University of
California Merced

MICROSCOPY IMAGE TO MOLECULAR MODELS: BRIDGING EXPERIMENTS AND SIMULATIONS

TRIBOLOGY

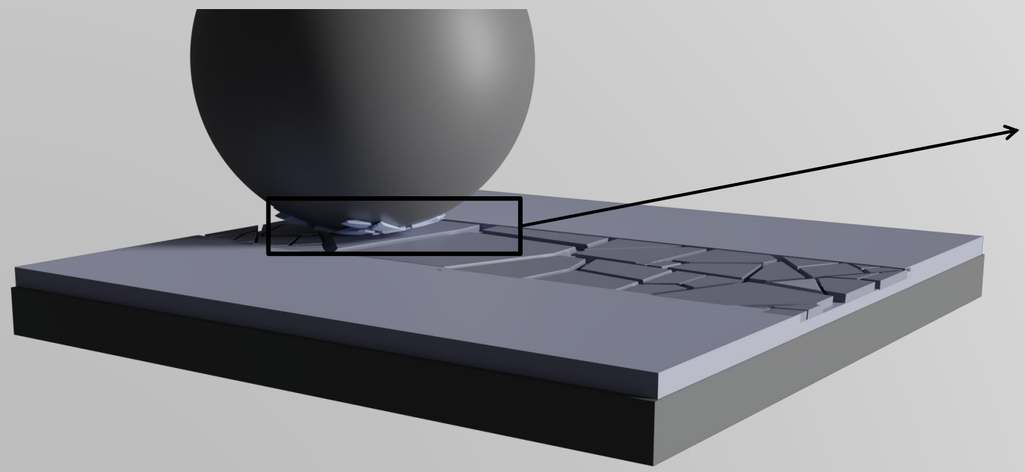
- Tribology can be defined as the science and technology of interacting surfaces in relative motion, and includes the study of friction, wear and lubrication – ScienceDirect

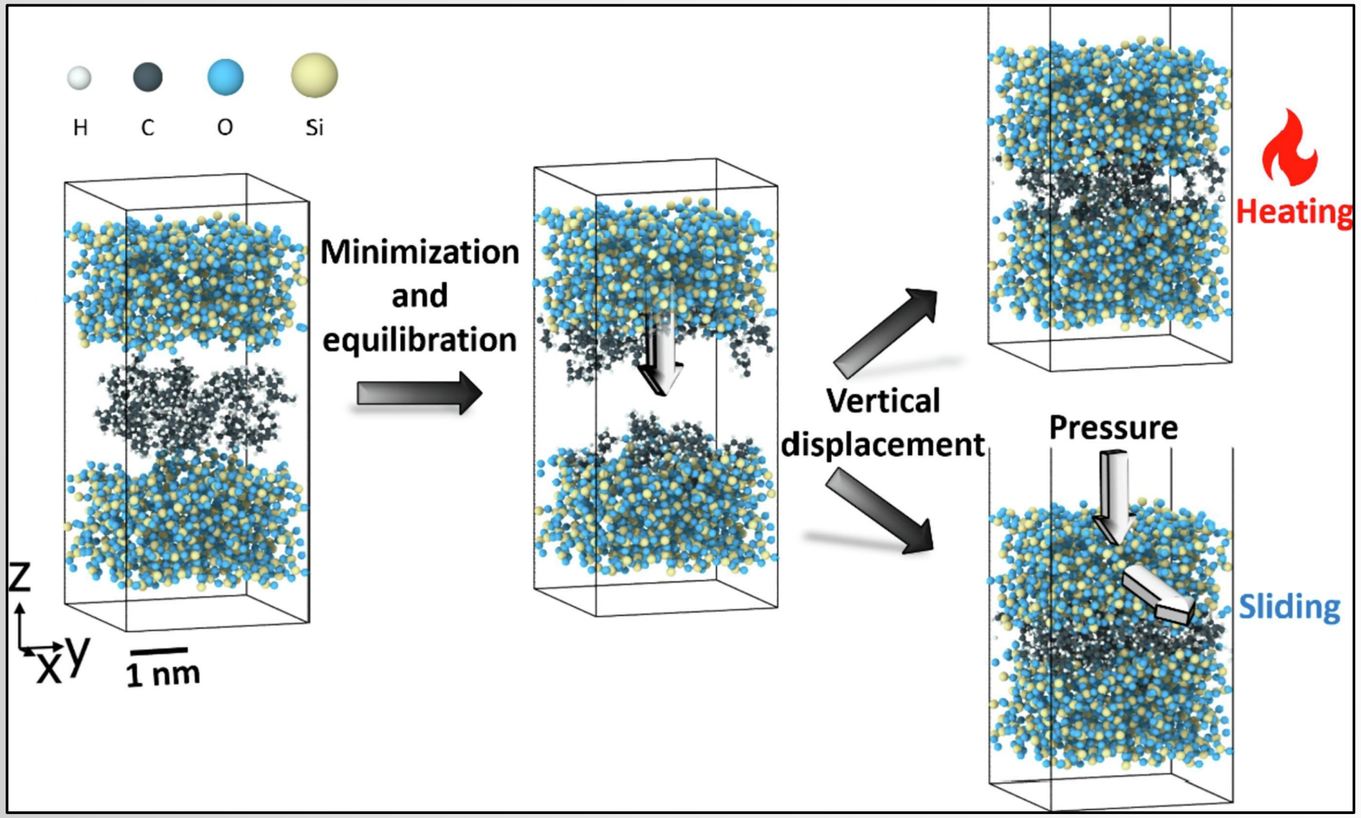
EXPERIMENTS

- In our laboratory, an exceptional team of experimentalists is dedicated to exploring the intricate dynamics of surface interactions.
- They meticulously investigate how various surfaces respond when subjected to specific lubricants, unveiling crucial insights that contribute to optimizing performance in diverse applications.

