhibit a small increase in relative contact when they are approaching their yield strain, which agrees with the results from ?? where the buckling reduces slightly towards the rupture strain.

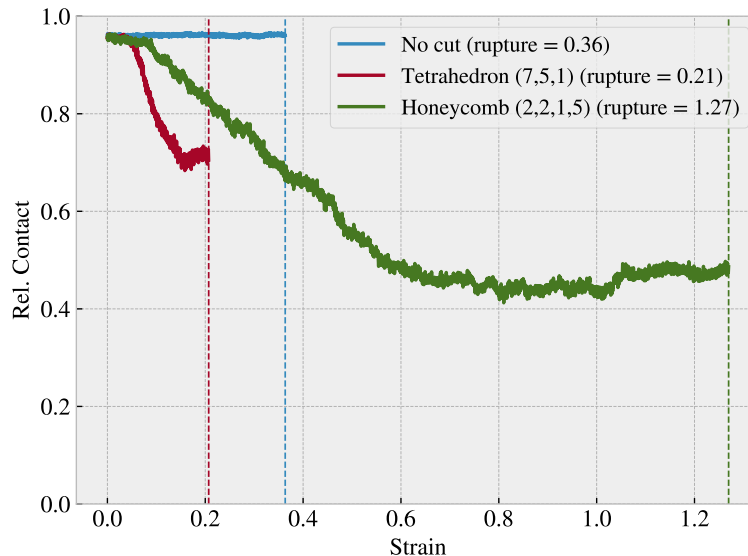


Figure 2.10: Relative contact, given as the relative number of atoms in the sheet being within chemical interaction range, vs. strain of the sheet. The cut-off for the interaction range is 4 \AA corresponding to $\sim 120\%$ the LJ equilibrium distance. No normal force is applied and temperature is kept at $T = 300 \text{ K}$.

Compare figure ?? to that of figure ?? where multiple simulations constitute the stretch-contact curve.

2.5 Investigating default parameters

We carry out a more extensive investigation of the friction dependence on temperature T , sliding speed v_{slide} , spring constant K , and timestep dt . This is done partly to understand how the dependencies relate to the theoretical, numerical and experimental results, and partly to understand how these parameters affect the stability of our system. We use the default parameters presented in ?? and investigate the results as we change parameters, one at a time. We keep the load at 1 nN . We consider the mean friction force, sampled from the last half of the simulation as described in ??, representing the kinetic friction. The results are shown in ??, where the shaded area (connected linearly) denotes the absolute error defined by the std as described in ??.

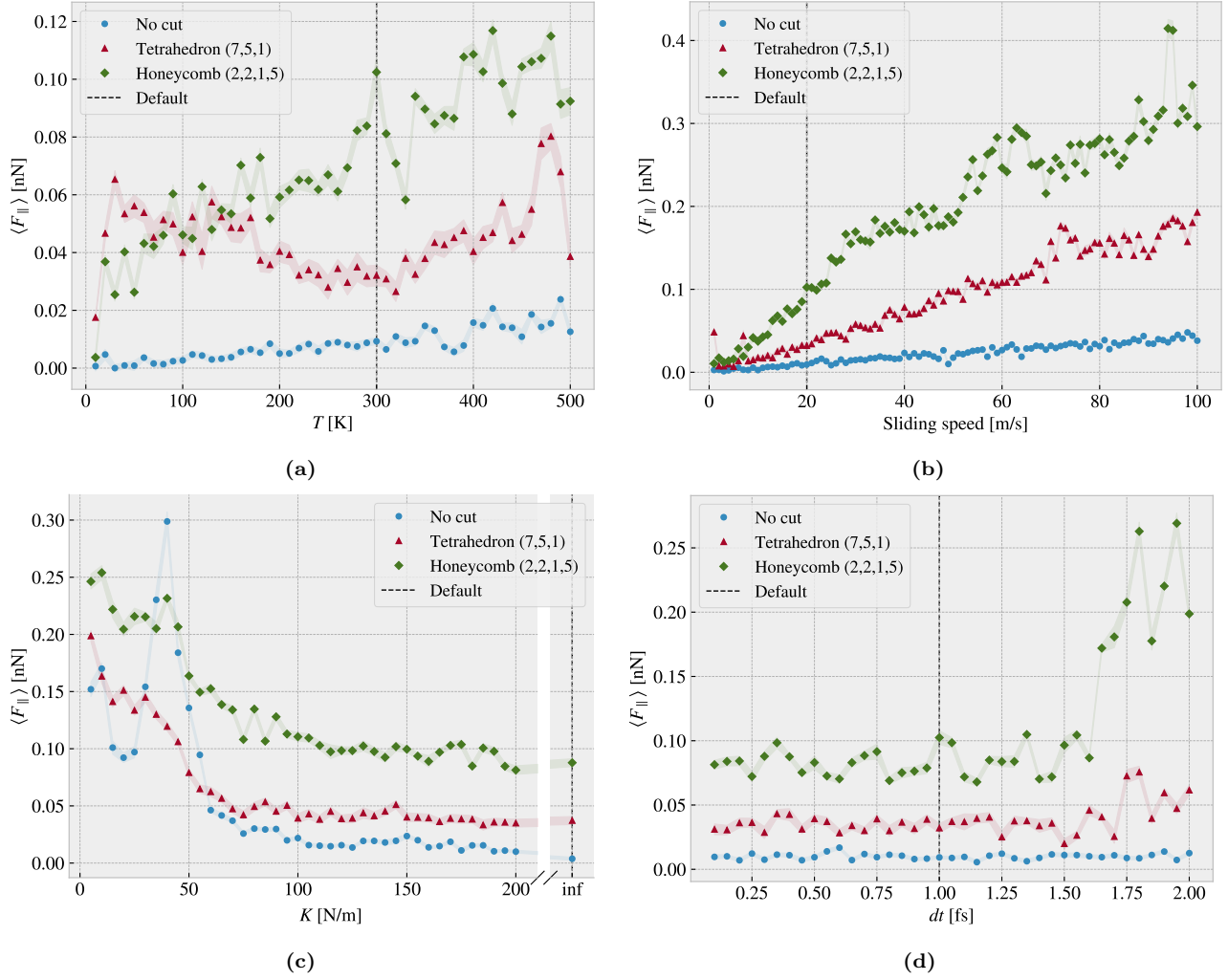


Figure 2.11: Main parameters investigation. Kinetic friction force

From the temperature investigation in ?? we find an increasing kinetic friction with temperature for both the non-cut sheet and the Honeycomb pattern. The Tetrahedron pattern shows both decreasing and increasing trends. The general trend shows a convex curve in the range (30–480 K) with a minimum around our default choice of 300 K, but with rapid fluctuations at the start (10–30 K) and end region (480–500 K). Similar fluctuations are also seen from the Honeycomb pattern, although it shows an underlying increasing trend throughout. When comparing the non-cut sheet and the Honeycomb pattern we observe that the slope for the increasing trend is high for the Honeycomb. From a theoretical and experimental point of view, we would expect a decrease in friction with temperature (see ??). However, an increasing trend is also observed in other MD simulation, for instance by Zhang et al. [21] sliding at 10 m/s, which is attributed to the high sliding speed associated with the ballistic motion. The default choice is initially based on the common choice of using the temperature $T = 300$ K. The non-cut and Tetrahedon friction seems to be rather stables around that point, but we do see some significant fluctuations for the Honeycomb pattern in this range. However, we do not regard this as a critical feature.

