SUPPLEMENTARY MATERIAL

The effect of density and surface topography on the coefficient of friction of polytetrafluoroethylene films

Mathew Brownell[1] and Arun K. Nair[1,2,*]

[1] *Multiscale Materials Modeling Lab, Department of Mechanical Engineering, University of Arkansas, Fayetteville, AR, USA.*

[2] *Institute for Nanoscience and Engineering, 731 W. Dickson Street, University of Arkansas, Fayetteville AR-72701.*

[*] Corresponding author, electronic address: nair@uark.edu; Phone: +479-575-2573, Fax: +479-575-6982

Convolutional neural network (CNN) architecture and validation

The convolutional neural network is written in Python [1] using the Pytorch [2] package and is described in Figure S1. Each convolutional layer uses a 2x2 filter size, a stride of 1, and a ReLu activation function. Max pooling layers have a pooling size of 2x2 and stride of 1. After the layers have been flattened, the density of the film is added to the flattened 128 filters to create 129 nodes, which are all fully connected to one single output (see Figure S1). The single output is compared to the coefficient of friction calculated during molecular dynamics tests to find the loss of the network. Parametric tests were performed on preliminary data to optimize network performance.

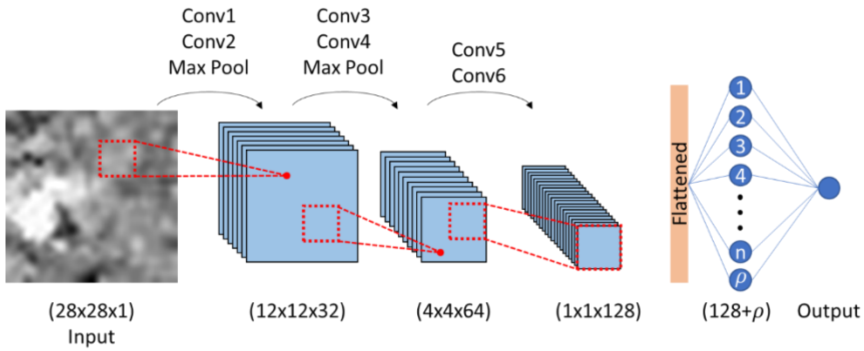

Figure S1 Convolutional neural network architecture. Notice that density (ρ) is added onto the fully connected layer once the filters are flattened.

A validation of the network was conducted by training and testing on the CIFAR-10 dataset [3], using the same network architecture except the number of outputs. A secondary network validation was performed on the AFM images classifying which annealing category the image belonged. The percent of correctly predicted images for the CIFAR-10 and AFM images were 64.41% and 91.53% respectively. The network presented throughout the rest of this work uses only one output, intended to predict the coefficient of friction of the input image.

Chain length and the effect on image resolution

Because we are attempting to use a CNN to predict the coefficient of friction of PTFE films, we need to design the type of images used as inputs. The size of the image was selected to be 28x28 pixels, which span a 92 nm square film. Because the number of pixels was selected to match a specific area of the film, the image input into the network have a limited resolution. Each pixel represents 3.28 nm of the model. When PTFE chain lengths of 54 Å are used, we reduce the number of pixels an individual PTFE chain spans, increasing the definition of the images. A PTFE chain with a length of 108 Å could span up to 4 pixels ($180 \div 32.8 = 3.29$), which would reduce the definition and decrease the networks ability to distinguish features on the surface of the film.

Indenter radius results and discussion

To compare with other studies, we investigate how the variation in indenter radius affects the COF. PTFE chains of 54 Å are used to create films with a density of approximately 1 g/cm3. Indenter radius varied from 8, 12, 16, 24, and 32 nm in diameter. Due to indentation on the film as well as stick slip between PTFE layers, the initial COF value was negative, however, after 20 Å each indenter had scratched past the initial indentation point and into more stable COF values (Figure S2A). The COF values at 3 nm are averaged and the standard deviation taken to plot the results in Figure S2B.