SIMULATIONS

- Experimental work gives us quantitative data on how different lubricants on different surfaces effect the tribological properties test specimens
- We pick up the torch from this point by delving into Molecular dynamics simulations where we can observe at an atomic level why the lubricants and surfaces are behaving as they are.

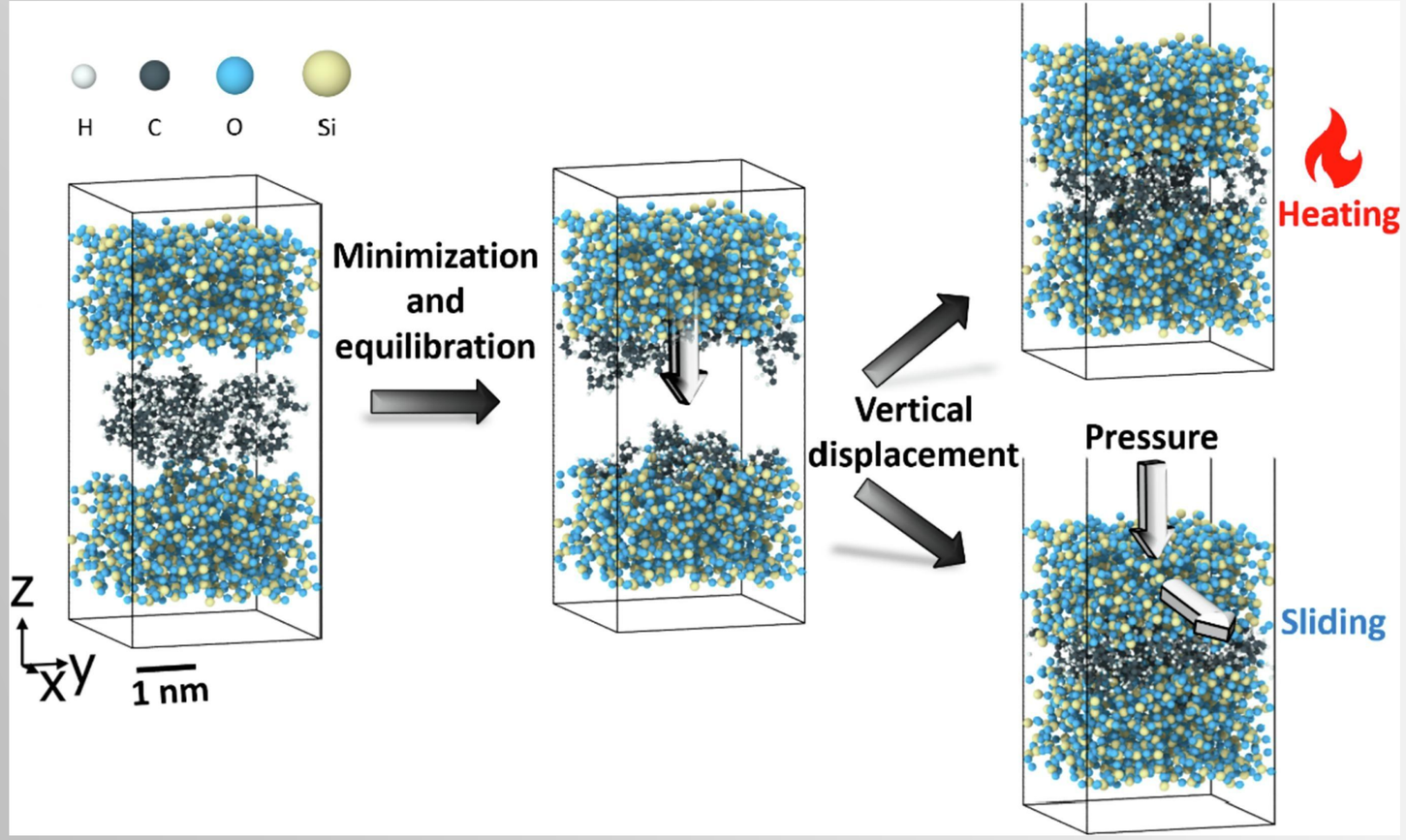




Bhuiyan, Fakhrul H., Seong H. Kim, and Ashlie Martini. 2022. *Applied Surface Science* 591 (July): 153209.