From the sliding speed investigation in ?? we generally find increasing friction with velocity. Due to the relatively high velocities used and the effects from the thermostat, we expect a viscous friction $F_k \propto v_{\text{sliding}}$ which matches rather well with these results. However, the Tetrahedron and Honeycomb sheets seem to fall slightly into a sublinear relationship as it approaches higher velocities. Furthermore, these sheets display indications of local fluctuations that could potentially be attributed to resonance effects, as discussed in relation to the phonon dynamics. Our choice of sliding speed at 20 m/s mainly reflects a consideration of computational cost, but the fact that no immediate resonance fluctuations appear in the proximity of this value supports the choice.

From the investigation of the spring constant parameter in ?? we observe a significant decrease in friction as the springs stiffen. This can be attributed to the transition from a stick-slip influenced regime to a smooth sliding regime as we saw for the force traces in ?. For soft springs the results are quite sensitive to the specific choice of spring constant which is especially seen for the non-cut sheet around $K = 40 \text{ N/m}$. Thus, in order to avoid this domain we settled for the infinitely stiff spring. This is also considered a more favorable option due to its ability to provide greater standardization of the simulations.

Finally, we consider the numerical stability of the result as we vary the simulation timestep in ?. The general trend shows a stable plateau below $\sim 1.5 \text{ fs}$ for which higher values show signs of arising instabilities for the cut sheets (Tetrahedron and Honeycomb). This mainly confirms that our choice of timestep is within a reasonable range. However, we do see some fluctuations which are more significant for the cut sheets.

The observed fluctuations suggest that randomness plays a role in our simulations and also indicate that the cut sheets are relatively unstable. Further investigation through varying the random seed for the initial velocity and thermostat could shed more light on this matter. In the meantime, we may consider these fluctuations as a sign that the uncertainty in our results is higher than what was estimated using the running mean and running std evaluation. For the Honeycomb sheet, these fluctuations are on the order $\pm 0.017 \text{ nN}$.

2.5.1 Computational cost

We run the simulations on a CPU cluster made available by the University of Oslo. This allows us to run multiple simulations at once and with each simulation running in parallel on multiple CPU cores as well. As we decide on the simulation parameters we must also consider the computational cost. When selecting simulation parameters, we also need to keep in mind the computational cost. Given that the chosen parameters will be applied to multiple simulations, any increase in computational time will be multiplied by the number of intended simulations, which is expected to be around 10,000. The computational cost is especially dependent on the timestep and the sliding speed as this will affect the number of computations. As an extension of the analysis in ?? we report on the computational times associated with temperature, sliding speed, spring constant and dt . By retrieving the computational time used for the parameter investigation in ?? we get the timing as shown in ?. Note that these timings are only based on a single simulation for each parameter as opposed to an average over multiple runs which is necessary for more reliable data.

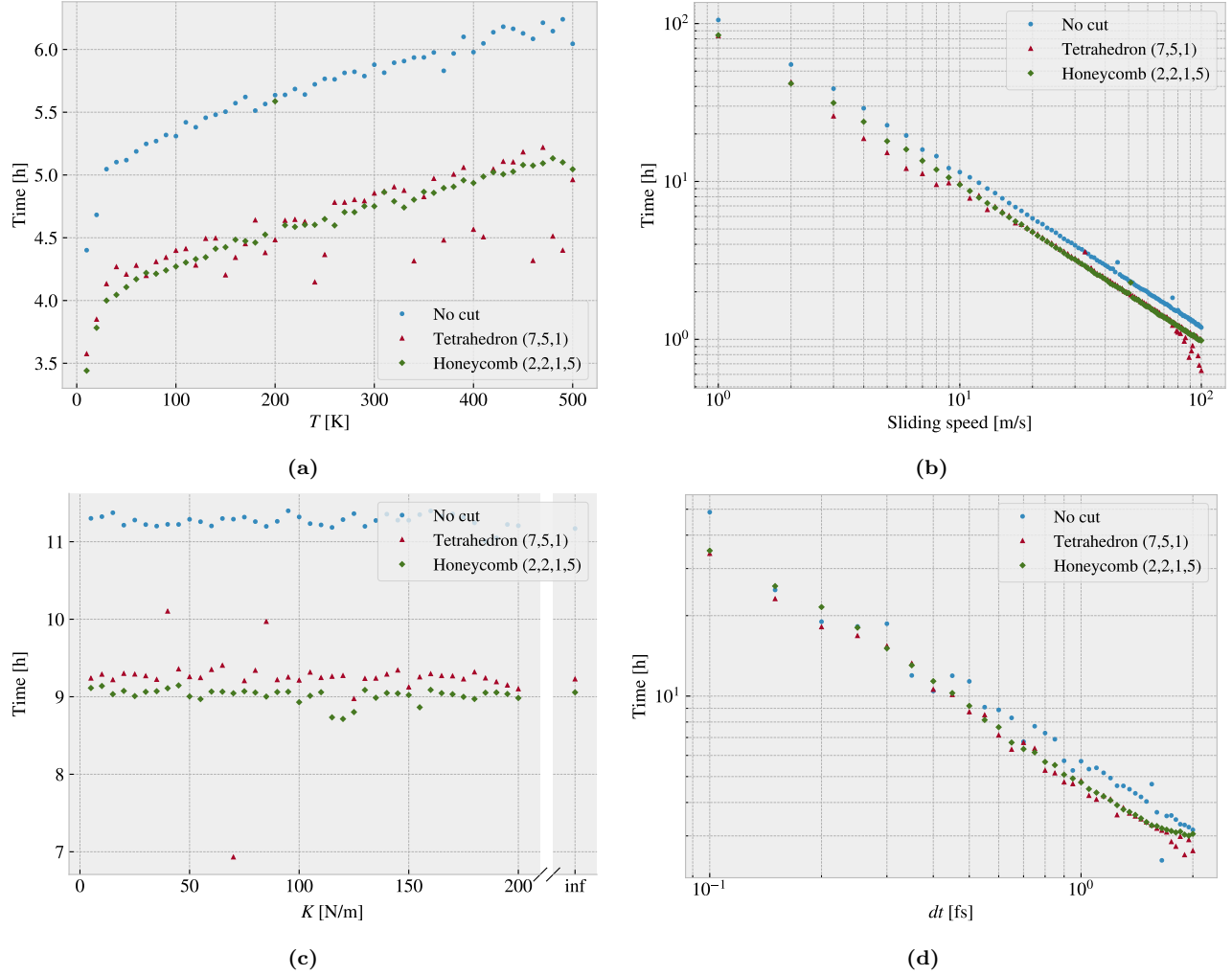


Figure 2.12: Computational cost related to temperature, sliding speed, spring constant and dt parameter in terms of CPU hours running on 16 cores on the cluster. Sliding speed follows $t \propto v^{-0.977 \pm 0.005}$ and dt follows $t \propto dt^{-0.87 \pm 0.02}$

The computational time is governed by the number of timesteps in the simulation and the time used per timestep. For a fixed sliding distance, the number of timesteps in the simulation are inversely proportional to sliding speed and similar inversely proportional to timestep dt . From the timings in ?? we find the sliding speed to obey this expectation rather well by $t \propto v^{-0.977 \pm 0.005}$ while the timing did not increase as strongly with timestep, falling below the $1/dt$ relation with $t \propto dt^{-0.87 \pm 0.02}$. Moreover, we find that increasing temperature also makes for an increased computation time. This can be attributed to an increase in the computation time associated with the force calculations. The rising temperature gives rise to more fluctuations in the system which might yield more atoms within the force calculation cutoffs for each computation. This kind of consideration can also be attributed to the reason for the deviating timing for dt . Finally, for the spring parameter, we did not see any noticeable effect on timing.

