Tuning friction properties of graphene sheets using kirigami inspired cuts and inverse design

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Project description

3 stages

1. Sheet kirigami: Alter graphene sheet using atomic scale cuts.
2. Forward simulation: Calculate frictional properties of the sheet using MD simulations.
3. Inverse design: Predict cut patterns based on frictional properties and optimize for desired properties.
   - Low / high friction coefficient.
   - Coupling between stretch and friction.

Motivation

Kirigami inspired cuts

Kirigami: Variation of origami with cuts permitted.

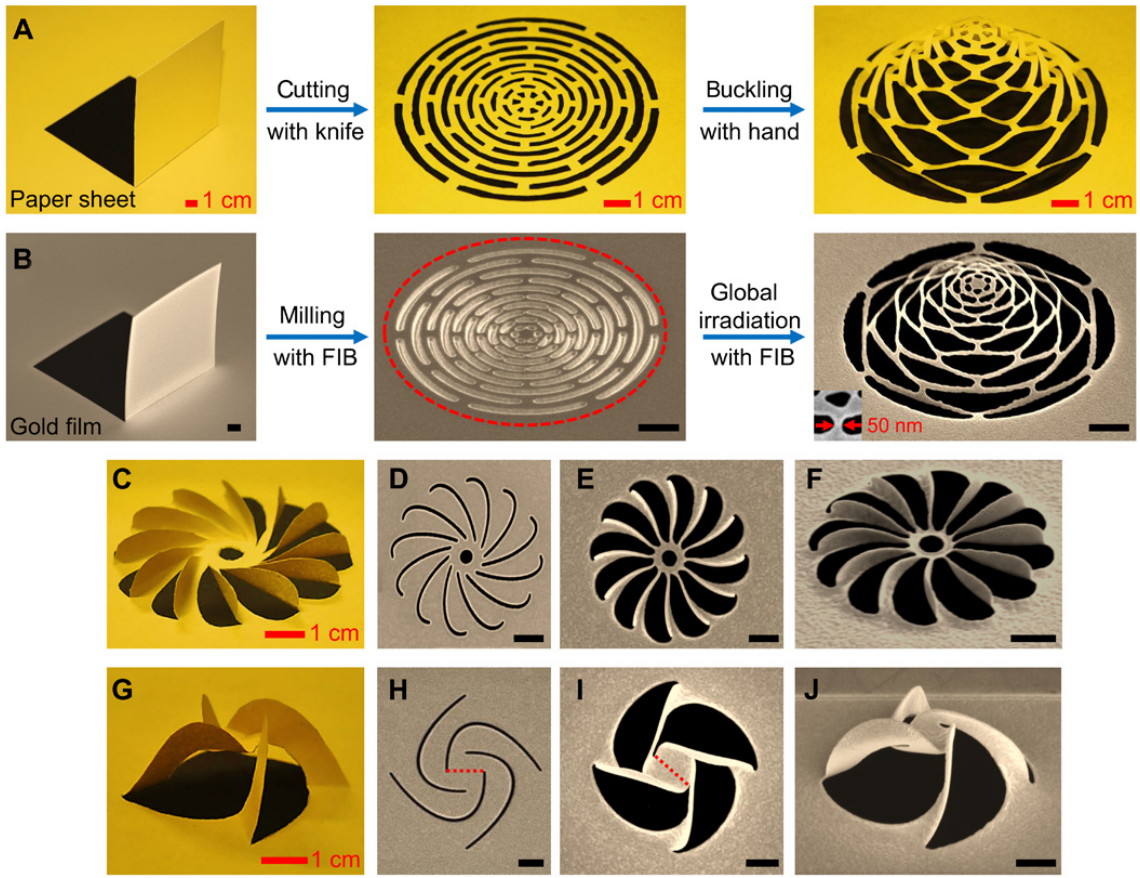

Figure: Exaple of transistion from macro- to nano-kirigami using a focused ion-beam (FIB) (Image courtesy of Nano-kirigami with giant optical chirality, ZHIGUANG LIU, 2018).

Motivation

Kirigami inspired cuts

Accelerated Search and Design of Stretchable Graphene Kirigami Using Machine Learning, Paul Z. Hanakata, 2018.

- Kirigami inspired cuts is used to tune **yield stress** and **yield strain** as a function of cutting pattern.
- A side effect is buckling into the third dimension.

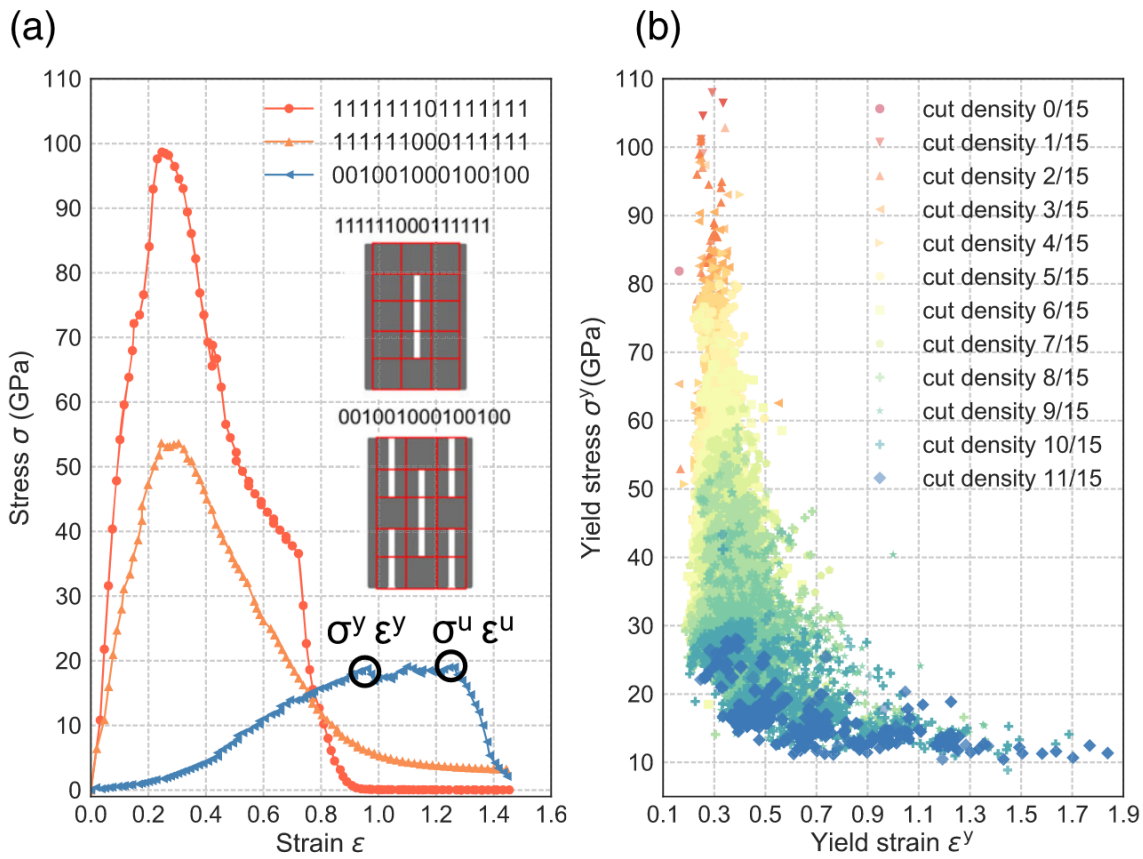

Figure: (a) Stress-strain plot of three representative kirigamis. Inset shows the "typical" kirigami cuts. (b) Yield stress as a function of yield strain for different configurations.

Motivation

Friction laws

- Stretching a sheet with cuts induces buckling into the third dimension.
- Friction lwas at different scales:

$$\text{Microscopic (Amontons' law): } F_f \propto F_N \quad (\text{ independent of } A),$$
$$\text{Nanoscale: } F_f \propto A = N_{at} \cdot A_{at},$$

where F_f is friction force, F_N normal force, A is the contact area and N_{at} is the average number of atoms in contact with an average contact area A_{at}.

Motivation

Nanomachine for negative friction coefficient

Coupling of friction force F_f, contact area A and normal force F_N.

$$\left.\begin{aligned} \text{Contact area} &: A_0 = k \cdot F_N \\ \text{Kirigami} &: A = A_0 - s_1 \cdot \text{stretch} \\ \text{Nanomachine} &: \text{stretch} = s_2 \cdot F_n \end{aligned}\right\} \Longrightarrow F_f \propto A = \underbrace{(k - s_1 \cdot s_2)}_{\mu} \cdot F_N$$

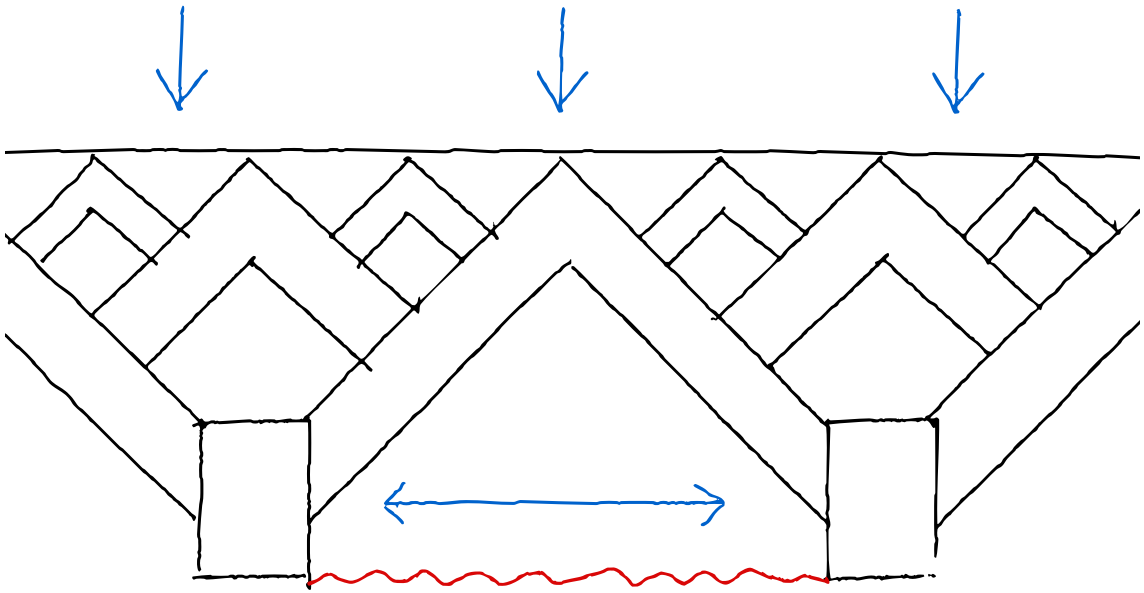

Figure: Sketch for nanomachine coupling normal force and stretch.