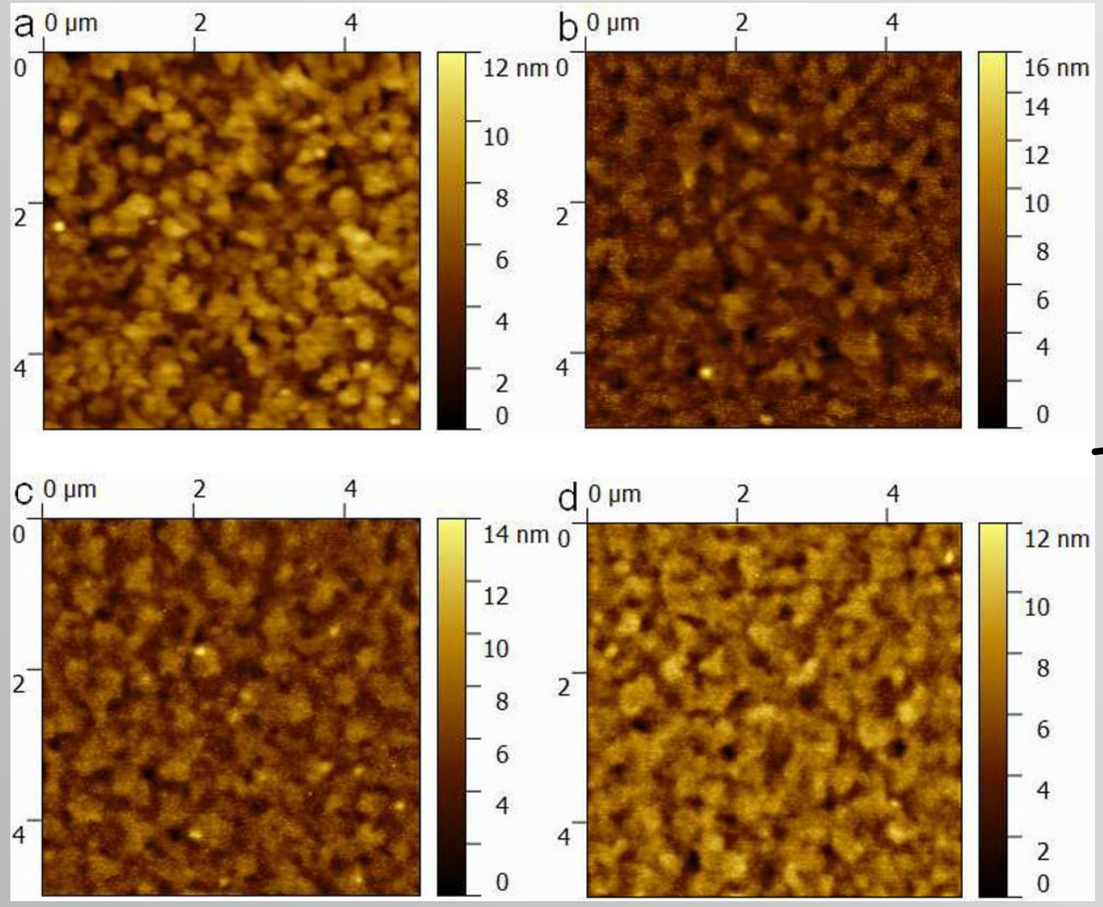
REPLICATING EXPERIMENTAL CONDITIONS

- In simulations, we are bound to thousands to few millions of atoms due to constrains imposed by computational resource
- Systems to be tested using simulations need to be modeled carefully considering the experimental phenomenon that we want to study

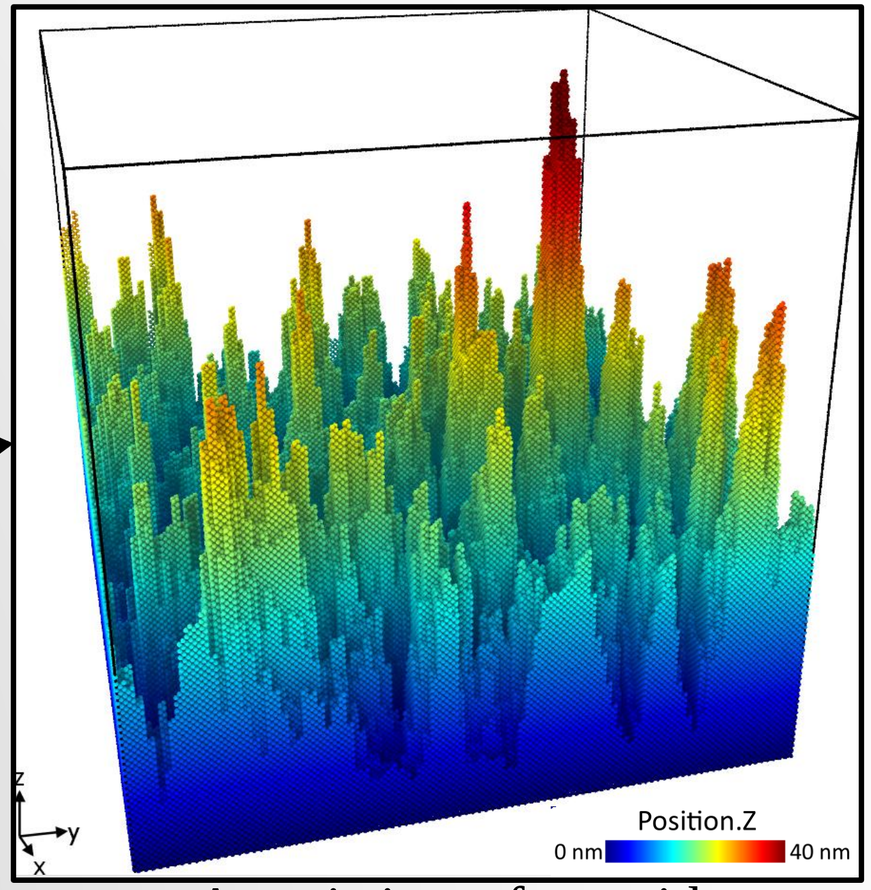


THE GOAL

- For my final project, I tackle a part of the challenge of designing realistic simulations by trying to create realistic surfaces