In general, we have selected our simulation parameters: temperature, sliding speed, spring constant, and timestep, based on numerical stability and computational cost. For the timestep, we found that a value of 1 fs, commonly used in similar studies [19, 20], produced stable results while higher values were prone to instabilities and lower values were computationally expensive. The sliding speed was chosen primarily based on computational cost, with a default value of 20 m/s being a reasonable compromise between computational efficiency and the lower values more commonly used in other studies. Although a lower sliding speed could lead to more commonly observed stick-slip motion, it represents a factor of 20 increase in computational time. Since stick-slip motion is out of reach based on the chosen sliding speed, we found that using an infinitely stiff spring $K = \infty$ was the

most reasonable option to ensure stable results. Finally, the temperature investigation did not provide much guidance for a specific choice, so we settled for the standard choice of room temperature $T = 300$ K.

2.6 Load and stretch dependencies

So far, we have carried out a general analysis of the system behavior under the influence of various simulation parameters. This lays the foundation for the remaining study as we now shift our intention towards the friction dependence of strain and load.

2.6.1 Pressure reference for normal load

We consider a load range of 0.1–10 nN which coincide with the general investigated range in other MD studies [17, 20]. In order to relate the magnitude of this load we provide a short calculation of the corresponding pressure. We will use the pressure underneath a stiletto-heeled shoe as a high-pressure reference from our macroscale perspective. The diameter of a stiletto-heeled shoe can be less than 1 cm [25], and hence an 80 kg man² standing on one stiletto heel, with all the weight on the heel, will correspond to a pressure

$$P = \frac{F}{A} = \frac{mg}{r^2\pi} = \frac{80 \text{ kg} \cdot 9.8 \frac{\text{m}}{\text{s}^2}}{(\frac{10^{-2} \text{ m}}{2})^2\pi} = 9.98 \text{ MPa}.$$

The fact that the pressure under a stiletto heel can get this high, actually greater than the pressure under an elephant foot, is an interesting realization in itself that is often used in introductory physics courses [26], but this also serves as a reasonable upper bound for human executed pressure. With a full sheet area of $\sim 21 \times 10^3 \text{ \AA}^2$ our load range of 0.1–10 nN corresponds to a pressure of 0.47–47 MPa which relates nicely to our macroscale reference. This pressure might be incompatible with various industrial purposes, but with no specific application in mind, this serves as a decent reference point. Notice, that if we consider a human foot with area 113 cm^2 [27] the pressure drops to a mere 70 kPa corresponding to only ~ 0.01 nN.

2.6.2 Strain dependency

We consider the effects of stretching the sheet using the non-cut, Tetrahedron (7, 5, 1) and Honeycomb (2, 2, 1, 5) sheet as used so far. For each configuration, we run a rupture test where the given sheet is stretched under zero load, but still under the influence of adhesion from the substrate. The rupture strain is then recorded, and multiple new simulations are initiated with strain values between zero and the rupture strain. For the sampling of the stretch values in the available range, we use a pseudo-uniform distribution, meaning that we divide the given interval into equal segments and pick a value from each segment by a uniform distribution. This is due to numerical limitations in LAMMPS³, but we find that this gives evenly spaced values which also carry some randomness. For the load we use 0.1, 1 and 10 nN.

First, we aim to reproduce the contact investigation from ???. We quantify the relative contact as described in ???, but we convert this into a single metric for a given simulation by considering the average of the last 50% of data points, similar to what we have done for the mean friction. We also adopt a similar method for quantifying the error (see ???). The results are shown in ??? where we observe a significant decrease in relative contact for the kirigami patterns which qualitatively agrees with the non-loaded continuous stretch simulation in ???. This result implies that the change in contact is not governed by a momentum effect during stretching, as each simulation now keeps the strain constant throughout the simulation. The absolute error for the mean rel. contact was generally quite low on the order of 0.01 for all configurations.

From an asperity theory point of view, this reduction in contact is theorized to induce a similar reduction in friction. However, when considering the kinetic friction in ??? we find that this is not the case. For the Tetrahedron and Honeycomb patterns, we find that the friction initially increases with a decreasing contact

²Yes, a man can certainly wear stiletto heels.

³In LAMMPS, we sample the various strain values by storing restart files during the straining of the sheet. The restart values are stored at specific timesteps governed by a LAMMPS variable. Such variables allow for a vector of uniform randomly chosen values, but unfortunately, we are not able to sort the vector for ascending values. This will lead to the script waiting to store each restart file according to the timesteps in the unsorted vector. As soon as the next timestep value is less than the current timestep the program will stop producing restart files and thus skip most of them. However, by first defining a series of intervals we can draw a uniform number for each interval without getting into trouble.

area. Yet, these are not simply inversely proportional as the friction force suddenly dips down and up again, in the strain range of 0.08–0.11 for the Tetrahedron and 0.73–1.05 for the Honeycomb pattern. When considering the non-cut sheet, we find that both the contact area and friction remain seemingly unaffected by strain. This indicates that the contact area is not a dominating mechanism for friction in our system, but the underlying mechanism might make for a correlation between a decreasing contact area and the non-linear friction-strain curve observed here. The latter point can be supported by the fact that the contact-strain and friction-strain curve both show signs of a discontinuous jump around a strain of 0.32. Since the non-cut sheet exhibits a flat friction-strain profile we cannot attribute the behavior to an increased tension either. The friction effect of tension of a graphene sheet has been investigated by Zhang et al. [23]. However, they report a decreasing friction with tension which qualitatively contradicts our observation as the direction of the effect is opposite. Instead, we might point to a commensurability effect or perhaps a change in the structural stiffness which is reported as an important feature by [28]. We observe that the initial friction value of the non-strained sheet varies across configurations, with the initial friction increasing from the non-cut sheet, through the Tetrahedron sheet, to the Honeycomb sheet. This is more evident from the parameter investigation from ?? We notice also that the two orders of magnitude increase in normal load did not make a significant difference in the results. The estimated absolute error marked by a shaded area in ?? were fairly low for both friction on the order 10^{-3} nN and relative contact on the order of 10^{-4} .