Motivation

Inverse design

- Inverse Design of Inflatable Soft Membranes Through Machine Learning
- Accelerated Search and Design of Stretchable Graphene Kirigami Using Machine Learning
- Designing complex architectured materials with generative adversarial networks

Stage 1 - Kirigami cuts

Choosing a cut pattern

- Kirigami design on macroscale.

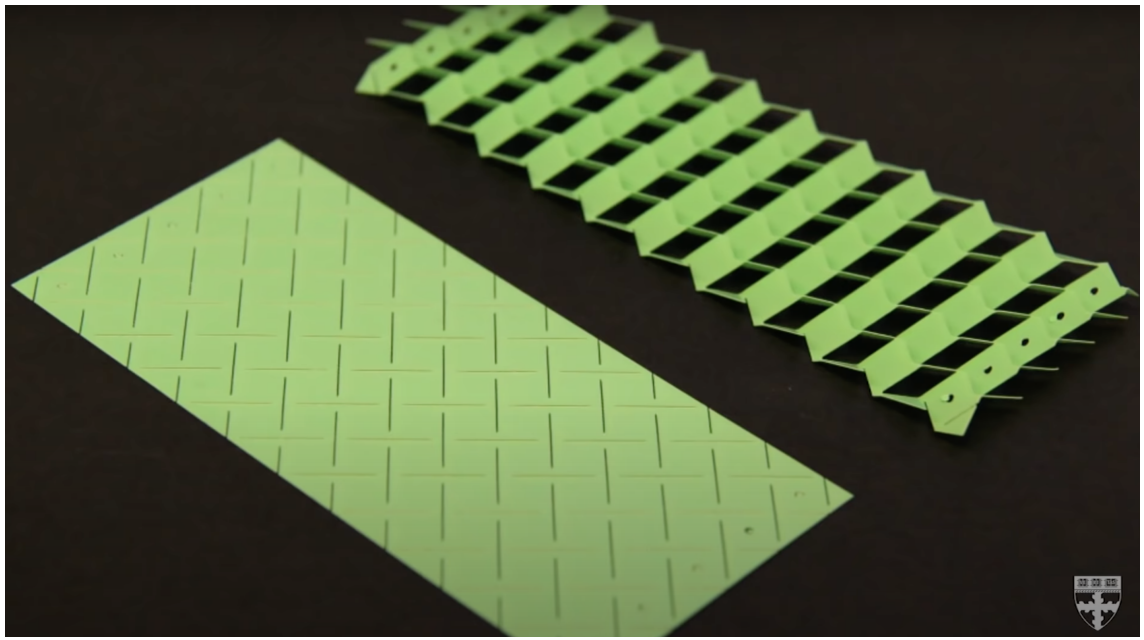

Figure: New pop-up strategy inspired by cuts, not folds - Leah Burrows, Harvard John A. Paulson School of Engineering and Applied Sciences

Stage 1 - Kirigami cuts

Choosing a cut pattern

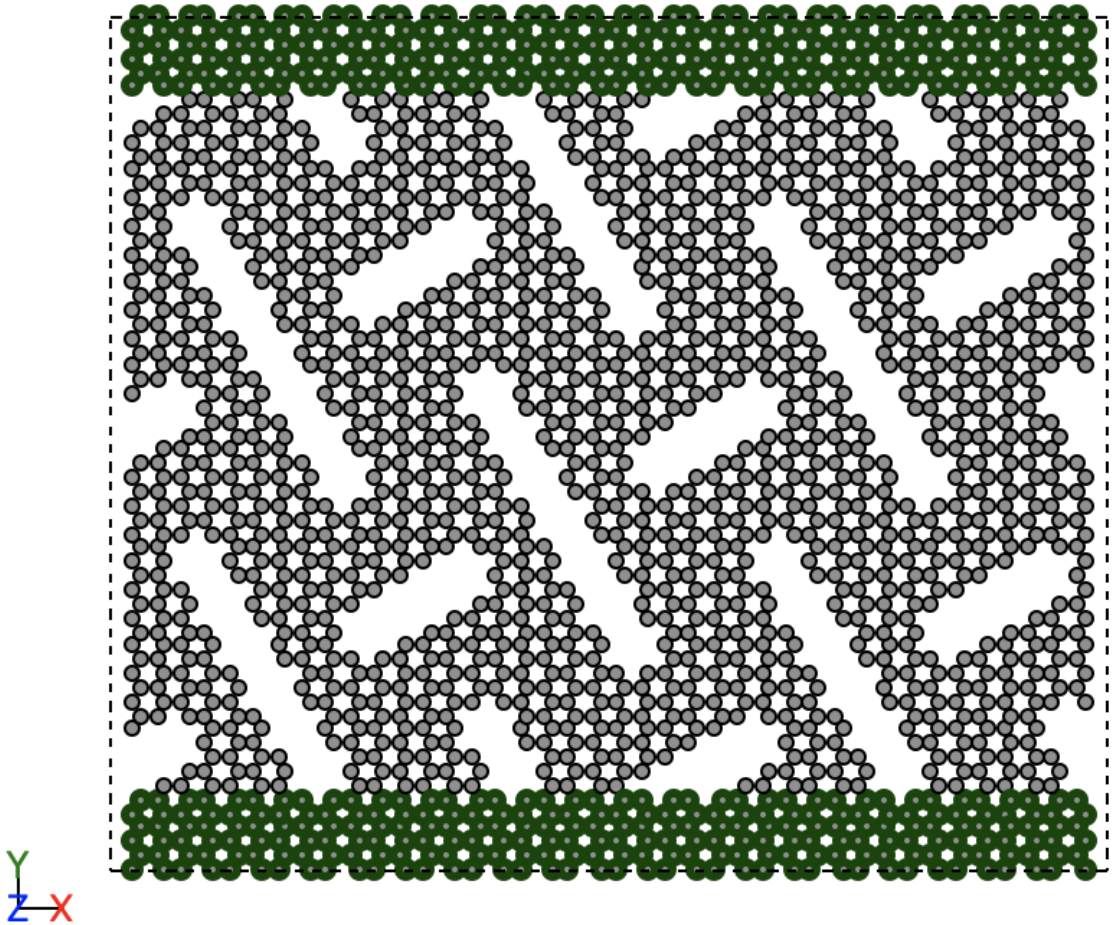

Figure: Example of cut pattern. The grey color marks the cutable sheet while green marks added blocks for stetching and dragging the sheet.

Stage 1 - Kirigami cuts

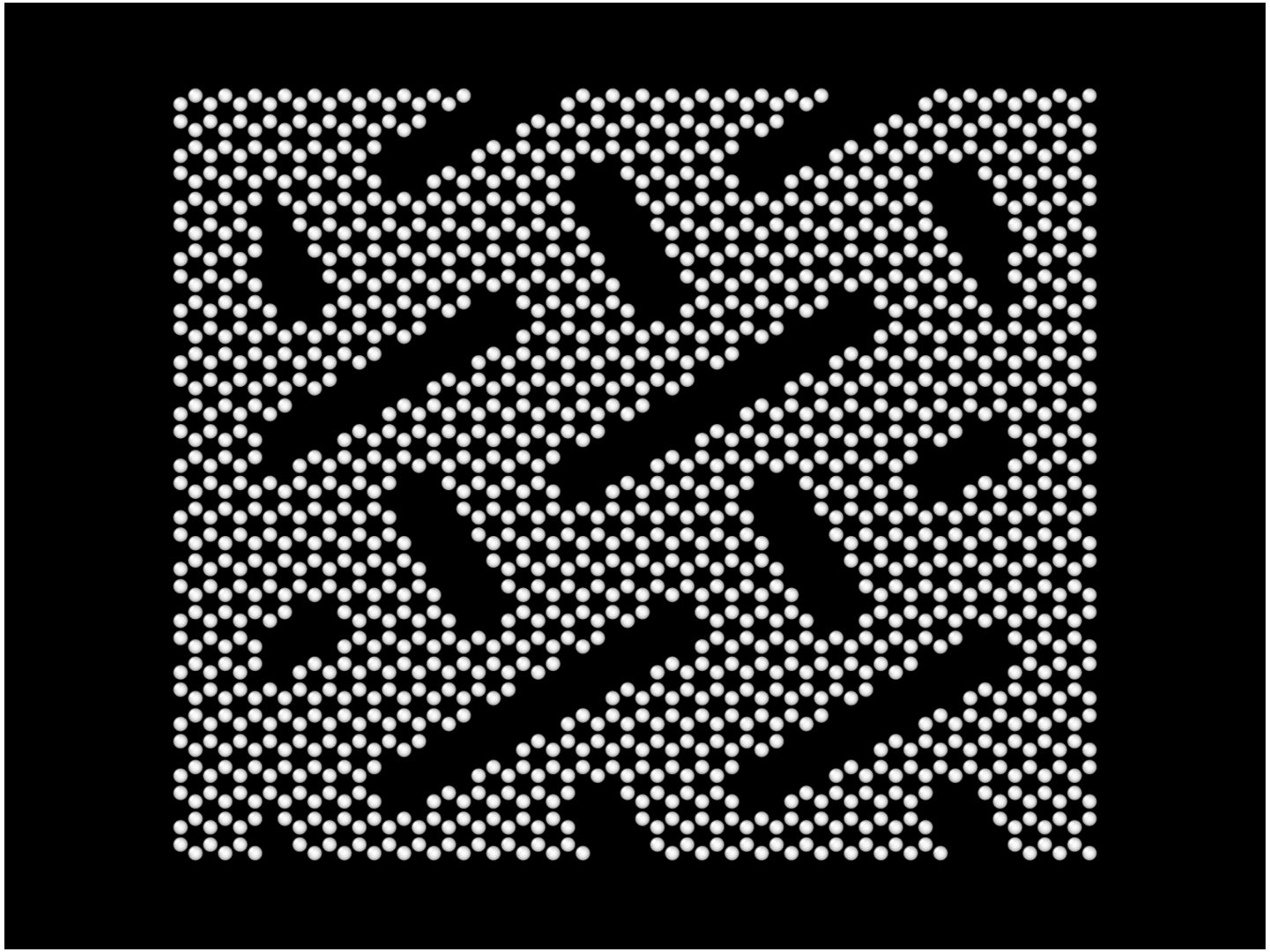

Figure: Kirigami sheet stretch in vaccuum.