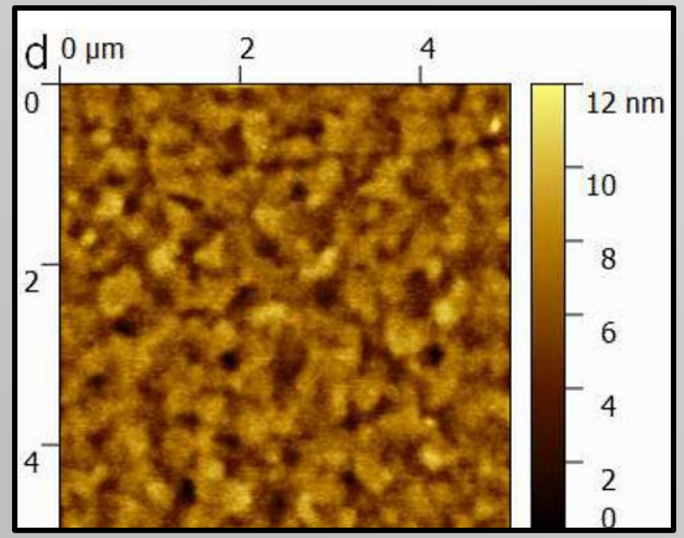
AFM image of a surface



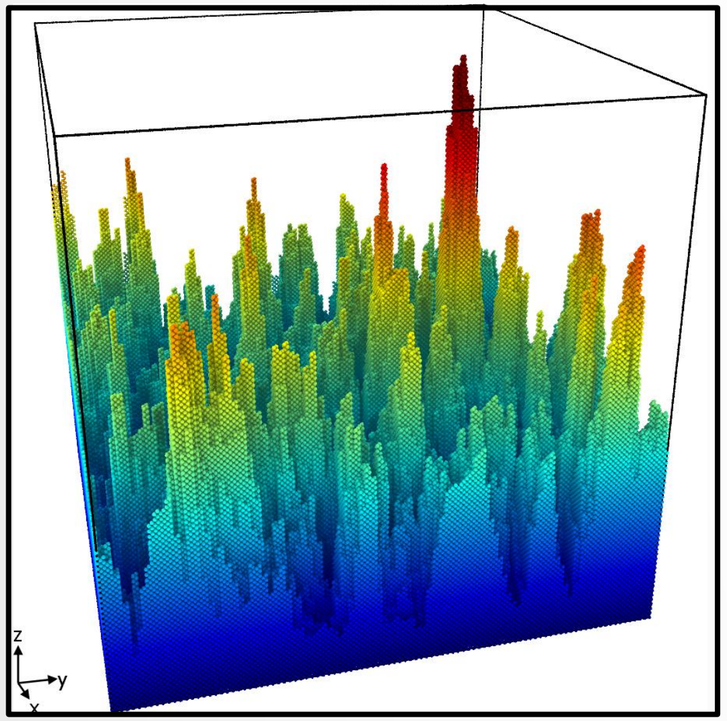
Atomistic surface with imprinted surface roughness

Ji, Wenyu, et. Al. *ACS Photonics* 4 (5): 1271–78.

FILLING IN THE GAPS



Some Python Magic



PYTHON MAGIC

- What packages to use?

```
import os
from PIL import Image
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
```

CONVERTING TO BLACK AND WHITE

- First, we write a function which converts the AFM image to black and white.

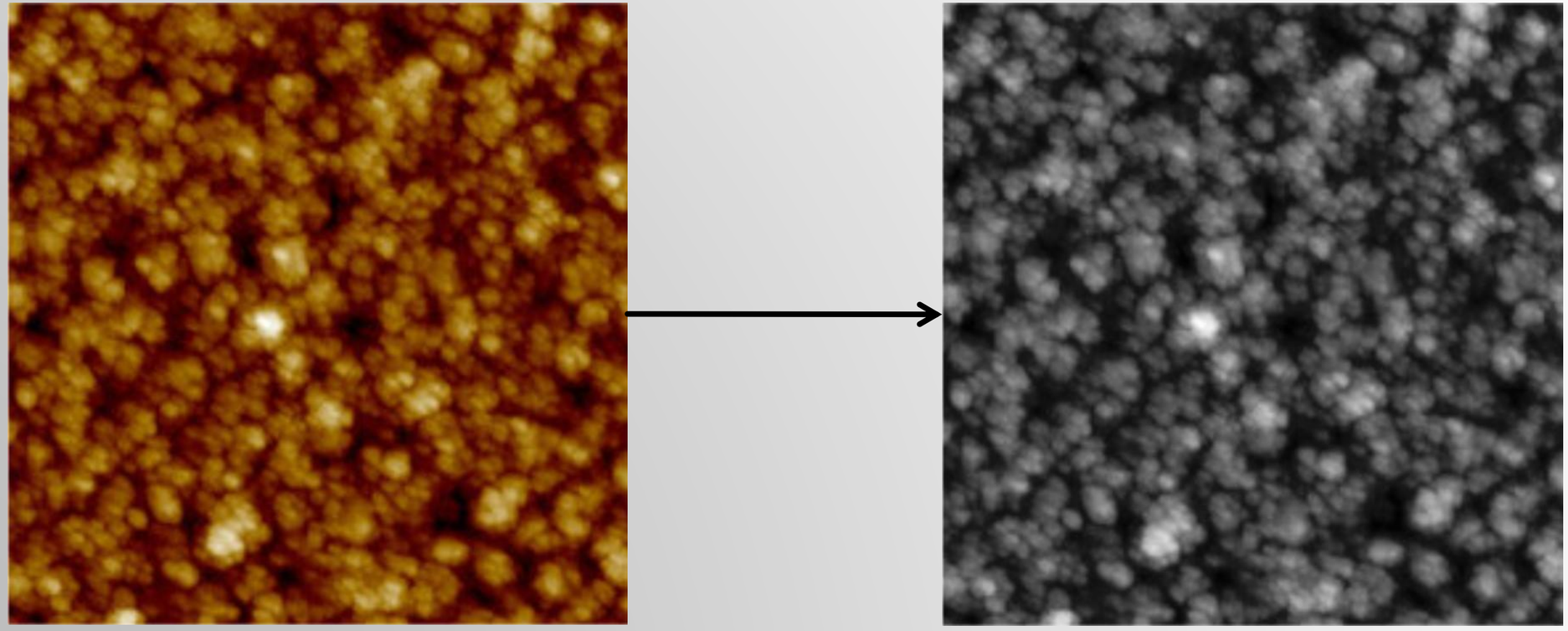
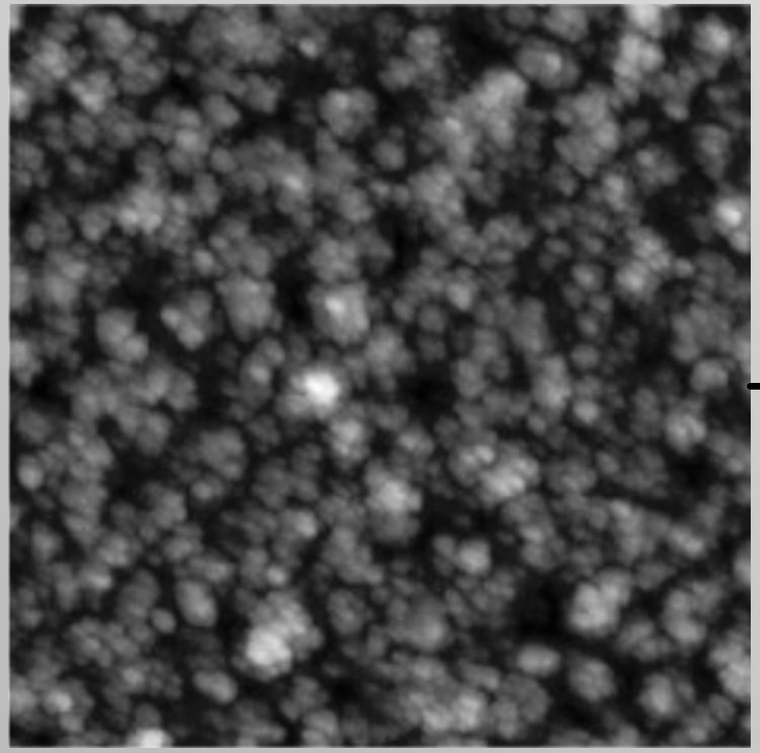