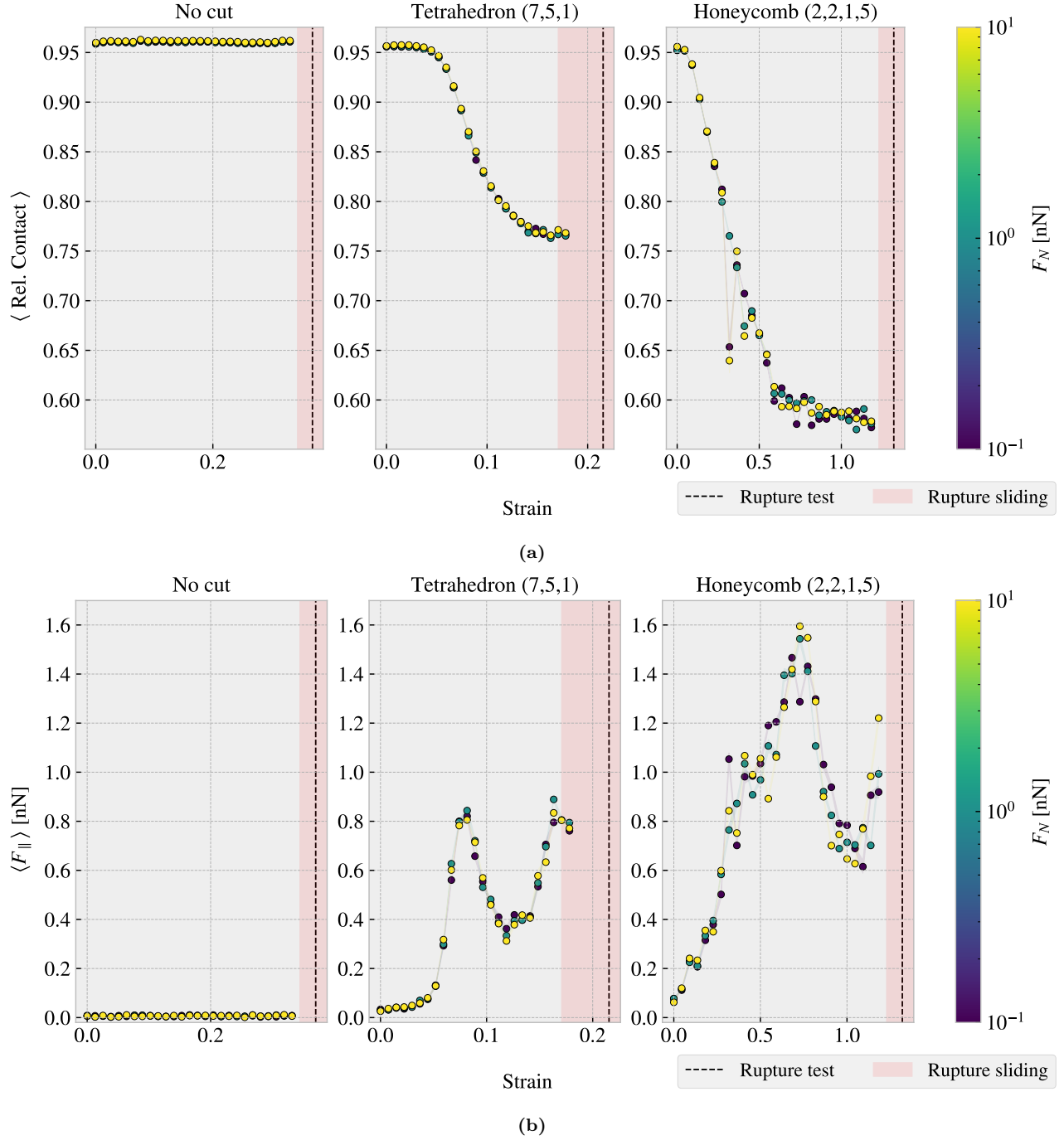


Figure 2.13: Average relative contact and average friction for multiple simulations, consisting of 30 stretch values sampled from a pseudo uniform distribution between 0 and the rupture point in combination with loads 0.1, 1 and 10 nN, for each of the configurations: non-cut, Tetrahedron (7, 5, 1) and Honeycomb (2, 2, 1, 5). The average is taken over the last half of the sliding phase. The red shade denotes the stretch range where ruptures occurred during sliding while the black-dotted line represent the rupture point in the no load rupture test. (a) The average relative contact defined as the relative number of atoms within a contact threshold of 4 Å to the substrate. The absolute error is on the order 0.01 (b) The average mean friction force parallel to the sliding direction. The absolute error for the mean friction is on the order 0.001–0.01 nN.
 Mention error for contact being on the order e-4–e-5

By considering the increase in friction from zero strain towards the first peak of the friction-strain curve we find that the Tetrahedron pattern exhibits a relative friction increase of ~ 27.7 while the Honeycomb pattern

exhibits a relative increase of ~ 22.4 . This is in itself a remarkable result, but considering that the friction drops almost as dramatically afterward makes for an even more unexpected behavior. For the Tetrahedron sheet the friction drops by ~ 0.51 nN during an increased strain $\Delta\varepsilon \sim 0.04$ while Honeycomb drops ~ 0.98 nN during a strain increase of $\Delta\varepsilon \sim 0.36$. These results are promising for the aim of demonstrating a negative friction coefficient for a system with coupled load and stretch. We will discuss this further at the end of this chapter in ??.

2.6.3 Load dependency

From the investigation of the stretch dependency we saw that increasing the normal load from 0.1 to 10 nN did not make a considerable impact on the friction in comparison to the effect associated with strain. One special feature of our system is that we only apply load to the pull blocks, and thus one might suspect this to be of importance. Therefore, we investigate the friction under varying loads for a non-cut sheet comparing the case of loading the pull block against a more traditional uniform loading of the sheet as shown in ??. Both load distributions show a seemingly non-dependent relationship between friction and load considering the size of our estimated error. Nonetheless, we do not see any indications that the uniform loading changes the qualitative behavior.

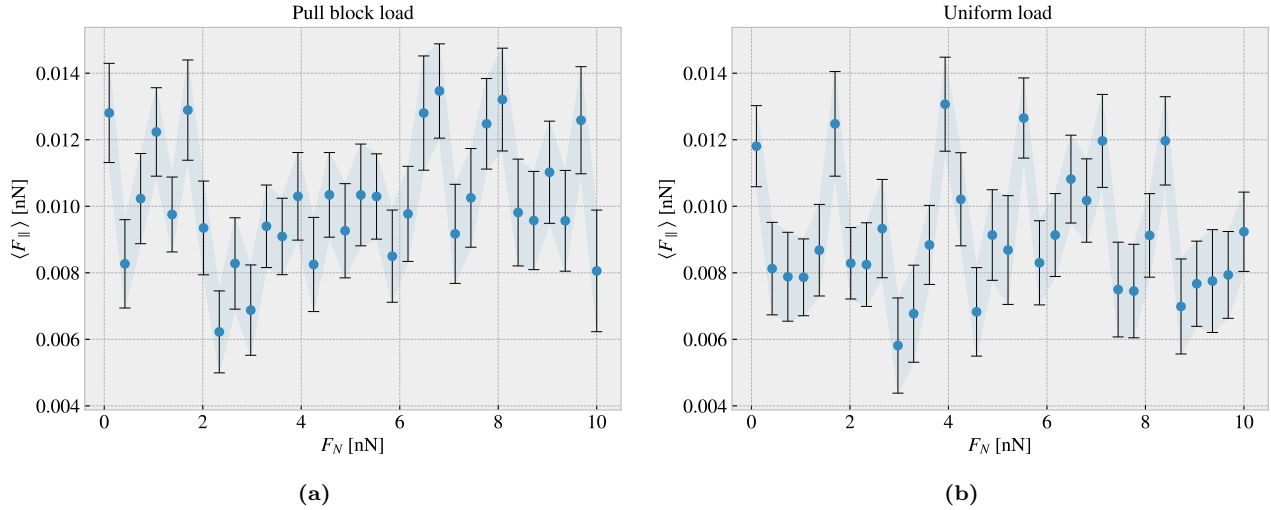


Figure 2.14: Multiple simulations of non-cut sheet under different load. Mean friction is plotted against load for two different variations of loading distribution. (a) Normal loading is applied to the pull blocks. (b) Normal loading is applied uniformly to the sheet.

In order to further investigate the friction dependency of normal load for the Kirigami patterns as they are stretched, we select a subset of stretch stages from ?? and perform additional simulations with a logarithmically increasing normal load in the extended load range 0.1–100 nN, using 30 load data points for each strain. The results are shown in ??. When spanning three orders of magnitude for the normal load we find some increase in friction with load. This goes for all patterns, but it is only really visible for the non-cut sheet as the values on the friction axis show a more narrow range. Notice that the load is plotted for a logarithmic axis which makes any seemingly linear trends on the figure sublinear. However, as the normal load approaches 100 nN we do start to see an increase that is more reminiscent of a linear relationship, but this is difficult to judge given that the change in friction is small in comparison to the noise in the data. Note that we omitted the error bars for visual purposes but they are on the same order of magnitude as shown in ??.