Stage 1 - Kirigami cuts

Investigating 3D buckling

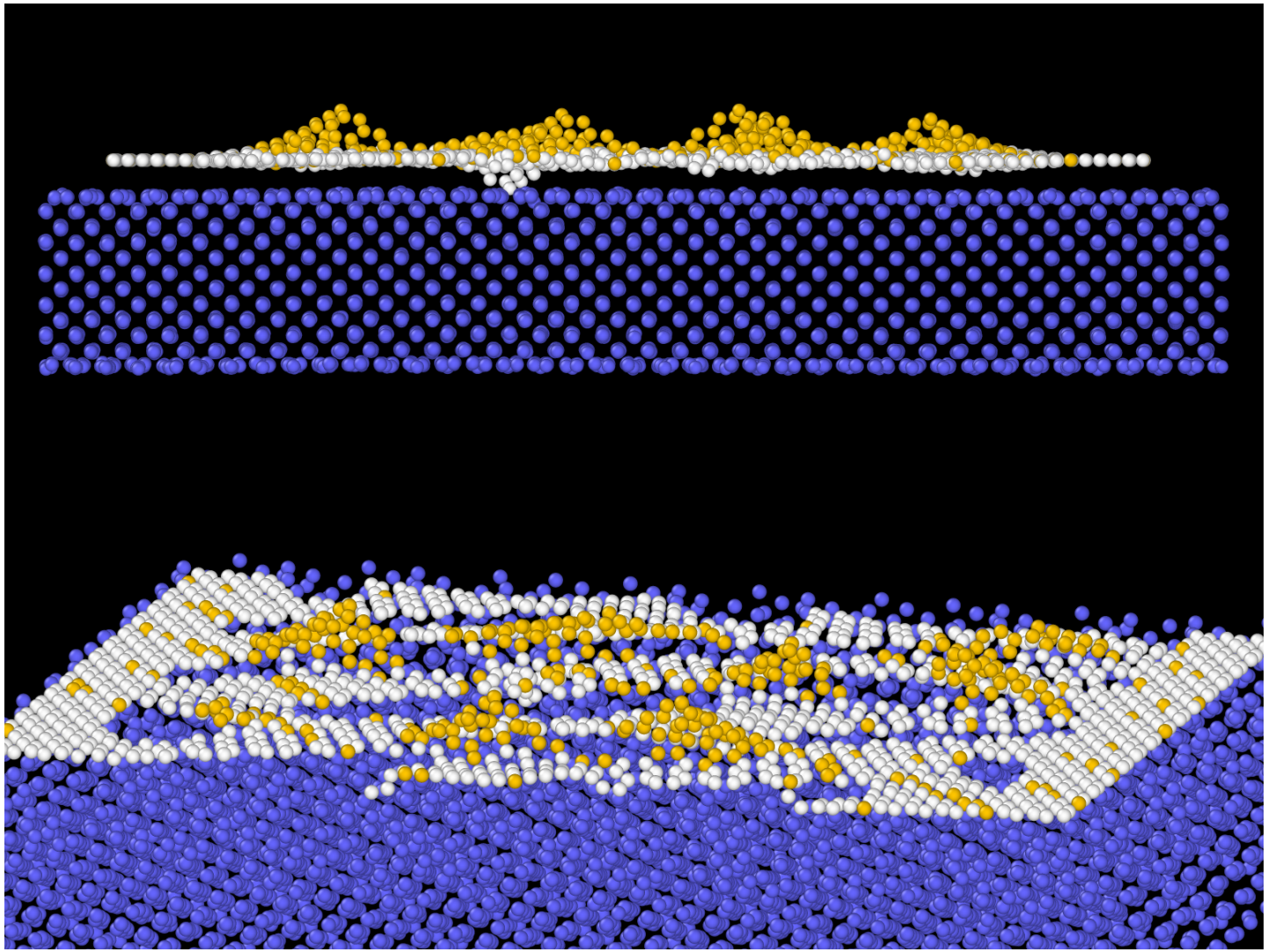

Figure: Kirigami stretch in contact with Si-substrate.

Stage 1 - Kirigami cuts

Investigating 3D buckling

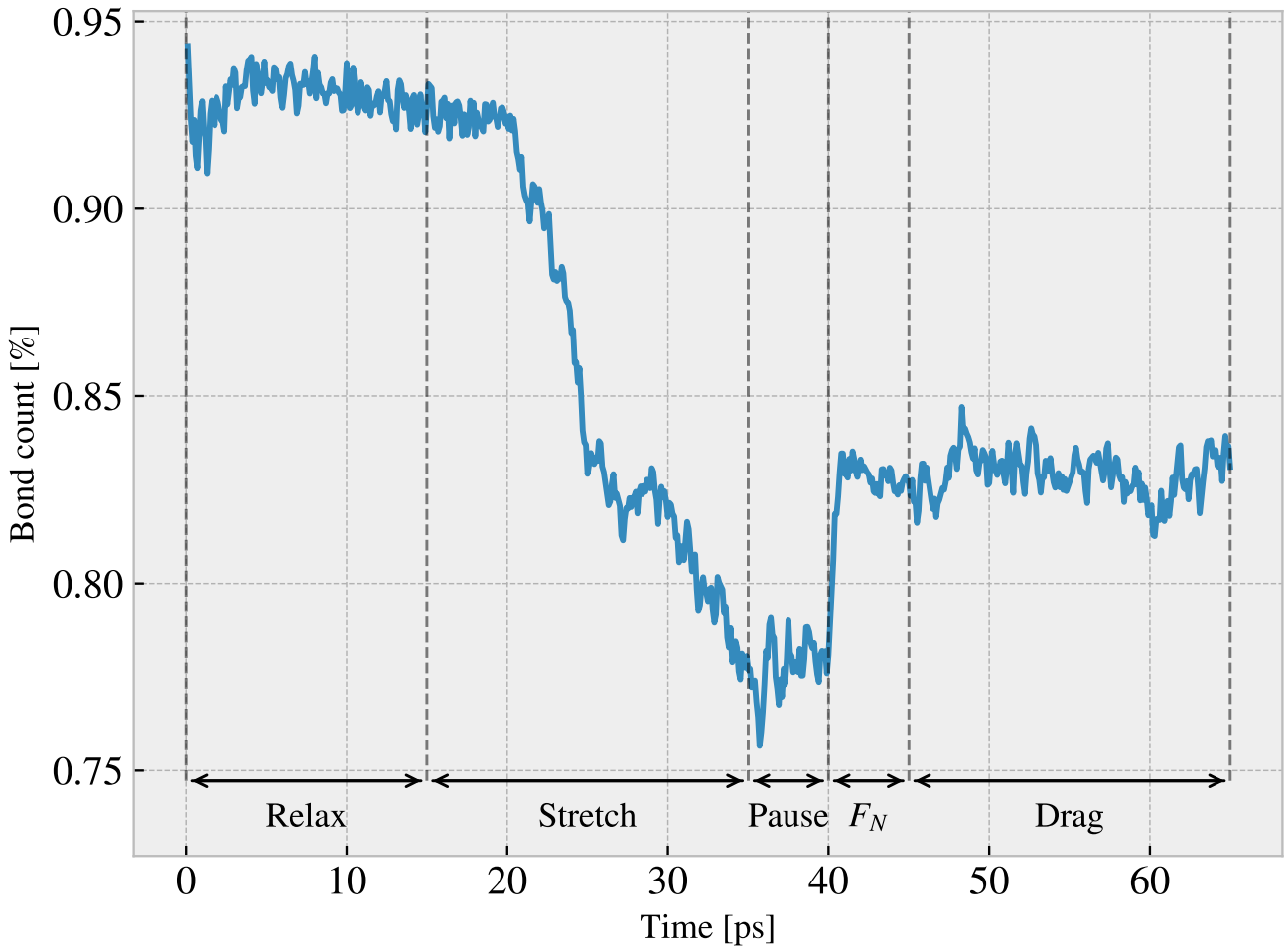

Figure: Contact area: number of C-Si bonds within a threshold distance of 110% the equlibrium distance in LJ the potential.