IMAGE TO COORDINATES

- Extract the coordinates from the image- with some extra steps
  - Normalizing coordinates along X and Y axis
  - Binning values along Z axis



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2   0.0009765625 0.0029296875 0.84
3   0.0009765625 0.0048828125 0.82
4   0.0009765625 0.0068359375 0.80
5   0.0009765625 0.0087890625 0.81
6   0.0009765625 0.0107421875 0.82
7   0.0009765625 0.0126953125 0.84
8   0.0009765625 0.0146484375 0.84
9   0.0009765625 0.0166015625 0.83
10  0.0009765625 0.0185546875 0.83
11  0.0009765625 0.0205078125 0.83
12  0.0009765625 0.0224609375 0.83
13  0.0009765625 0.0244140625 0.84
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15  0.0009765625 0.0283203125 0.85
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17  0.0009765625 0.0322265625 0.86
18  0.0009765625 0.0341796875 0.84
19  0.0009765625 0.0361328125 0.85
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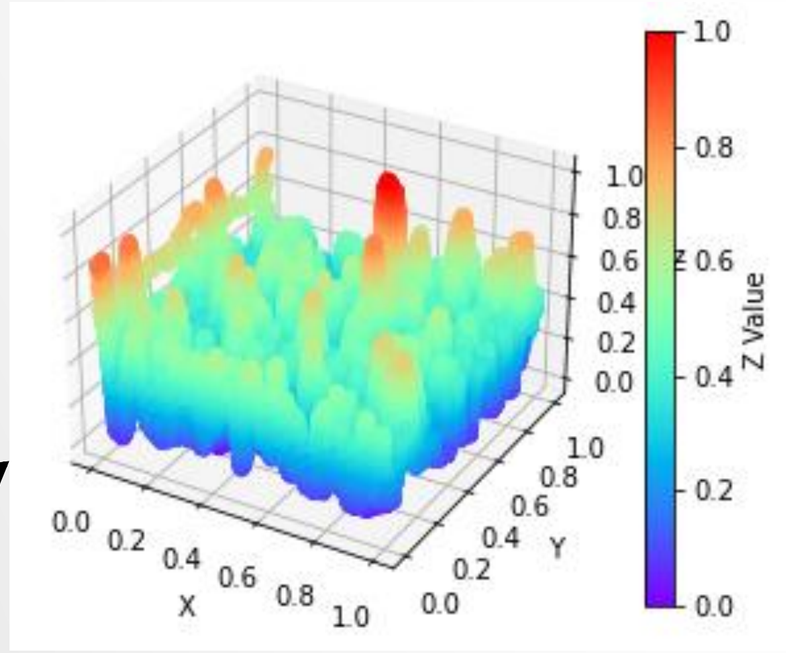
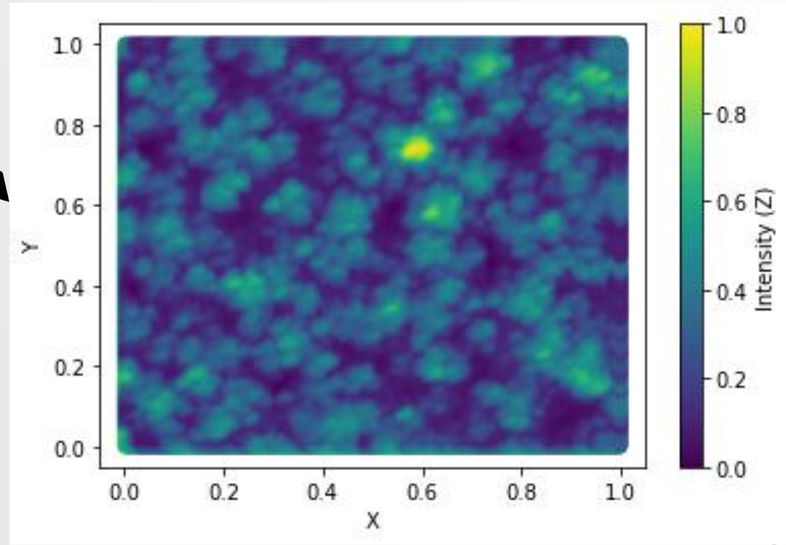
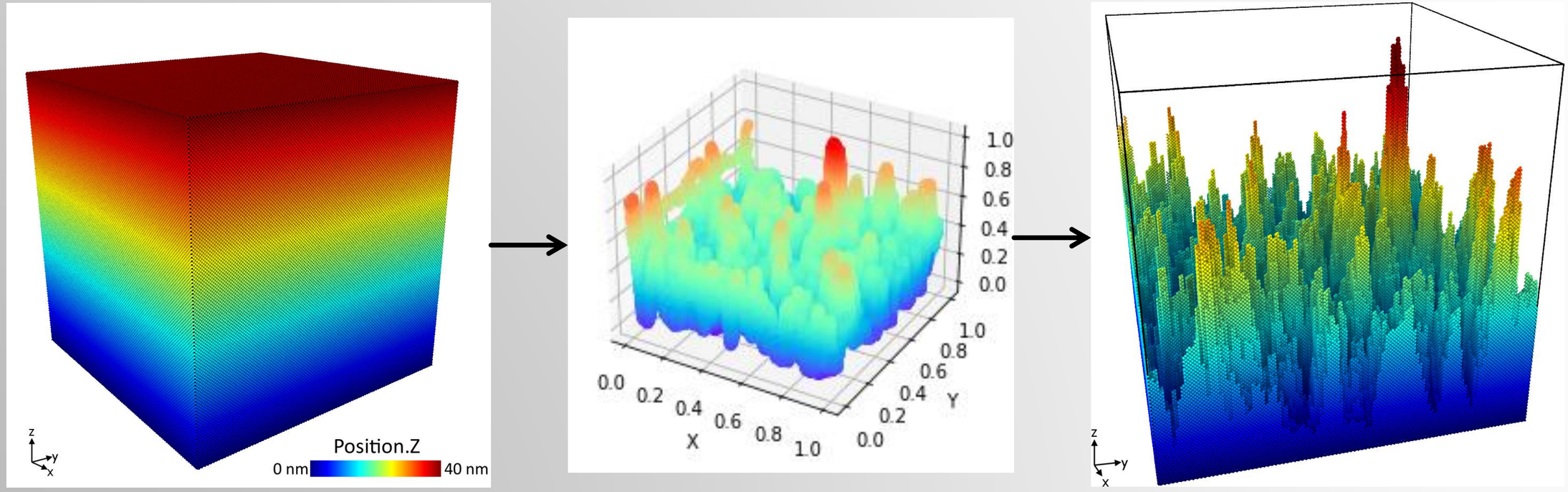