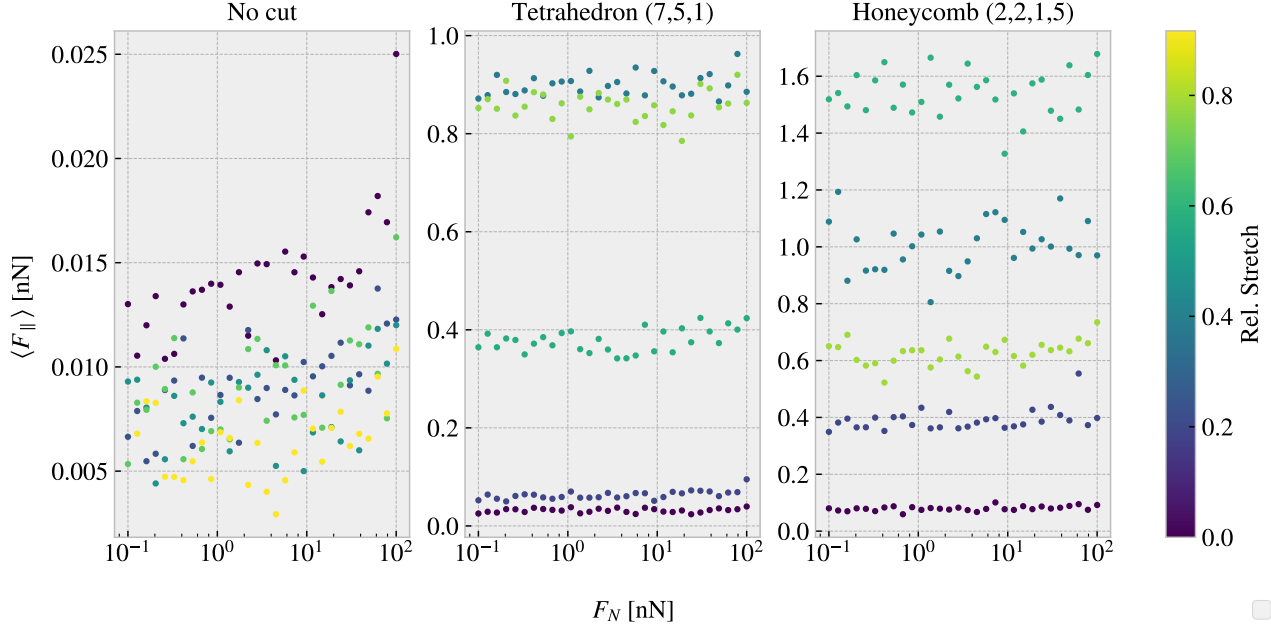


Figure 2.15: Mean friction force vs. load in the range 0.1–100 nN, for the non-cut, Tetrahedron (7, 5, 1) and Honeycomb (2, 2, 1, 5) sheet respectively, at different stretch stages relative to their rupture point.

From the friction measurements in ?? we see that the non-cut sheet generally produces a friction force in the order of 0.005–0.0025 nN throughout the 0.1–100 nN load range. Using a ratio based friction coefficient definition ??, $\mu_1 = F_{\text{fric}}/F_N$, this would lead to a coefficient roughly in the range

$$\mu_1, \text{ ??}: \quad \text{No cut} \sim [10^{-4}, 0.13], \quad \text{Tetrahedron} \sim [4 \times 10^{-4}, 8.7], \quad \text{Honeycomb} \sim [9 \times 10^{-4}, 15.2].$$

However, these values mainly reflect the poorness of this definition, as we find the values to diverge at low load and decrease towards high load due to the lacking linear relationship and an offset in the load curve corresponding to a finite friction at zero load. This offset is drastically enhanced for the Kirigami patterns under strain. Due to the small changes in friction compared to the noise in the data, it is not sensible to calculate the slope dF_{fric}/dF_N as a function of load. Nonetheless, if we force a linear fit for the whole range and use the second definition ?? as $\langle \mu_2 \rangle = \Delta F_{\text{fric}}/\Delta F_N$, we get average coefficients in the range

$$\mu_2, \text{ ??}: \quad \text{No cut} \sim [4, 9] \times 10^{-5}, \quad \text{Tetrahedron} \sim 5 \times [10^{-5}, 10^{-4}], \quad \text{Honeycomb} \sim [1, 9] \times 10^{-4},$$

depending on the strain values. These numbers should be interpreted cautiously, but we can take it as a rough estimate of the friction coefficient being on the order 10^{-4} – 10^{-5} . This relates to the finding by [29] who reported a seemingly non-existing relationship between friction and normal load with change in friction that corresponds to friction coefficients in the range 10^{-3} – 10^{-4} when using the slope definition ?. This supports the idea that the graphene sheet does in fact exhibit superlubric behavior in these conditions. Moreover, the fact that the increase with load is relatively unaffected by the stretching points to the fact that the strain-induced effect mainly shifts the load curve towards higher friction but does not significantly alter its slope.

2.6.4 Prospects of a negative friction coefficient

Considering the results from ?? and ?? we find that strain-induced friction effects, on the order of $/SI1nN$, are generally dominating in comparison to load-induced effects on the order of 0.01 nN given a load range of 10^2 nN. This is promising for the idea of achieving a negative friction coefficient for a nanomachine system that couples load and strain. By applying load on the nanomachine we would increase both the load and the strain on the sheet simultaneously. However, since the friction dependency to strain dominates in comparison to load effects such a system can be designed entirely by considering the strain dependency. The friction coefficient is by our definition (??) given as the slope of the friction F_f vs. normal force F_N curve. Hence, for two points

$\{(F_{N,1}, F_{f,1}), (F_{N,2}, F_{f,2})\}$, $F_{N,1} < F_{N,2}$ we can evaluate the associated friction coefficient $\mu_{1,2}$ as

$$\mu_{1,2} = \frac{F_{f,2} - F_{f,1}}{F_{N,2} - F_{N,1}} = \frac{\Delta F_f}{\Delta F_N}.$$

If we neglect load effects $F_f(F_N, \varepsilon) \sim F_f(\varepsilon)$ and consider a coupling $\varepsilon = RF_N$ with linear coupling ratio R we get

$$\mu_{1,2}(\varepsilon_1, \varepsilon_2) = \frac{\Delta F_f(\varepsilon_1, \varepsilon_2)}{\frac{1}{R}(\varepsilon_2 - \varepsilon_1)} = R \frac{\Delta F_f(\varepsilon_1, \varepsilon_2)}{\Delta \varepsilon}. \quad (2.1)$$

When considering the ratios found for the reduction in friction with strain for the Tetrahedron and Honeycomb patterns in ?? we find the corresponding coupled system friction coefficients to be

$$\text{Tetrahedron: } R \frac{-0.51 \text{ nN}}{0.04} = -R \cdot 12.75 \text{ nN}, \quad \text{Honeycomb: } R \frac{-0.98 \text{ nN}}{0.36} = -R \cdot 2.72 \text{ nN}$$

This showcases that we might be able to utilize the strain effect to achieve a negative friction for the system of coupled strain and load

Chapter 3

Negative friction coefficient

For the final part of this thesis, we concern ourselves with a proof of concept approach for the designing of a negative friction coefficient. From the pilot study (??) we found the two investigated patterns to have a non-linear relationship with strain which is hypothesized to yield a negative friction coefficient in a coupled system system of load and strain for certain load ranges. We will investigate this hypothesis further in this chapter.