Stage 2 - MD measurements

Friction force

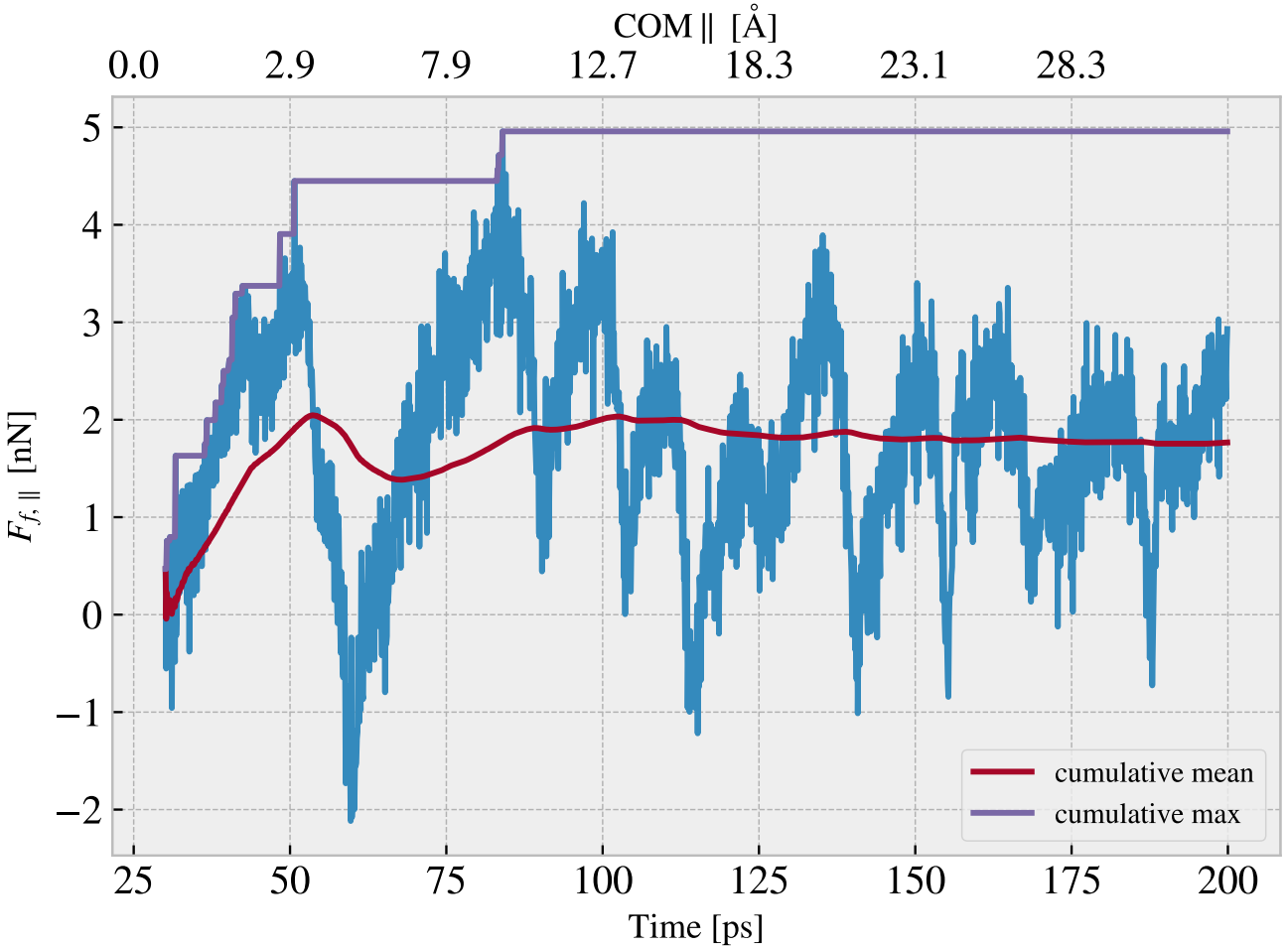

Figure: Friction force parallel to drag direction with normal force $F_N = 200$ nN. Drag distance = 40 Å

Stage 2 - MD measurements

Friction force

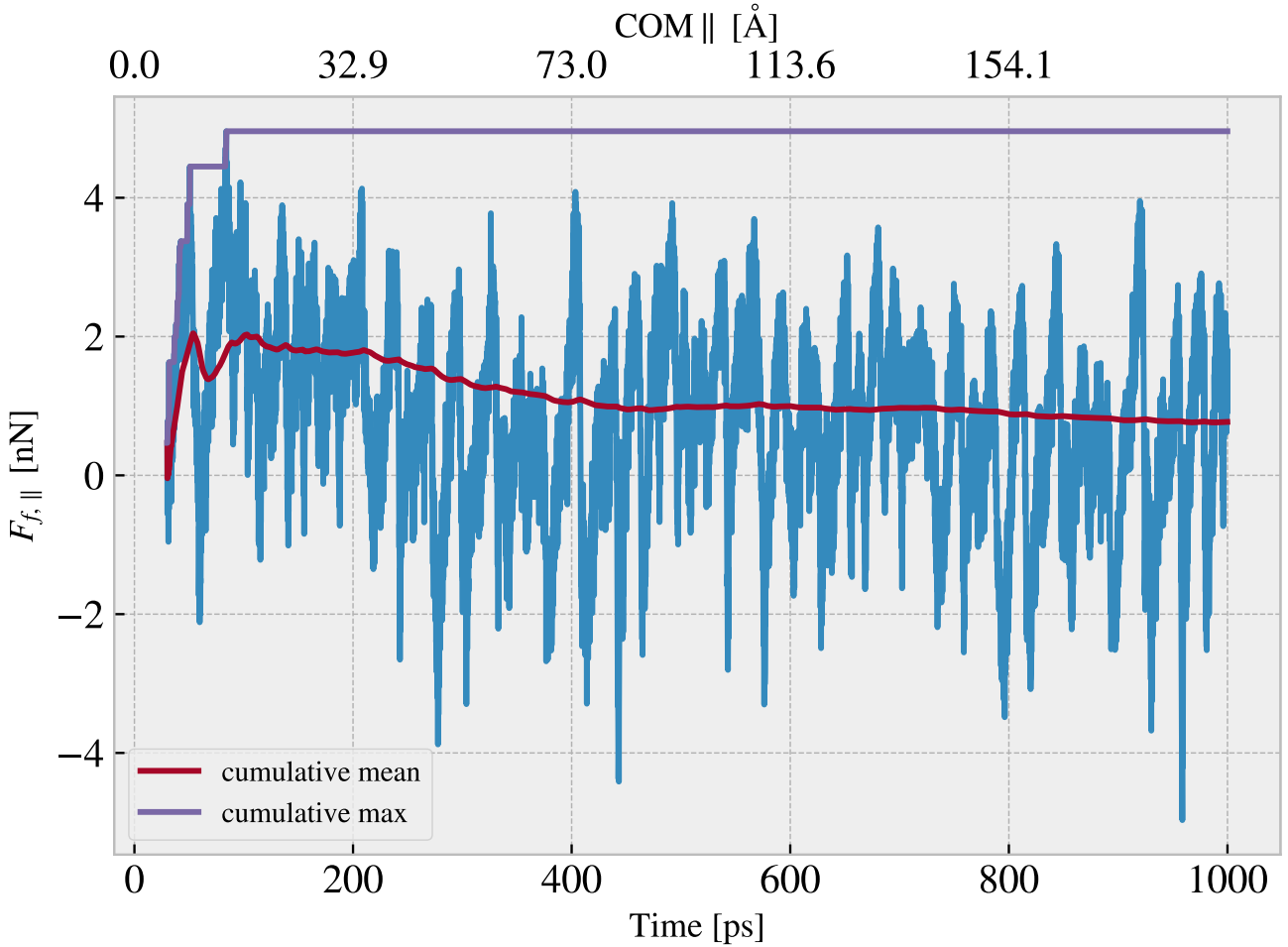

Figure: Friction force parallel to drag direction with normal force $F_N = 200$ nN. Drag distance = 200 Å.

Stage 2 - MD measurements

Contact area

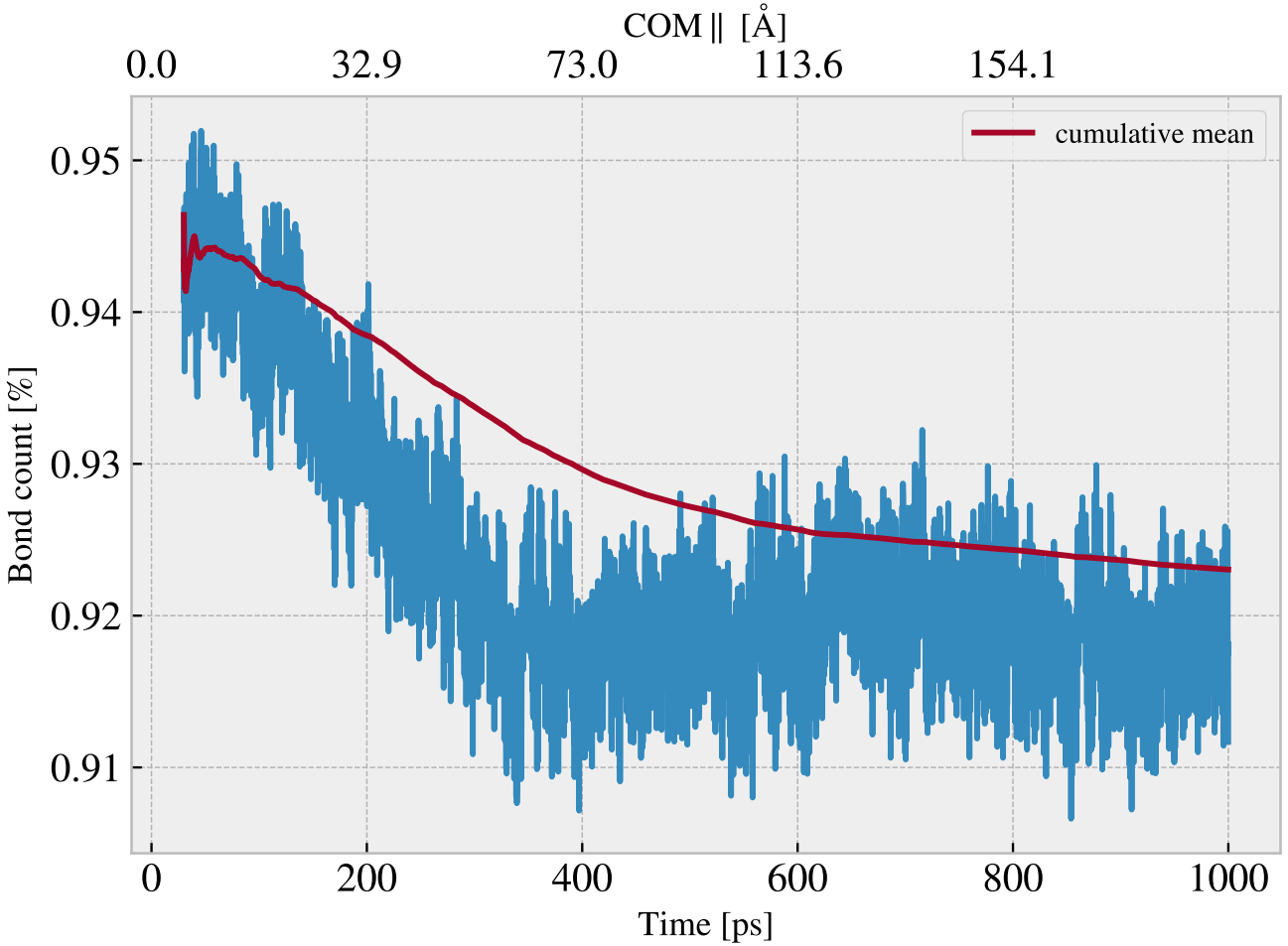

Figure: Contact bond count with normal force $F_N = 200$ nN. Drag distance = 200 Å.