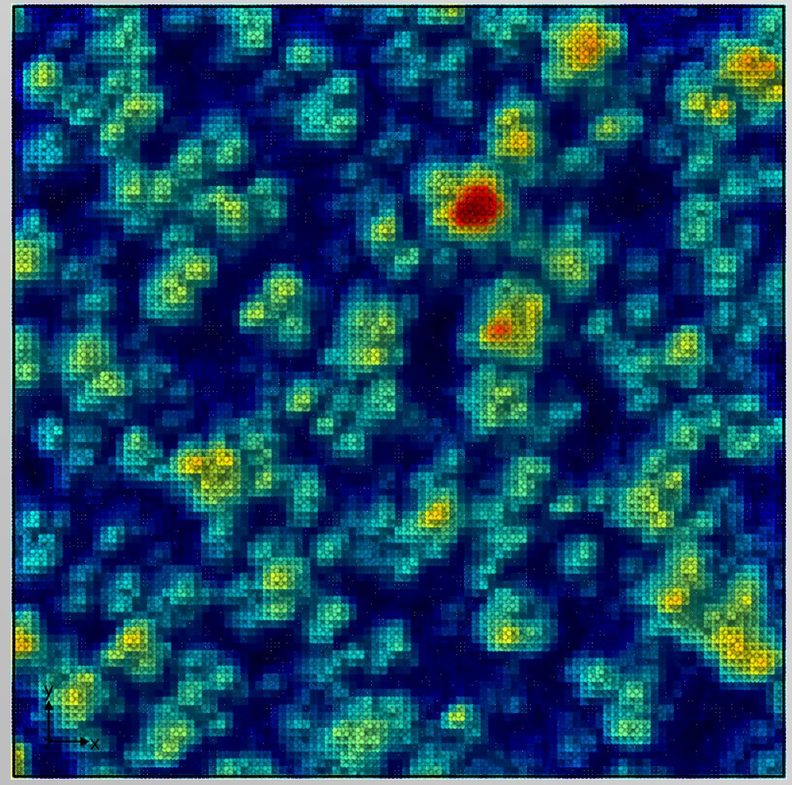
BASE STRUCTURE IMPORT AND PROCESSING

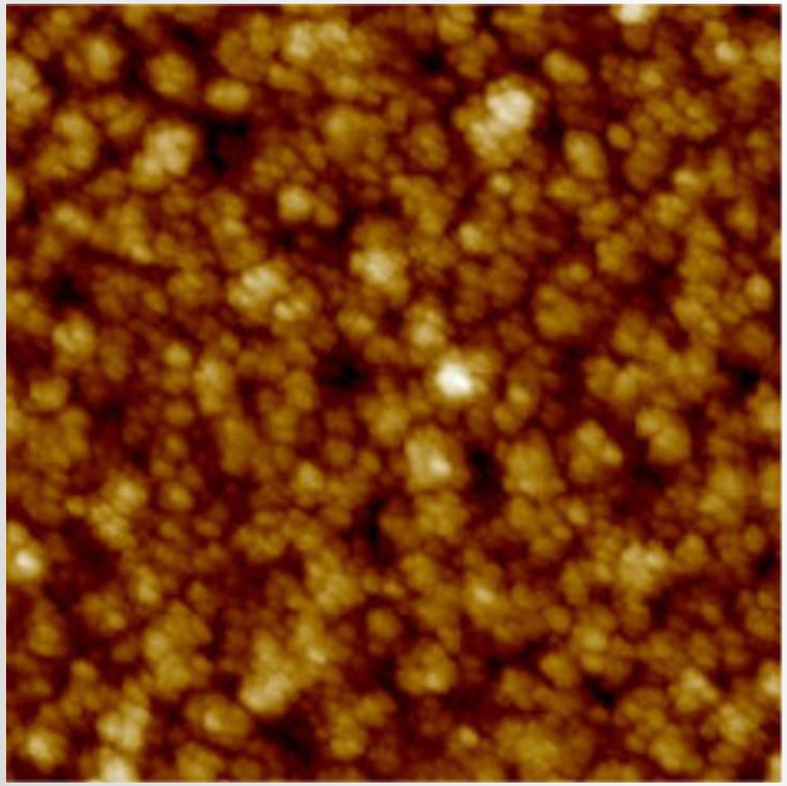
- Next, we import the base structure from which we will make the final structure by removing atoms
- Then we use the 3D point data obtained from the AFM image and use it to select out atoms we need to remove to create the final structure



SANITY CHECK