3.1 Nanomachine coupling

We do not attempt to simulate the dynamics of any nanomachine desings, but we propose that a coupling could be achieved, for instance by following a design as sketched in ??. Such a design could perhaps be achieved by rigging carbon nanotubes in a similar configuration.

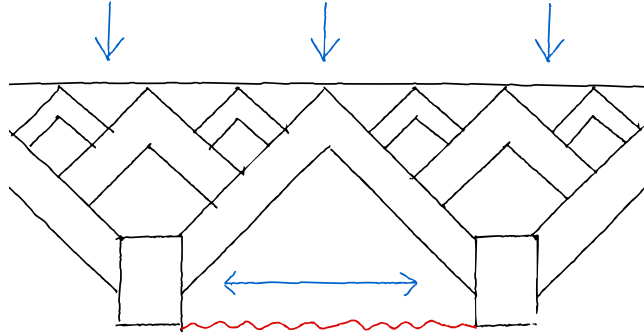


Figure 3.1: Working sketch for nanomachine

We mimic the nanomachine coupling by implementing a load-depending tension force to our MD simulations. So far, we have kept the pull block spaced by a fixed distance throuhout the simulations, but now we let the pull blocks move relative to each other under the influence of this tension force between the blocks. The tension force F_t is modeled to be linearly coupled to normal load F_N by a factor T which represents the ratio for the load to strain coupling. We find that a ratio of $T = 6$ will provide the necessary tension for achieving a full strain range (till rupture) within the loading range used so far in our study. Notice that this coupling scheme is slightly different than that proposed in ?? where we assumed a coupling between load and strain $\varepsilon = RF_N$. This is done to provide a standardized description of the proposed nanomachine for which the relation between tension and strain will depend on the specific Kirigami sheet. We use the Tetrahedron (7, 5, 1) and Honeycomb (2, 2, 1, 5) from the pilot study and perform multiple simulations for different loads. We sample 100 pseudo uniform normal force values in the $[0, 15]$ nN which corresponds to a tension force of $[0, 90]$ nN. For the Tetrahedron pattern we increase the load by a speed of 0.015 nN/ps. Due to a rapid change in the strain-tension curve for the Honeycomb pattern we reduced the loading speed to 0.0015 nN/ps and added additional data points to the sparsely populated strain range. By considering the strain-load curve we map compare the results

from the pilot study ?? by mapping the strain values to the corresponding load values of our coupled system. The results are shown in ??.

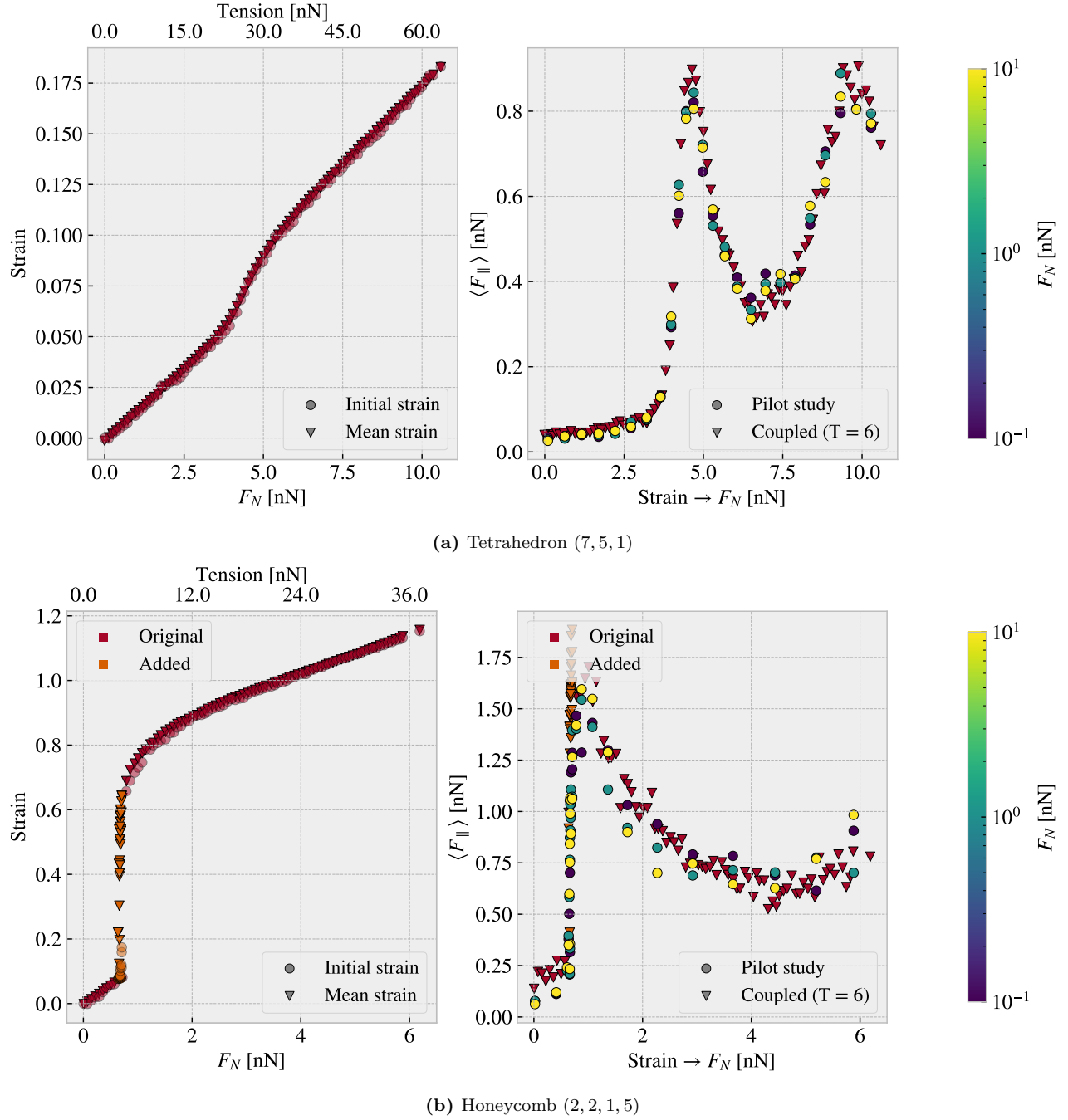


Figure 3.2: Evaluation of the friction response for a coupled system using (a) the Tetrahedron (7, 5, 1) and (b) Honeycomb (2, 2, 1, 5) pattern. The pull blocks are allowed to move relative to each other under the influence of a tension force F_t modeled as $F_t = RF_N$ for normal load F_N and a ratio $R = 6$. The right panel shows the friction vs. stretch curve in comparison to the locked pull block system and constantly defined normal from the pilot study (?). The left panel shows the strain-tension curve. For the Honeycomb pattern, we added more data points in the region where the strain-tension curve changed rapidly.