Stage 2 - MD measurements

Contact area

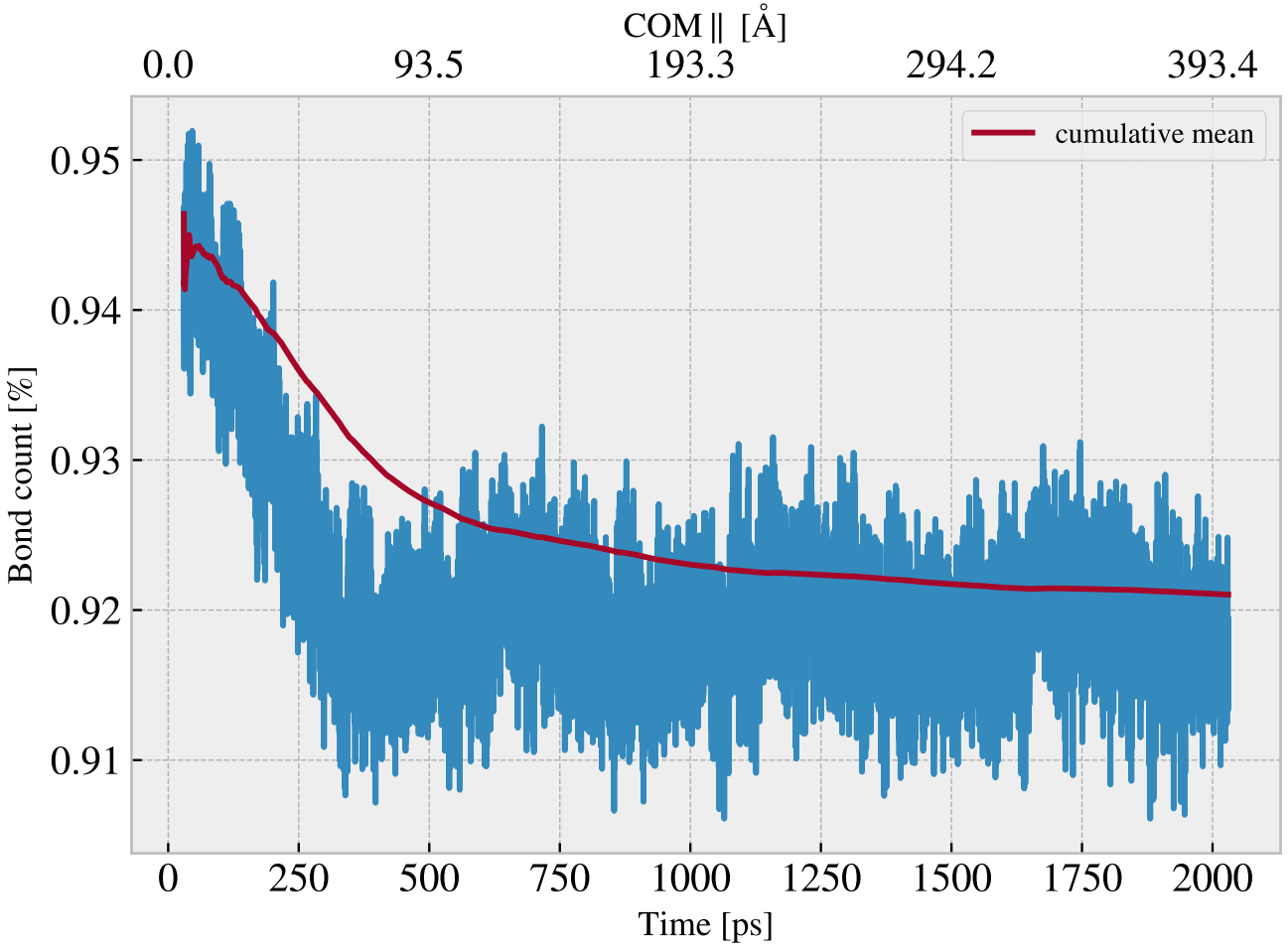

Figure: Contact bond count with normal force $F_N = 200$ nN. Drag distance = 400 Å.

Stage 2 - MD measurements

Parameters

Category	**Parameter**	**Range**
Physical (free)	Temperatur	[0, 300] K
	Drag speed	$[1, 20]$ m/s
Physical (ML input)	Cut configuration	No ruptures
	Scan angle	$[0, 90^\circ]$
	Streth amount	$[0, 20]$ %
	Normal force	$[10, 200]$ nN
MD settings	Relax and pauses	$\sim$ 10 ps
	Sretch speed	$[0.5, 0.1]$ %/ps
	Drag spring constant	$[10, \infty]$ N/m
	Drag length	$[50, 400]$ Å
	Sheet size	$\sim 62 \times 75$ Å

Table: Relevant parameters and approximate ranges

Stage 2 - MD measurements

...