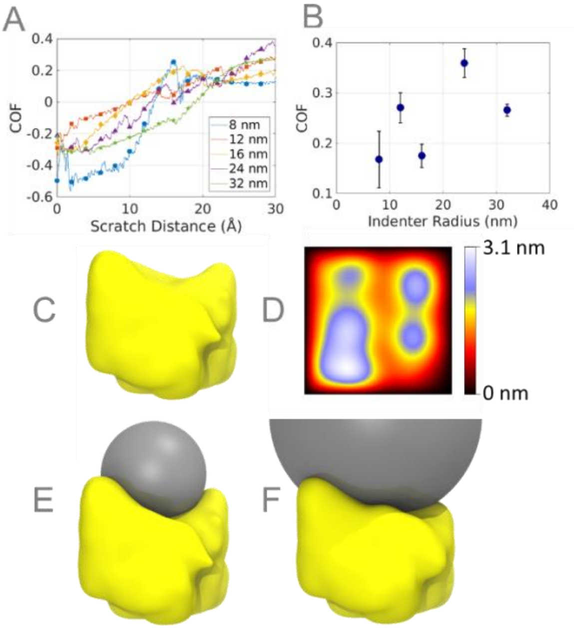

Figure S2 A) Plot of COF vs scratch distance. B) Plot of the COF vs indenter radius. C) Image of the center of the PTFE film before indentation and scratch. D) Topography map of the center of the PTFE film before indentation and scratch, showing the peaks and valleys each indenter would contact during indentation. E) Image of 8 nm indenter showing the indenter sitting within the peaks and F) 16 nm indenter sitting on top of the peaks.

The 8 nm indenter experienced a change in the COF at the midpoint of the scratch due to the topography of this particular model (Figure S2 C&D). The 8 nm indenter sits inside the valley surrounded by the peaks of the PTFE film (Figure S2 E), but the indenter sits on top of all the valleys when it is as large as 16 nm (Figure S2 F) To capture how the COF changes with topography in further simulations, we selected the 12 nm indenter radius because it was small enough to observe the COF changes due to topography height, but not too small to result in major spikes of COF values.

To ensure our models were accurately representing PTFE films, a spherical indenter with a radius of 120 nm was used to calculate the COF of films and compare to experimental results. The maximum COF calculated from our simulations with a larger indenter tip was 0.064, within the range of experimental films created similarly to the ones used to form our CG models, which report COF values between 0.06-0.1 [4].

Comparison of 3 nm and 30 nm scratch length

Because we are attempting to simulate data to use in a machine learning program, the amount of time each simulation can run must be kept short. By decreasing the time to perform simulations, we can create more data which is necessary in a CNN. Additional scratch tests were performed to investigate the differences between a 3 and 30 nm scratch length. During these scratch tests we observed the transient regime to be within the first 2 nm. The last 1 nm which we present in the manuscript contains the beginning of the saturated values of the COF. For the duration of the 30 nm scratch, the COF closely follows the surface topography, as seen in Figure S3 A.

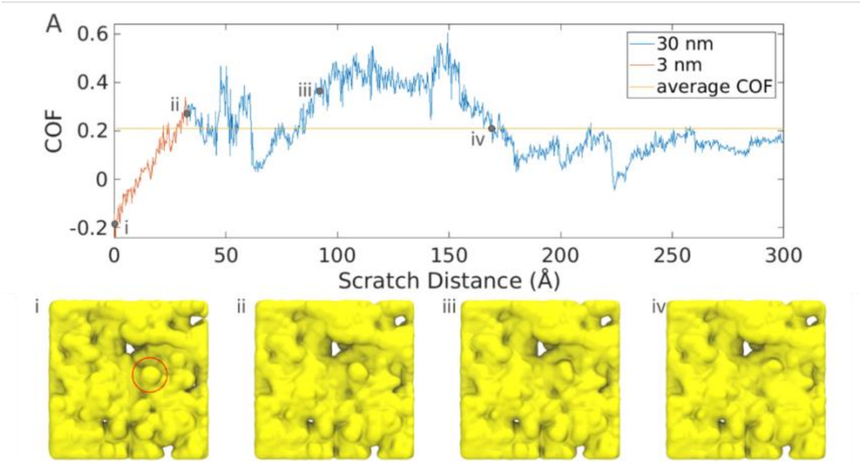

Figure S3 A) Plot of the coefficient of friction of a 54 Å chain model scratched for 300 Å (blue). The results for the first 30 Å are used in the CNN. After the first 20 Å, the COF exhibits behavior particular to the topography of the film. i) The initial PTFE film surface with a red circle surrounding the asperity which causes the increased COF observed from the 30-200 Å scratch distances. ii) The topography of the PTFE film after 30 Å. iii) The asperity has begun to be flattened under the indenter, and the coefficient of friction climbs. iv) The asperity is completely flattened, and the coefficient of friction has decreased to what it once was in the first 30 Å of scratch.

Characterization of film dataset

Characterization on the coarse-grained models was accomplished to better understand the relationship between the coefficient of friction and the film topography. In each model we performed a characterization in the same line where the indentation and scratch were performed (Figure S4 A). A film profile is shown in Figure S4 B, and the center-line average, the variance, and the skewness are shown for all models (Figure S4 C-D). Our results show a significant difference in the centre line average and variance between the 0-minute annealed models and the others, however, the 4- and 8-minute models are very similar.