Generally, we observe from ?? that the data points of the coupled system aligns reasonable well with the mapped data points from the pilot study. This indicates that the simultaneous loading and straining of the

system does not suppress the underlying mechanism governing the non-linear trends. For the Tetrahedron pattern we find an almost linear strain-tension curve which makes for a recognizable trend in the friction-load curve similar to that seen in the friction-strain curve in ???. In both cases, we also notice that the initial and the mean strains aligns rather well. This suggest that the sliding does not contribute to a significantly increased tension in the sheet which would otherwise lead to an increased strain as well. For the Honeycomb pattern, we find an interesting trend for the strain-tension curve. At low tension, the curve of the strain is increasing seemingly linearly with strain, but a drastic increase in strain happens at a tension of 4.5 nN ($F_N = 0.75$ nN) transitioning from a strain of roughly 0.08 to 0.7. Eventually this settles off into a linear trend before reaching the rupture point. This reflects the reason for decreasing the loading speed and adding more data points to fill this gap in strain-tension curve. The rapid increase in the strain-load curve makes for a similar rapid increase in the friction-load curve as well. Hence we find that the Honeycomb coupled system essentially exhibit an intial discontinuous increase in friction with load, which is then followed by a longer region of decreasing friction with load. When considering the simulation frames in ??? we notice that the strain range covered in this transition aligns rather well with the unfolding of the honeycomb pattern. We have previously noted that the Honeycomb pattern unfolds in segments buckling one at a time. We observe that this unfolding is initiziated after passing a minimum tension. During the unfolding phase the friction increases, but immediately after friction decrease with further straining. Once again, this highlights that this transition might of interest for further investigations in order to get a better understanding of the underlying mechanisms being in play.

From the results in ??? we have found that our proposed coupled system, based on a $T = 6$ tension-load coupling, demonstrates a significant negative friction coefficient in certain load regions. By considering the maximum and minimum friction points along the friction-strain curve we find that this correponds to minimal friction coefficients μ_{\min} on the order of

$$\text{Tetrahedron: } \mu_{\min} \sim \frac{0.31 \text{ nN} - 0.90 \text{ nN}}{6.55 \text{ nN} - 4.65 \text{ nN}} = -0.31 \quad \text{Honeycomb: } \mu_{\min} \sim \frac{0.53 \text{ nN} - 1.88 \text{ nN}}{4.31 \text{ nN} - 0.71 \text{ nN}} = -0.38. \quad (3.1)$$

This result supports that the use of Kirigami sheet in a coupled system can be used to achieve a negative friction coefficients. In the pilot study (??) we estimated the Tetrahedron pattern to exhibit a coeffient following $-R12.75$ nN smaller than the Honeycomb following $-R2.72$ nN. From the results in ??? we find that the resulting coefficients a closer in value which we attribute to the difference in the strain-tension curve. However, we notice that both values can be scaled by increasing the strain-load coupling T , which would make for a more negative slope.

Chapter 4

Summary

The work presented in this thesis covers several topics (find a better opening line). We have created an MD simulation which enabled us to study the frictional behavior of a graphene sheet sliding on a Si substrate. In addition, we have created a numerical framework for creating Kirigami design patterns and introducing these into the friction simulations. This was used to study the effects of the out-of-plane buckling induced by a selected pair of Kirigami designs in comparison to a non-cut sheet under the influence of strain. Further, we have created a dataset of various Kirigami designs for the scope of investigating the possibilities with Kirigami design. We have investigated the possibility to use machine learning on this dataset and attempted an accelerated search. Finally we look into the prospects of achieving a negative friction coefficient for a system with coupled load and stretch. In this chapter we will summarize the findings and draw some conclusions. We will also provide some topics for further research.

4.1 Summary and conclusions

4.1.1 Design MD simulations

We have designed an MD simulation for the examination of friction for a graphene sheet sliding on a silicon substrate. The key system features were the introduction of the pull blocks, defined as the end regions of the sheet with respect to the sliding direction, which was utilized for applying normal load and sliding the sheet. The pull blocks were made partly rigid and used to employ a thermostat as well. Similarly, we divided the substrate into three parts with the lowermost part being rigidly locked in place, the middle part reserved for a thermostat and the upper part remaining free from further modifications. By an analysis of the friction forces from a sliding simulation we settled on a standardization of the kinetic friction metric as the mean value of the last half of the sliding simulation. This was measured with respect to the sliding distance and for the full sheet (including the pull blocks). We defined the uncertainty of the measurements through the standard deviation of the running mean. We found that the assessment of static friction was ambiguous for our simulation and did not pursue this further. From the analysis of the force traces, friction force vs. time, we identify the friction behavior in our simulation domain as being in the smooth sliding regime. This is further supported by a demonstration of a transition to stick-slip behavior for softer springs and lower sliding speed which points toward our system being in the ballistic sliding regime. By conducting a more systematic investigation of the effects of temperature, sliding speed, spring constant and timestep, we settled on standardized choices based on numerical stability and computational cost. We found that friction increased with temperature which disagrees with experimental and theoretical considerations but matches other MD. This is attributed to simulation conditions corresponding to a ballistic regime. We choose a room temperature 300 K as a standard choice. We found friction to increase with velocity as expected with some signs of phonon resonance sliding speeds as well. We chose a rather high velocity of 20 m/s mainly for the consideration of computational cost. For the spring constant, we found decreasing friction with increasing stiffness of the springs which is associated with the transition from a stick-slip-influenced regime toward smooth sliding. The choice of an infinitely stiff spring was made from a stability assessment. Finally, we confirmed that a timestep of 1 fs provides reasonable numerical stability. However, some fluctuations were observed, especially for the Honeycomb pattern, which might be interpreted as a sign of a higher uncertainty than expected on the order of ± 0.017 nN.

4.1.2 Design Kirigami framework

We have designed a numerical framework for creating Kirigami designs. By defining an indexing system for the hexagonal lattice structure we were able to define the Kirigami designs as 2D matrix for numerical implementation. We digitalized two different macroscale designs, which we named the *Tetrahedron* and *Honeycomb* pattern respectively, that successfully produced out-of-plane buckling when stretched. Through a numerical framework we could create an ensemble of perturbed variations which gave approximately 135k configurations for the Tetrahedron pattern and 2025k patterns for the size of the sheet used in our study. When considering the possibility to translate the patterns this gave roughly a factor 100 more of unique perturbations. We also created a framework for creating Kirigami designs through a random walk. This was further controlled by introducing features such as bias, avoidance of existing cuts, preference to keeping a direction and procedures to repair the sheet for simulation purposes. The capabilities of the numerical framework for generating Kirigami designs was far larger than the capabilities for producing MD designs within the time constraint of this thesis. Thus we believe that this contains the possibility to benefit more extended studies and for the creation of a larger dataset.

4.1.3 Control friction using Kirigami

We have investigated the friction behavior of a non-cut sheet in comparison to the Tetrahedron and Honeycomb pattern under various strain and load. Initially we observed that straining the Kirigami sheet resulted in an out-of-plane buckling in vacuum. When adding the substrate to the simulation this translated to a reduced contact area with strain. We find the Honeycomb sheet buckled the most resulting in a reduction of the contact area to approximately 43%. The non-cut sheet did not produce any significant buckling in comparison. However, when considering the friction effects we found that friction generally increased with strain which contradicts the asperity theory hypothesis of decreasing friction with decreasing contact area. Moreover, the friction-strain curve exhibited highly non-linear trends with strong negative slopes as well as shown in ???. The non-cut sheet did not reveal any significant dependency on the strain. This led us to the conclusion that the contact area nor tension alone (for a non-cut sheet) can be regarded as a dominant mechanism for friction in the graphene sheet system. When considering the dependency with load we generally found a weak dependency which can be associated to friction coefficients on the order of 10^{-4} – 10^{-5} even though we could not confirm any clear relationship. This is best attributed to the superlubric state of the graphene sheet on the substrate. The slope of the friction-load curves was also not affected by the straining of the Kirigami sheet which led us to the conclusion that the strain-induced effects are dominant in comparison to load-related effects. By proposing a linear coupling between load and strain with ratio R we find that the results allow for negative friction coefficients for the Tetrahedron pattern on $-R \cdot 12.75$ nN and Honeycomb $-R \cdot 2.72$ nN.