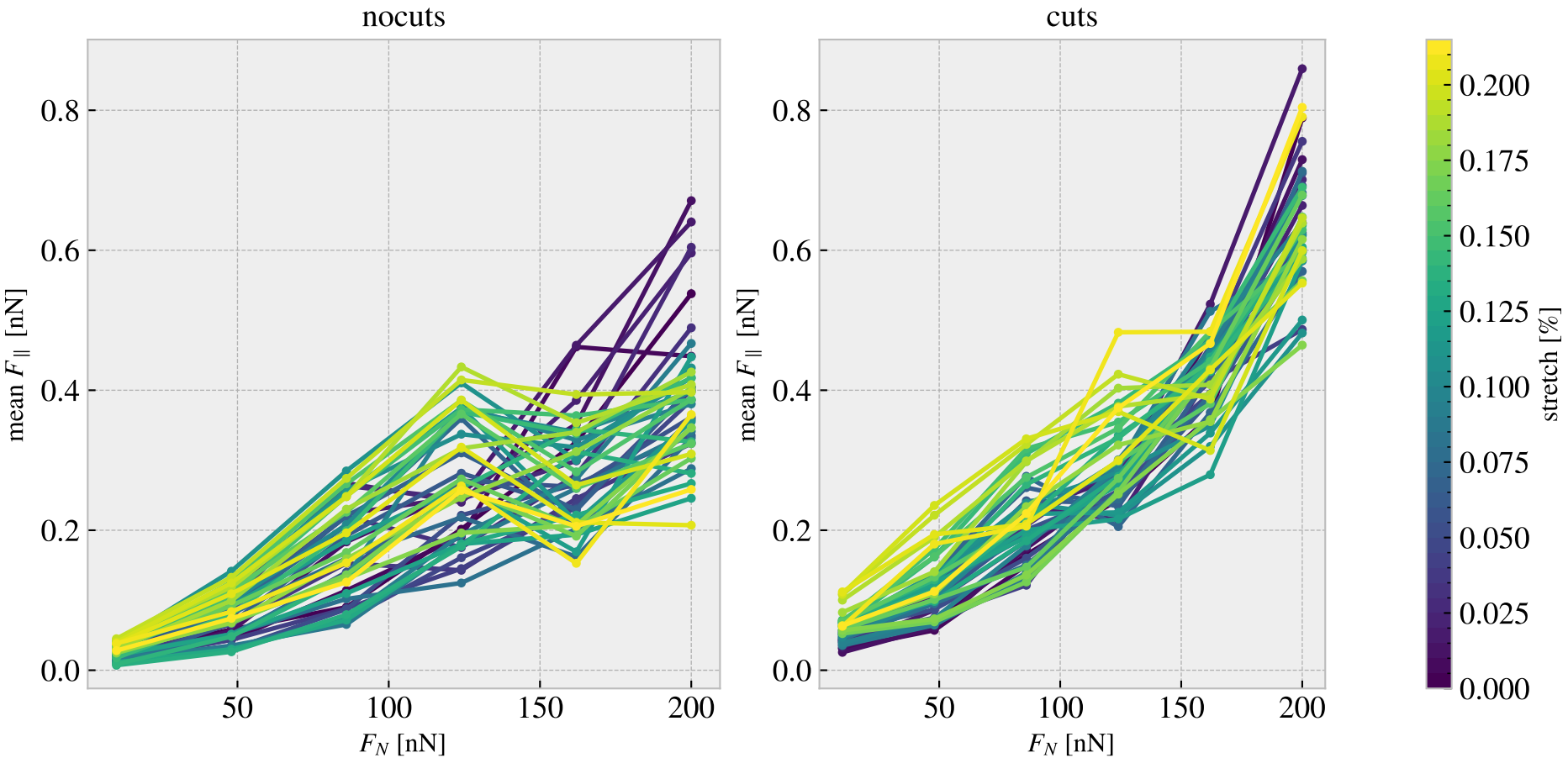

Figure: caption

Stage 2 - MD measurements

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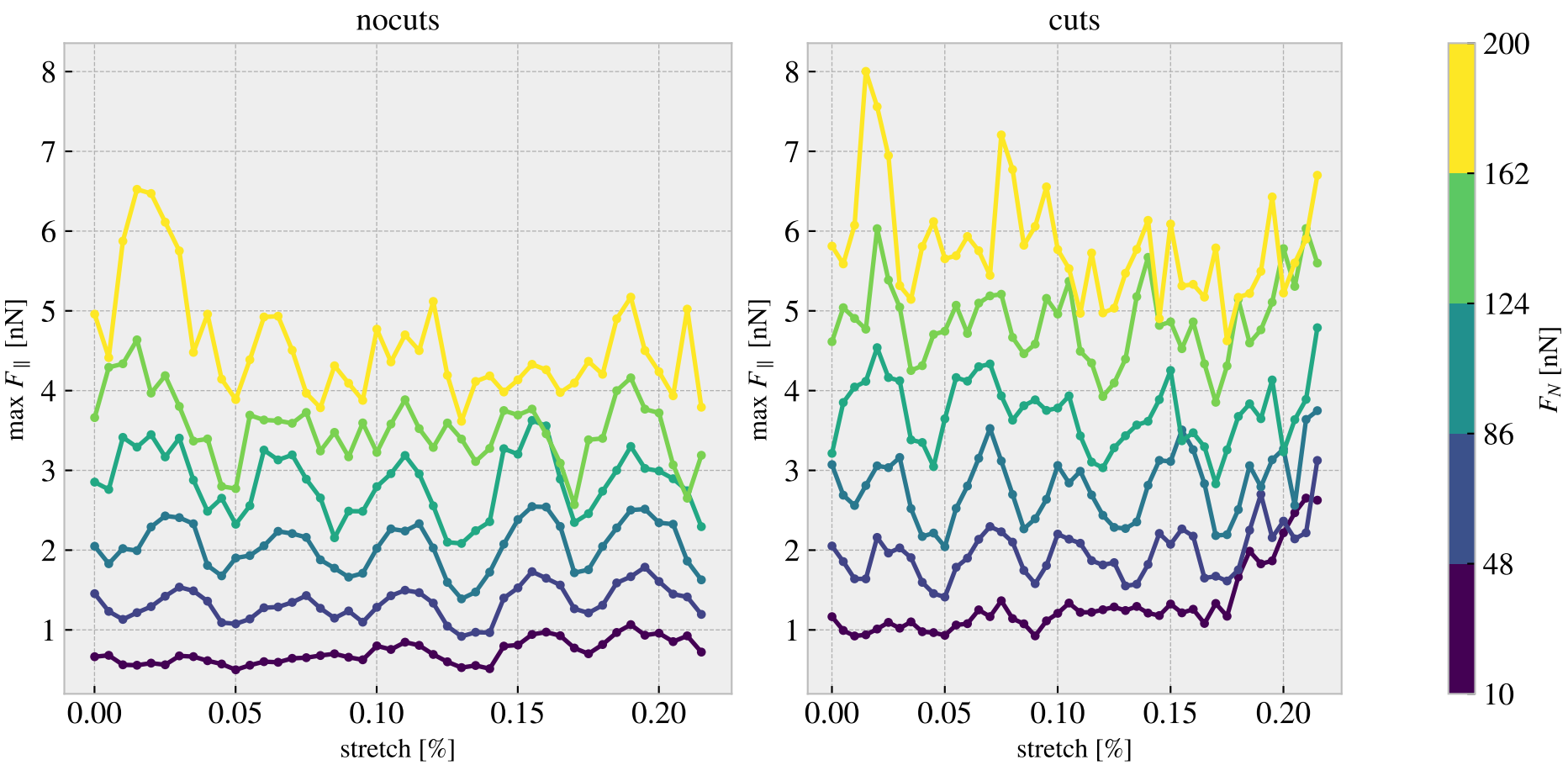

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Stage 2 - MD measurements

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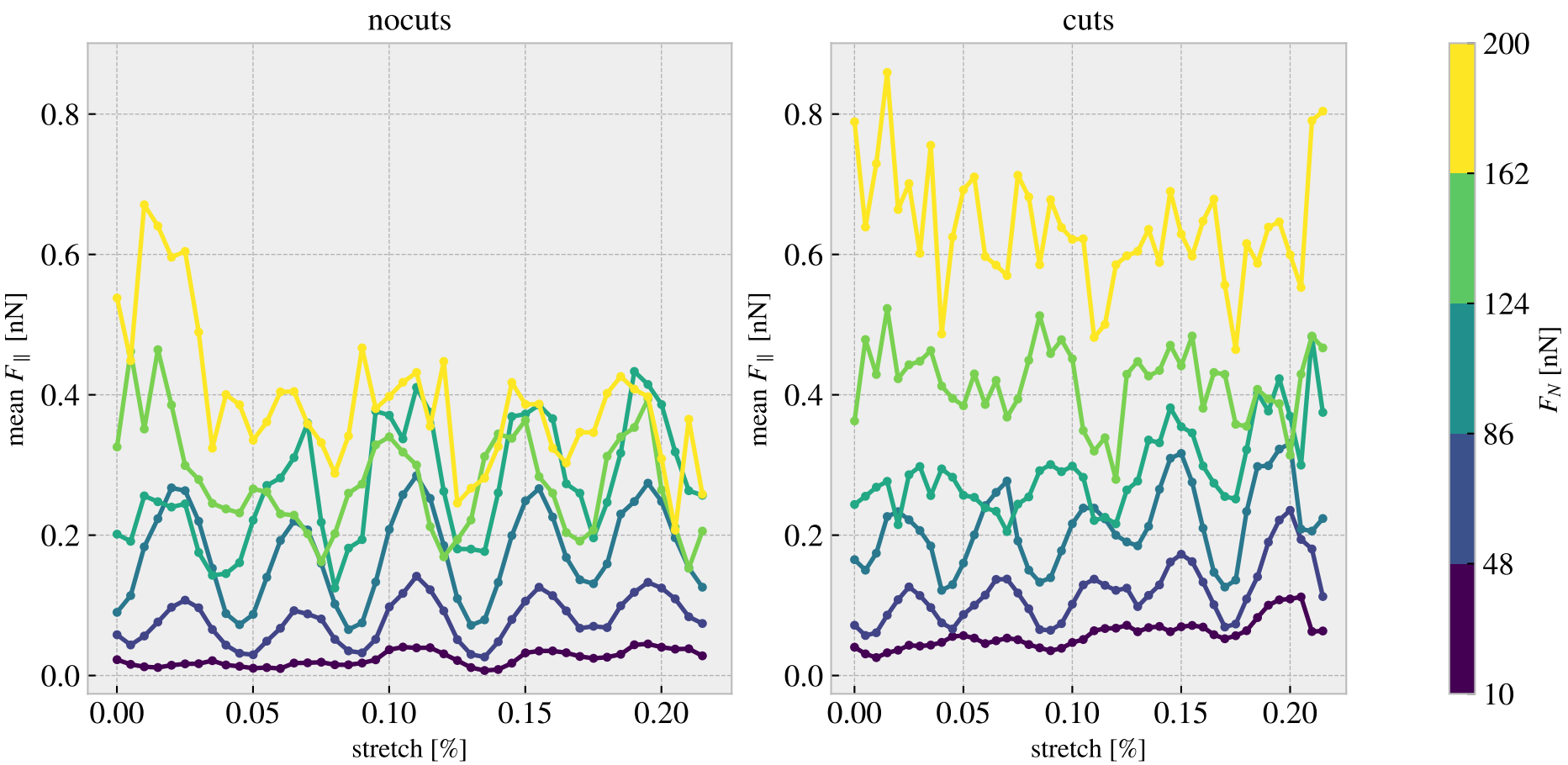

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Stage 2 - MD measurements

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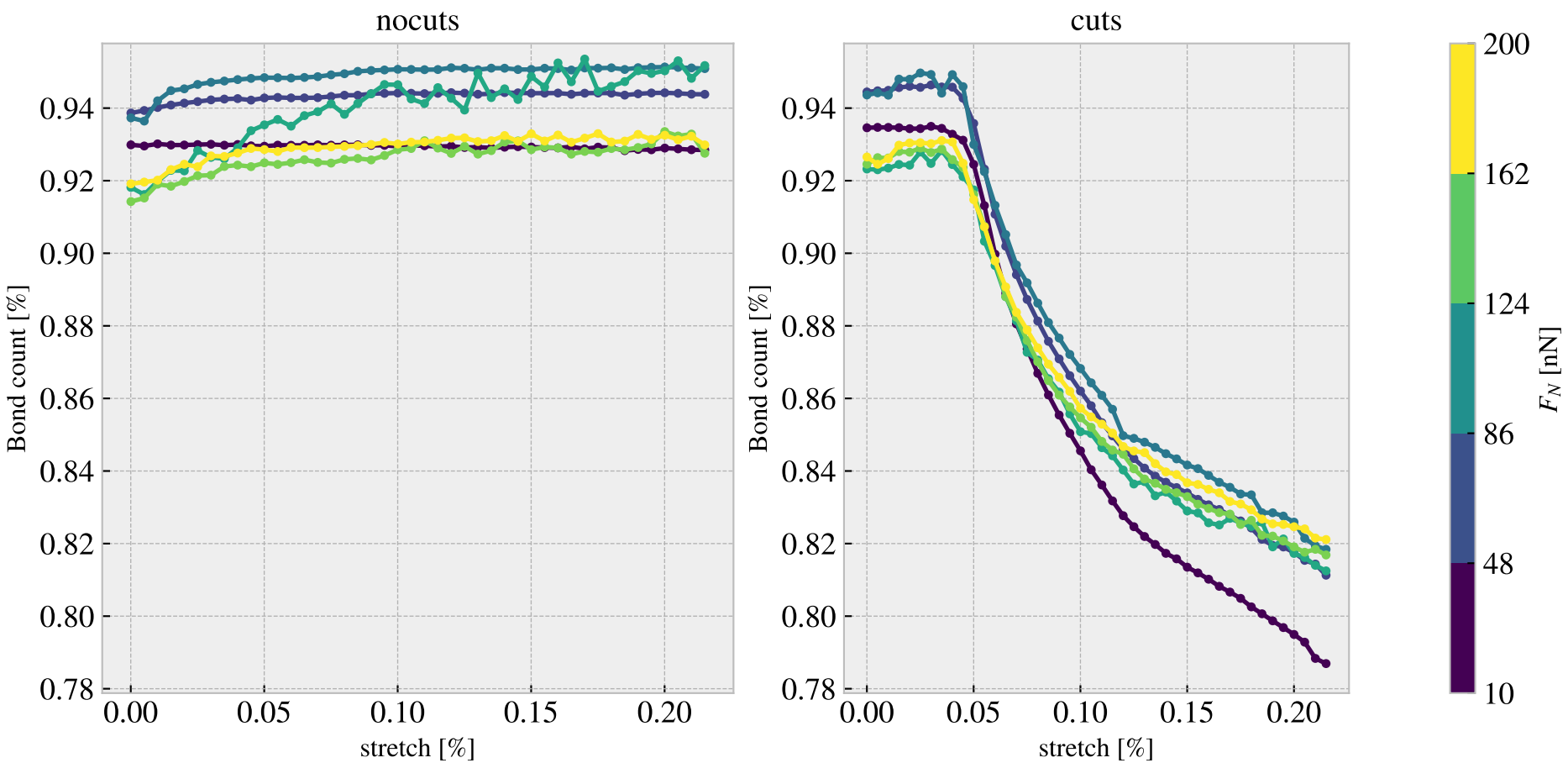