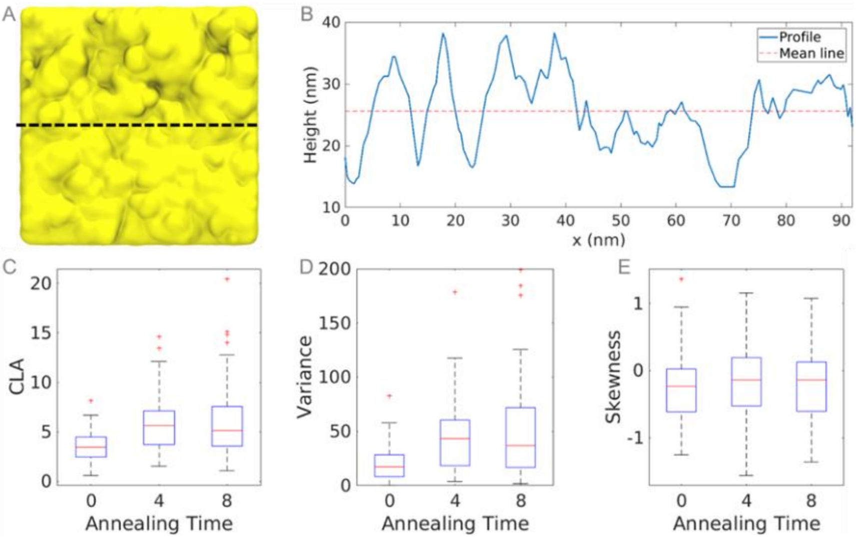

Figure S4 A) Image of a coarse-grained model based on a 0-minute annealed PTFE film. A line is drawn through the film where the scratch on the film is performed. B) Film characterization showing the profile at the point where the scratch is performed. C) Statistics of the center-line average of the entire dataset. D) Statistics of the variance of the entire dataset. D) Statistics showing the skewness of the entire dataset.

Internal fiber orientation image creation

The atom coordinates of each model are used to create images as input into the CNN. An image is initialized in Python using 0 as the default image color. The atom coordinates of each model are imported and looped through to find the maximum height of the model in each pixel of the initialized image. The resulting image is normalized to the total maximum height from all models and used as input into the CNN.

To create the images of the internal fiber orientation of each model, the model height is divided into quarters and the maximum atom height which can contribute to the image height is capped at each quarter interval, resulting in four separate images. The four images represent the topography of the particle and the internal structure of the particle at three different heights. This allows the network to view the internal fiber orientation of the models and results in a better percent of correct COF predictions after training and testing.

Internal fiber orientation simulations

Based on the results in the manuscript, we investigate how internal fiber orientation affects the COF of films with identical topographies. We used a single 0-minute annealed model and removed the bottom 10 nm of PTFE chains, and replace them with a PTFE film where all chains are oriented in the same direction. One film with parallel and one with perpendicular chains to scratch direction, are both equilibrated and scratched as described in the manuscript. The results of the COF values from these films varies depending on the internal chain orientation. The COF values where internal chains are oriented parallel to the scratch direction have a lower COF than a random orientation, which is lower than a perpendicular orientation. Results are represented graphically in Figure S5 A, showing the trends in the COF values. Figure S5 B-D show the random, parallel, and perpendicular internal fiber orientation of the area where scratch is performed in the film.

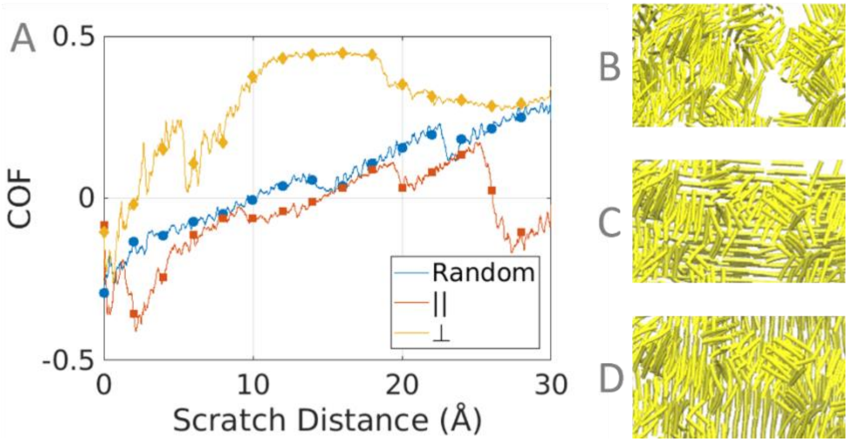

Figure S5 A) Plot of the coefficient of three identical film topographies with varying internal fiber structure. B) Image of the random internal fiber orientation in the area where scratch is performed. C) Image of the parallel fiber orientation. D) Image of the perpendicular fiber orientation.

References

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