- Next, we import the base structure from which we will make the final structure by removing atoms



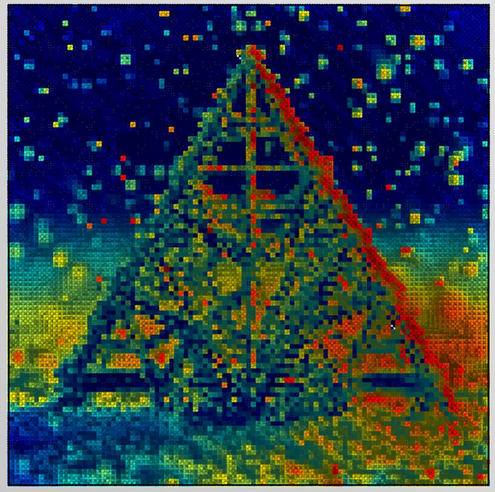


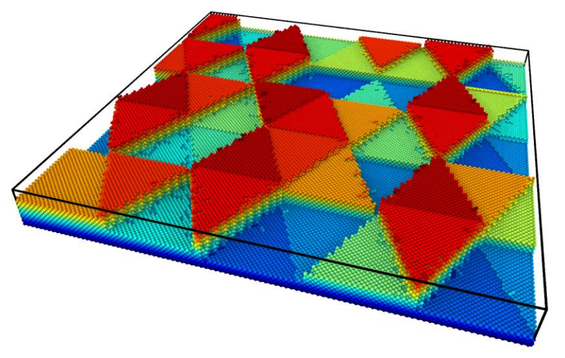
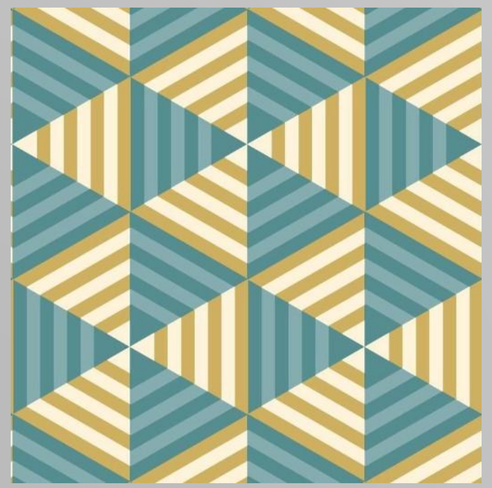
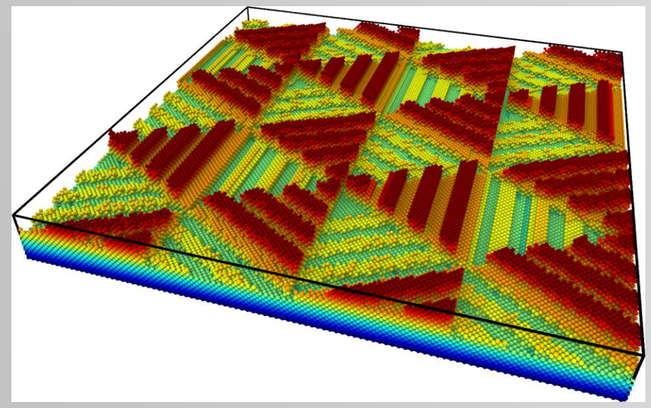
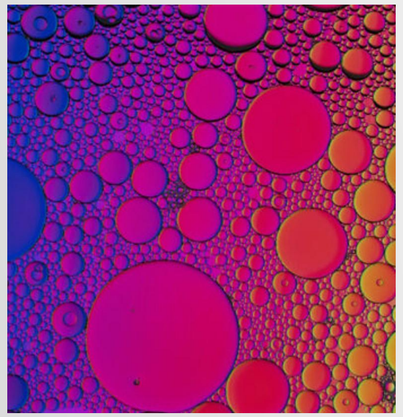
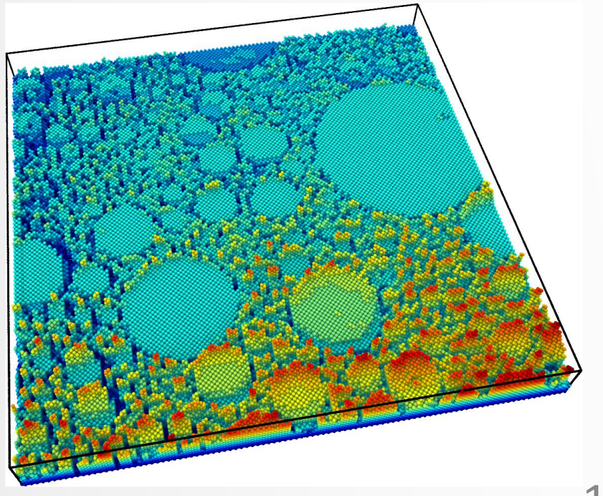
LIMITATIONS AND NEXT STEPS