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Stage 2 - MD measurements

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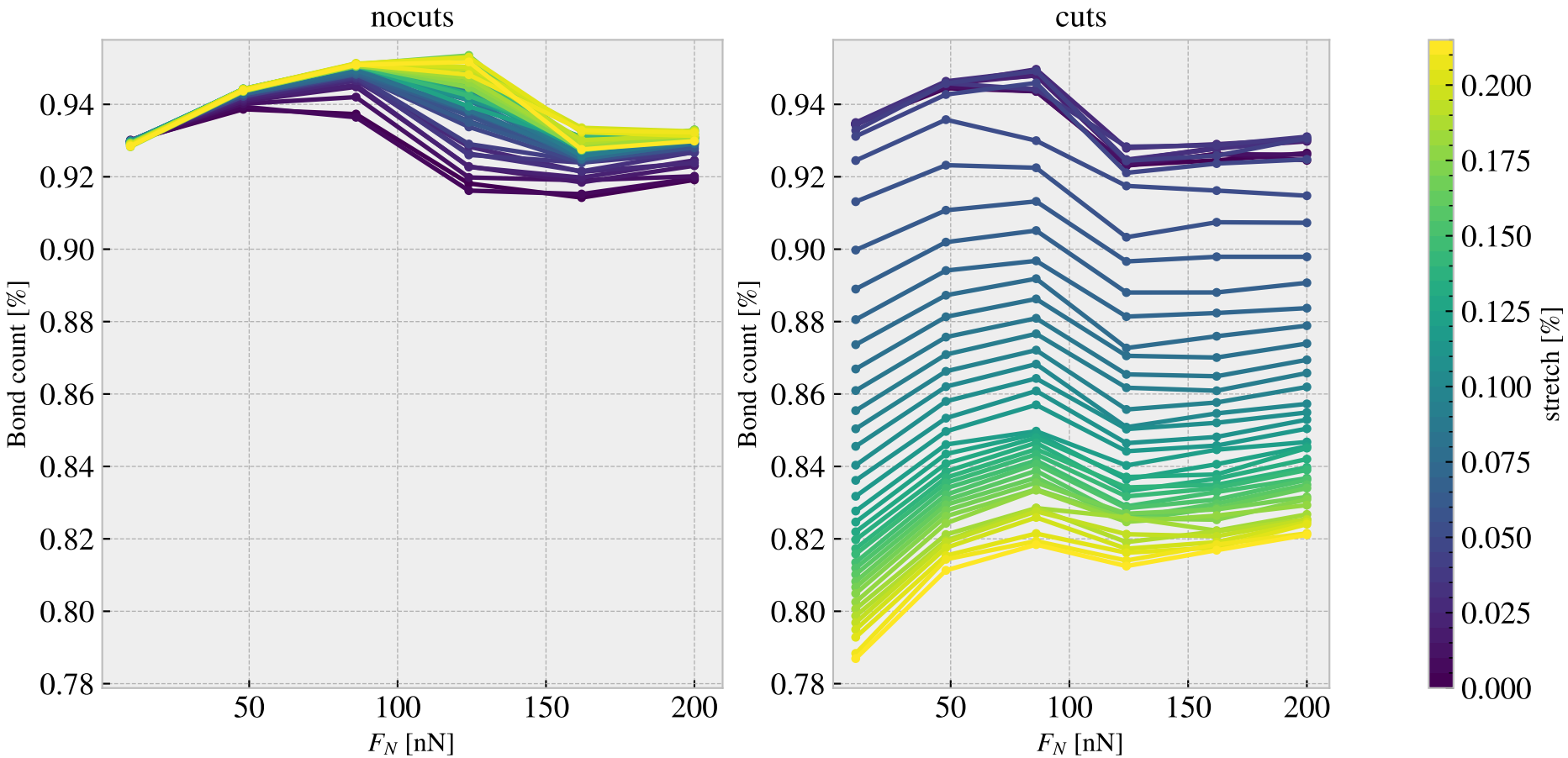

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Stage 2 - MD measurements

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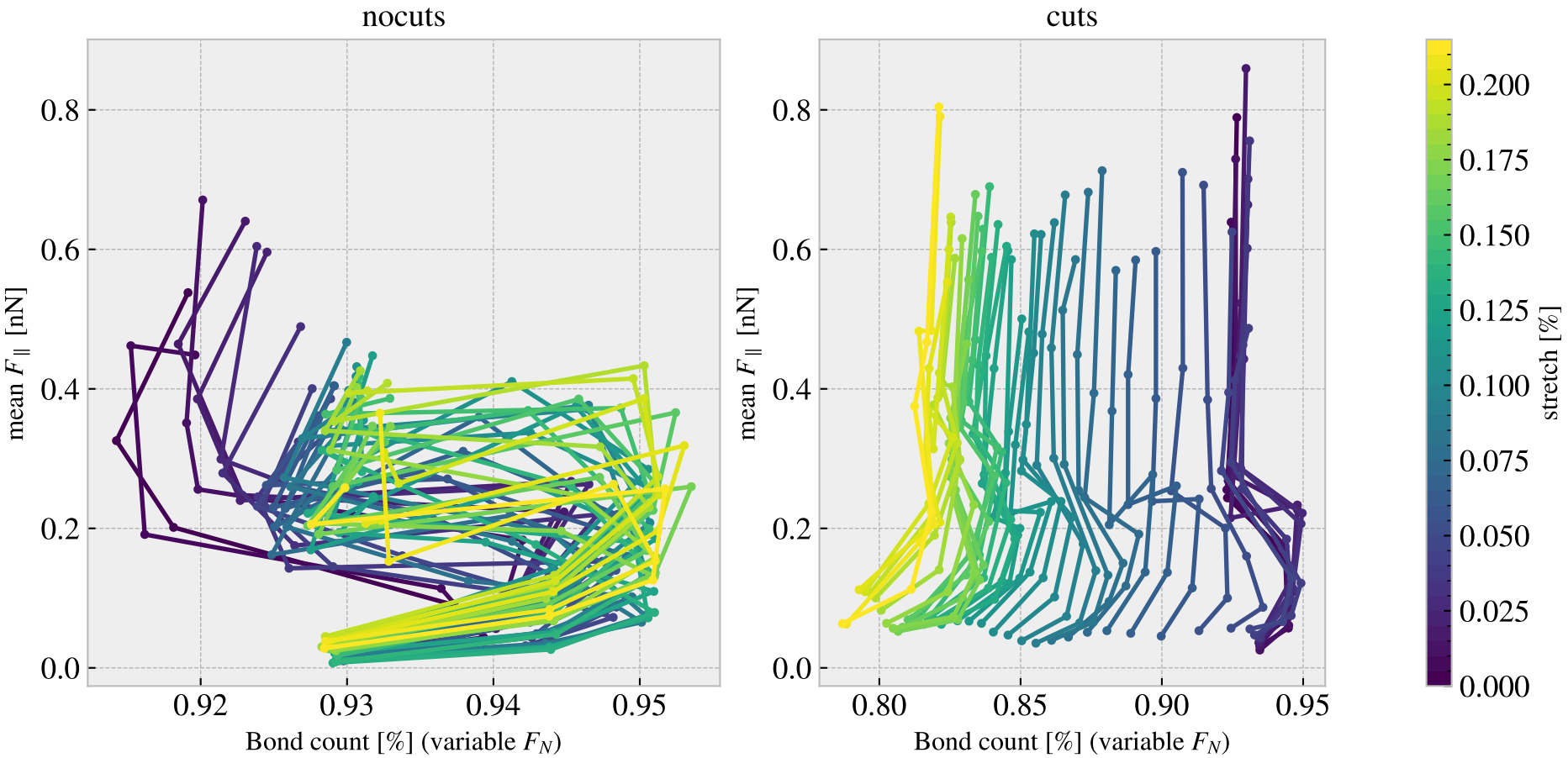