4.1.4 Capture trends with ML

With the use of MD simulations, we have generated an extended dataset of 9660 data points based on 216 Kirigami configurations (Tetrahedron: 68, Honeycomb: 45, Random walk: 100, Pilot study: 3) under various strains and normal loads. The dataset reveals some general correlations with mean friction, such as a positive correlation to strain (0.77) and porosity (0.60), and a negative correlation to contact area (-0.67). These results align with the findings from the pilot study suggesting that these features are relevant, but not necessarily the cause, of the observed phenomena. By defining the friction property metrics: $\min F_{\text{fric}}$, $\max F_{\text{fric}}$, $\max \Delta F_{\text{fric}}$ and max drop (maximum decrease in friction with strain), we investigated the top candidates within our dataset. From these results, we found no incentive of the possibility to reduce friction with the Kirigami approach since the non-cut sheet provided the lowest overall friction. Regarding the maximum properties, we found an improvement from the original pilot study values and with the Honeycomb pattern producing the highest scores. This suggests that the data contains some relevant information for optimization with respect to these properties. Among the top candidates, we found that a flat friction-strain profile is mainly associated with little decrease in the contact area and vice versa.

For the machine learning investigation, we have implemented a VGGNet-16-inspired convolutional neural network with a deep “stairlike” architecture: C32-C64-C128-C256-C512-C1024-D1024-D512-D256-D128-D64-D32, for convolutional layers C with the number denoting channels and fully connected (dense) layers D with the number denoting nodes. The final model contains 1.3×10^7 and was trained using the ADAM optimizer for a cyclic learning rate and momentum scheme for 1000 epochs while saving the best model during training based on the validation score. The model validation performance gives a mean friction R^2 score of $\sim 98\%$ and a rupture

accuracy of $\sim 96\%$. However, we got lower scores for a selected subset of the Tetrahedon ($R^2 \sim 88.7\%$) and Honeycomb ($R^2 \sim 96.6$) pattern based on the top 10 max drop scores respectively. These scores were lower despite the fact that the selected set was partly included in the training data as well and the fact that the hyperparameter selection favored the performance on this selected set. Thus we conclude that these selected configurations, associated with a highly non-linear friction-strain curve, represent a bigger challenge for machine learning prediction. One interpretation is that these involve the most complex dynamics and perhaps that this is not readily distinguished from the behavior of the other configurations which constitutes the majority of the data set. By evaluating the ability for the model to rank the dataset according to the property scores we found in general a good representation of the top 3 scores for the maximum categories, while the minimum friction property ranking was lacking. We attribute this latter observation to a higher need for precision in order to rank the lowest friction values properly which the model did not possess.

In order to provide a more true evaluation of the model performance we created a test set based on MD simulations for an extended Random walk search. This test revealed a significantly worse performance than seen for the validation set with a two-order of magnitude higher loss and a negative friction mean R^2 score which corresponds to the prediction being worse than simply guessing on a constant value based on the true data mean. However, by considering one of the early hypertuning choices, regarding architecture complexity, we evaluated the model when prioritizing mainly for the lowest validation loss. This gave similar performance on the test set which indicates that it is not simply a product of a biased hypertuning process, since we based our choices on the selected configuration set (which overlapped with the training data). Instead, it points to the fact that our original dataset did not cover a wide enough configuration distribution to accurately capture the full physical complexity of the Kirigami friction behavior.

4.1.5 Accelerated search

Using the ML model we performed two types of accelerated search. One by evaluating the property scores of an extended dataset and another with the use of the genetic algorithm approach. For the extended dataset search we used the developed pattern generators to generate $135\text{ k} \times 10$ Tetrahedon, $2025\text{ k} \times 10$ Honeycomb and 10 k Random walk patterns. For the minimum friction property, the search suggests a favoring of a low cut density (low porosity) which aligns with the overall idea that the dataset does not provide an incentive for further friction reduction. The maximum properties resulted in some minor score increases but the suggested candidates were overlapping with the original dataset. By investigating the sensitivity to translation of the Tetrahedron and Honeycomb patterns we found that the model predictions varied drastically with pattern translation. This can be attributed to a physical dependency since the edge of the sheet is effected by this translation. However, due to the poor model performance on the test set, we find it more likely to be a model insufficiency arising from a lacking training dataset.

For the genetic algorithm approach, we investigated the optimization for the max drop property with respect to starting population based on the result from the extended dataset accelerated search, and some random noise initializations with different porosity values. This approach did not provide any noteworthy incentive for new design structures worth more investigation. In general, the initialization of the population itself proved to be a more promising strategy than the genetic algorithm. However, this is highly affected by the uncertainty of the model predictions, and thus we did not pursue this any further. By considering the Grad-CAM explanation method we found that the model predictions sometimes seem to pay considerable attention to the top and bottom edge of the configurations. This is surprising since these are not true edges but are connected to the pull blocks in the simulation. Despite the uncertainties in the predictions, we argue that this might be attributed to thermostat effects from the pull blocks and thus we note this as a feature worth more studying.

4.1.6 Negative friction coefficient

By enforcing a coupling between load and stretch, mimicking a nanomachine attached to the sheet, we investigated the load curves arising from loading of the Tetrahedron (7, 5, 1) and Honeycomb (2, 2, 1, 5) pattern from the pilot study. The non-linear trend observed for increasing strain carried over to the coupled system as well producing a highly non-linear friction-load curve. This demonstrates a negative friction coefficient **say something about the values.**

4.2 Outlook / Perspective

Having successfully demonstrated a non-linear effect on friction with increasing strain of the sheet our results invite a series of further studies to investigate this relation. First of all, it would be valuable to investigate how the friction-strain curve depend on temperature, sliding speed, spring constant, and on load for an increased range $F_N > 100nN$. This is especially interesting in the context up conditions leading to a stick-slip behavior as our results were carried in the smooth sliding. Moreover, it would be important to verify that the choices for relaxation time and pauses are not critical for the qualitative observations as well as trying a different interatomic potential for the graphene and perhaps an entirely different substrate material. Especially the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential for the modeling of the graphene sheet might be of interest. The effects from excluding adhesion (the LJ interaction) can also be useful for the investigation of the observed phenomena.

In order to get a better understanding of the underlying mechanism for the friction-strain relationship we might investigate commensurability effects further by varying the scan angle. we might also consider investigating the friction-strain relationship under a uniform load to get insight into whether the loading distribution is of importance. Another topic worth studying is the relation to scale. Thus it would be interesting to study size effects but also further look into edge effects by translating the pattern. With this regard, we would also suggest a more detailed study of the effect from the thermostat in the pull blocks which is suggested to have a possibly importance by judging from the machine learning model Grad-CAM analysis.

For machine learning, we can either try to extend the data set to resolve the issue of the model not being generalized enough. We can also create a dataset for a single kirigami design and include some of the mentioned physical variables above and attempt to use machine learning for unraveling these relations. In that context we would advice for as more detailed investigation of machine learning techniques. If succesfull this would invite a study of inverse design methods such as GAN or diffusion models.

- How is this behavior effected by scaling?
- How does the distirbution of normal load effect the Kirigami friction behavior?
- Things to vary: load range, scan directions, adhesive forces, longer relaxation time, different potential (AIREBO)
- Investigate if the contact area is effecting the friciton non-linear by turning of friction force for atoms corresopnding to those that lift of from the sheet during the out-of-plane buckling.
- Investigations of commensurability effects.
- Study dependency of translation of the patterns as suggested by the ML results.
- Investigate effects from pull blocks...
- Investigate effects from the thermostat since the top and bottom edges was shown interest by the model prediction.

Appendices

Appendix A

Appendix A

Appendix A

Appendix B

Appendix B

Appendix C

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