- The method I developed requires normalization of the image data and the atomistic data, this disregards the actual height of the roughness- for now the quick workaround is using the base structure having z height equal to the roughness height mentioned in literature
- In atomistic simulations we generally use periodic boundaries, as of now my code does not have periodicity- for my next step I will look into algorithms to create periodic images from non periodic images to solve this problem

STRENGTHS

- The code I made is agnostic to input image and input structure crystallinity, this allows me to make imprint any image over any atomistic surface

LIVE DEMO

- Let's paint the Mona Lisa with atoms

THANK YOU

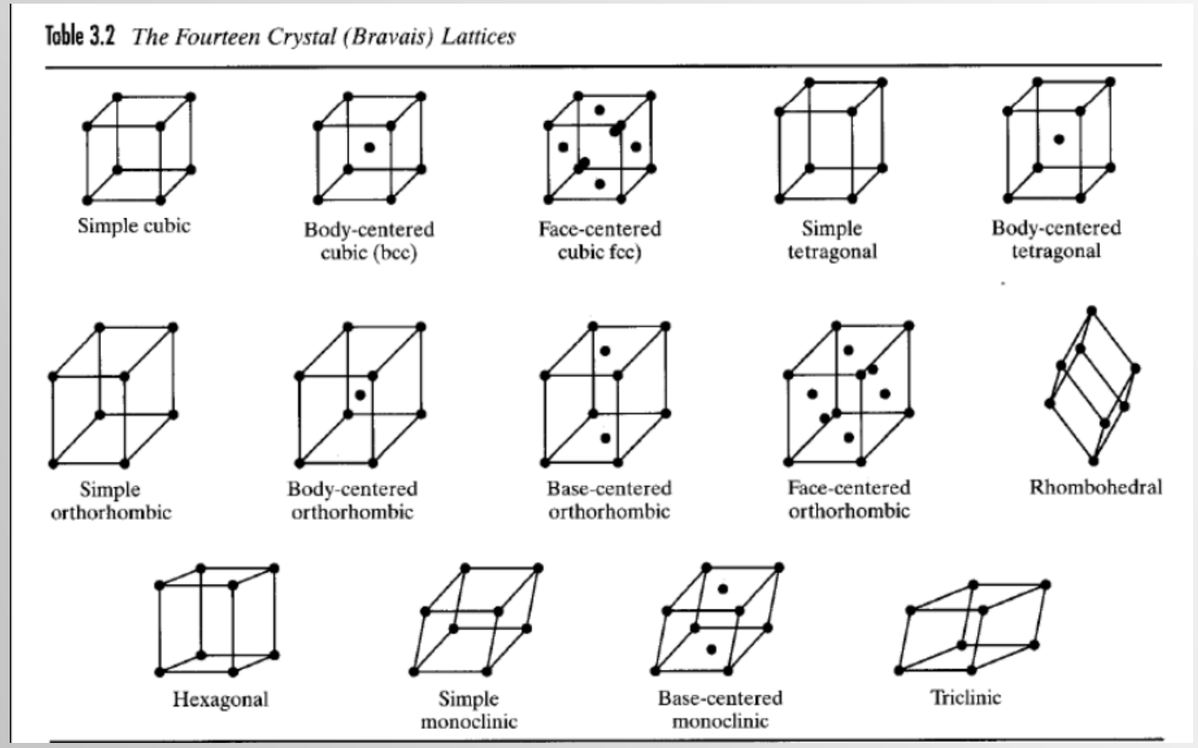
Special thanks to ChatGPT

University of California Merced

Martini Research Group

STRUCTURE VARIATIONS

- The base structure we need may be of different structures- ranging from crystalline lattices like FCC or BCC all the way to amorphous surfaces, this makes defining the structures much more difficult



HANDELING STRUCTURAL VARIATIONS

- Normalizing coordinates and snapping proxy identifiers of atoms into grids