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Stage 2 - MD measurements

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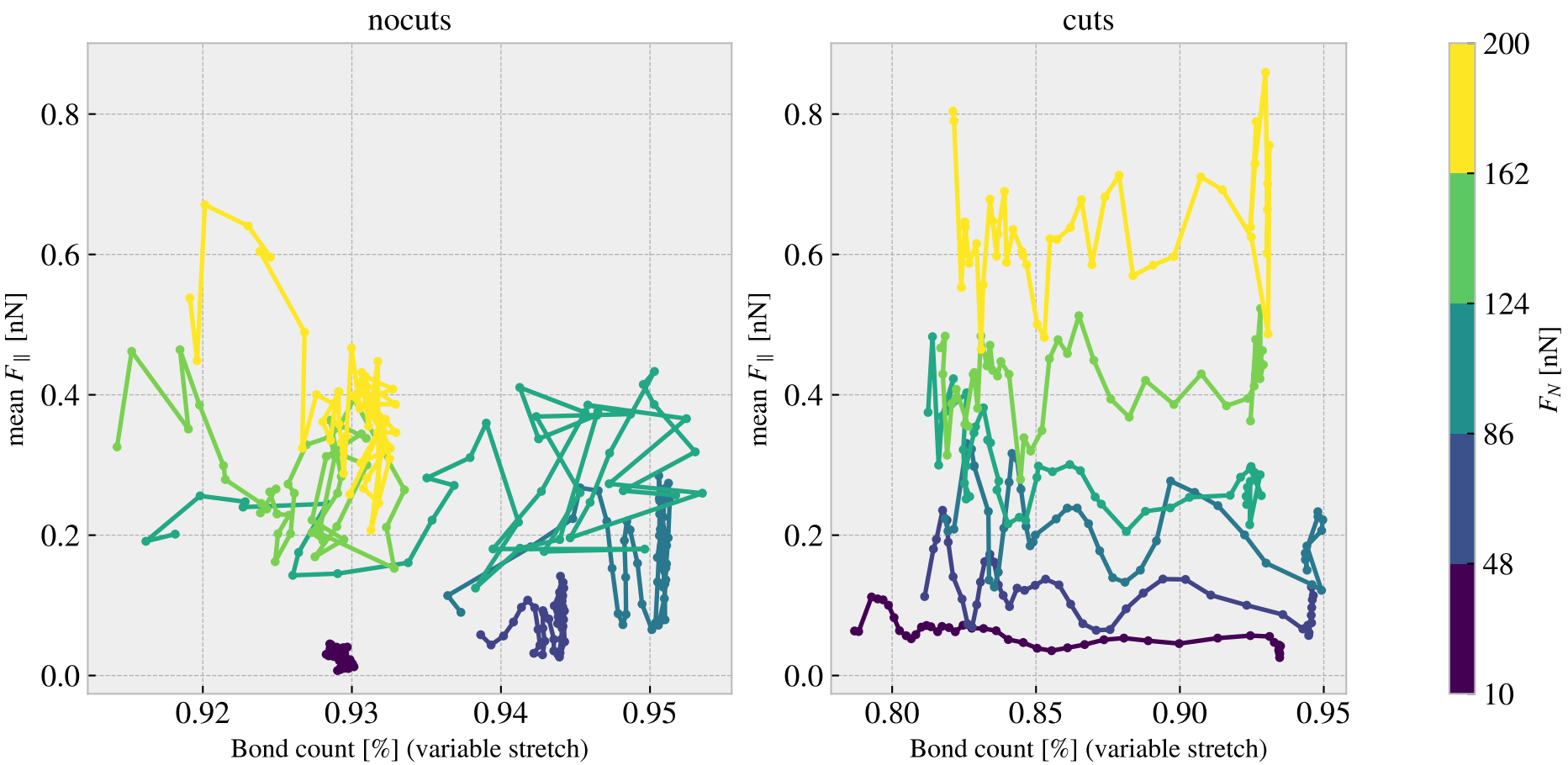

Figure: caption

Stage 2 - MD measurements

Static non-bonded regions

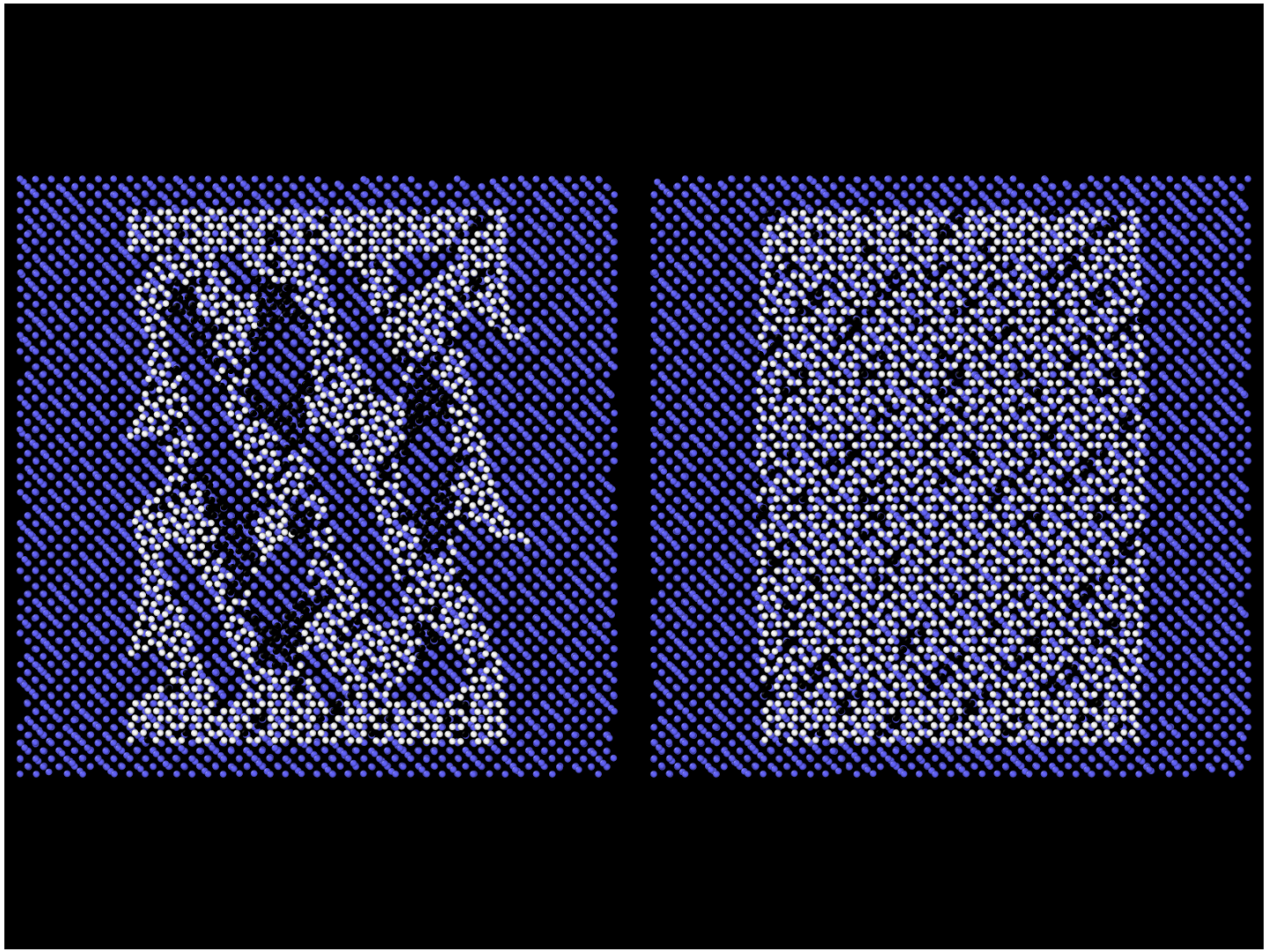

Figure: Stretch = 22 %, $F_N = 200$ nN, Drag length = 200 Å.

Paragraphs of Text

Sed iaculis dapibus gravida. Morbi sed tortor erat, nec interdum arcu. Sed id lorem lectus. Quisque viverra augue id sem ornare non aliquam nibh tristique. Aenean in ligula nisl. Nulla sed tellus ipsum. Donec vestibulum ligula non lorem vulputate fermentum accumsan neque mollis.

> *Sed diam enim, sagittis nec condimentum sit amet, ullamcorper sit amet libero. Aliquam vel dui orci, a porta odio.*
> *— Someone, somewhere...*

Nullam id suscipit ipsum. Aenean lobortis commodo sem, ut commodo leo gravida vitae. Pellentesque vehicula ante iaculis arcu pretium rutrum eget sit amet purus. Integer ornare nulla quis neque ultrices lobortis.

Lists

Bullet Points and Numbered Lists

- Lorem ipsum dolor sit amet, consectetur adipiscing elit
- Aliquam blandit faucibus nisi, sit amet dapibus enim tempus
  - Lorem ipsum dolor sit amet, consectetur adipiscing elit
  - Nam cursus est eget velit posuere pellentesque
- Nulla commodo, erat quis gravida posuere, elit lacus lobortis est, quis porttitor odio mauris at libero

1. Nam cursus est eget velit posuere pellentesque
2. Vestibulum faucibus velit a augue condimentum quis convallis nulla gravida

Blocks of Highlighted Text

Block Title

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Integer lectus nisl, ultricies in feugiat rutrum, porttitor sit amet augue.

Example Block Title

Aliquam ut tortor mauris. Sed volutpat ante purus, quis accumsan.

Alert Block Title

Pellentesque sed tellus purus. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos himenaeos.

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Multiple Columns

Subtitle

Heading

1. Statement
2. Explanation
3. Example

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Integer lectus nisl, ultricies in feugiat rutrum, porttitor sit amet augue. Aliquam ut tortor mauris. Sed volutpat ante purus, quis accumsan dolor.

Table

Subtitle

Treatments	Response 1	Response 2
Treatment 1	0.0003262	0.562
Treatment 2	0.0015681	0.910
Treatment 3	0.0009271	0.296

Table: Table caption

Definitions & Examples

Definition

A prime number is a number that has exactly two divisors.

Example

- 2 is prime (two divisors: 1 and 2).
- 3 is prime (two divisors: 1 and 3).
- 4 is not prime (three divisors: 1, 2, and 4).

You can also use the `theorem`, `lemma`, `proof` and `corollary` environments.

Theorem, Corollary & Proof

Theorem (Mass–energy equivalence)

$E = mc^2$

Corollary

$x + y = y + x$

Proof.

$\omega + \phi = \epsilon$ □

Equation

$$\cos^3\theta = \frac{1}{4}\cos\theta + \frac{3}{4}\cos 3\theta \tag{1}$$

Verbatim

Example (Theorem Slide Code)

```
\begin{frame}
\frametitle{Theorem}
\begin{theorem}[Mass--energy equivalence]
$E = mc^2$
\end{theorem}
\end{frame}
```

Slide without title.

Citing References

An example of the `\cite` command to cite within the presentation:

This statement requires citation [Smith, 2022, Kennedy, 2023].

References


John Smith (2022)
Publication title
Journal Name 12(3), 45 – 678.


Annabelle Kennedy (2023)
Publication title
Journal Name 12(3), 45 – 678.

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Smith Lab

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- Jennifer
- Yuan

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The End

Questions? Comments?