

Supporting Information

Morphology prediction for polymer blend thin films using machine learning

Bishnu R¹, Rabibrata Mukherjee², Nandini Bhandaru^{1*}, Arnab Dutta^{1*}

¹Chemical Engineering Department, Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus, Jawahar Nagar, Medchal District, Hyderabad-500078, Telangana, India

²Instability and Soft Patterning Laboratory, Department of Chemical Engineering, Indian Institute of Technology (IIT) Kharagpur-721302, India

Content:

S1: AFM images used for model development

S2: AFM images used for model validation

S3: Impact of substrate surface energy on model accuracy

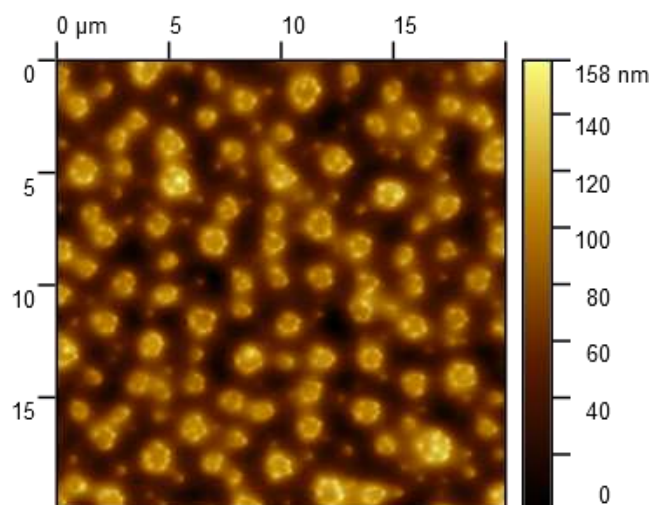
*Corresponding author: Email: nandini@hyderabad.bits-pilani.ac.in (Nandini), arnabdutta@hyderabad.bits-pilani.ac.in (Arnab). Tel: +9140 66303571 (Nandini), +9140 66303758 (Arnab).

S1: AFM images used for model development

All 80 AFM images used to develop the machine learning model are given below along with the critical parameters extracted using the Gwyddion software for each of these images. These parameters were used in Figure 2 to label the actual morphology for each of the images.

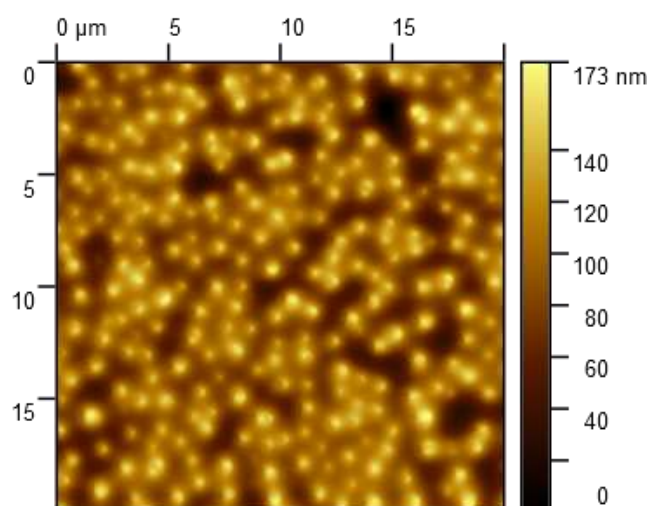
Aspect ratio for each image is calculated using the following formula:

$$\text{Aspect Ratio} = \frac{\text{Average morphology diameter}}{\text{Average morphology height}}$$



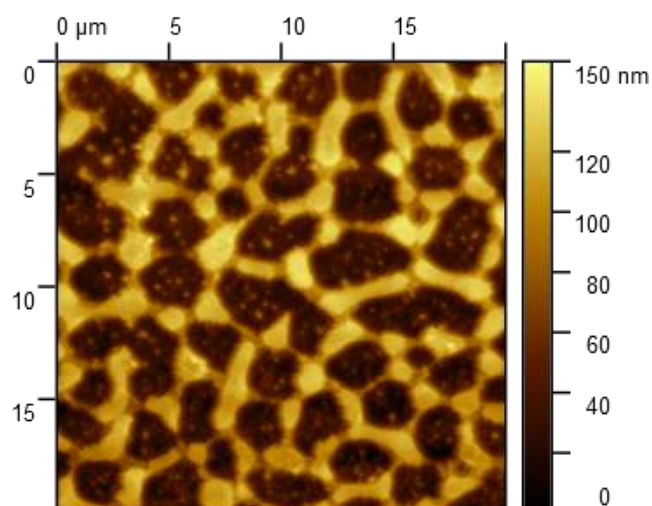
Sample: 1 (Morphology: Column)

1. Area fraction of PMMA (%): 23.69
2. Average morphology diameter (nm): 813.4
3. Average morphology height (nm): 103.2
4. Aspect ratio: 7.88



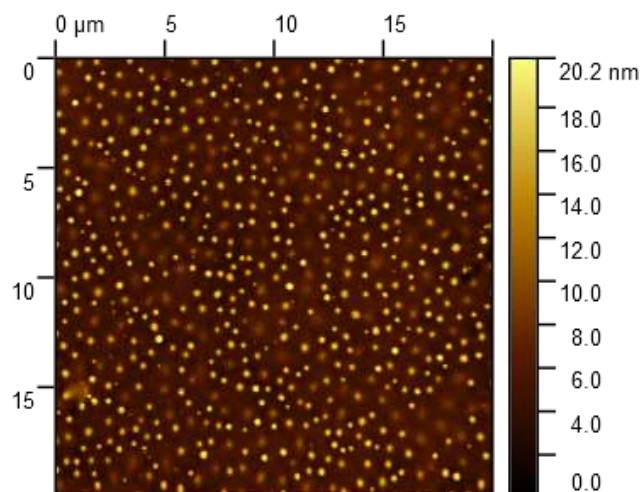
Sample: 2 (Morphology: Column)

1. Area fraction of PMMA (%): 15.08
2. Average morphology diameter (nm): 442.9
3. Average morphology height (nm): 148.5
4. Aspect ratio: 2.98



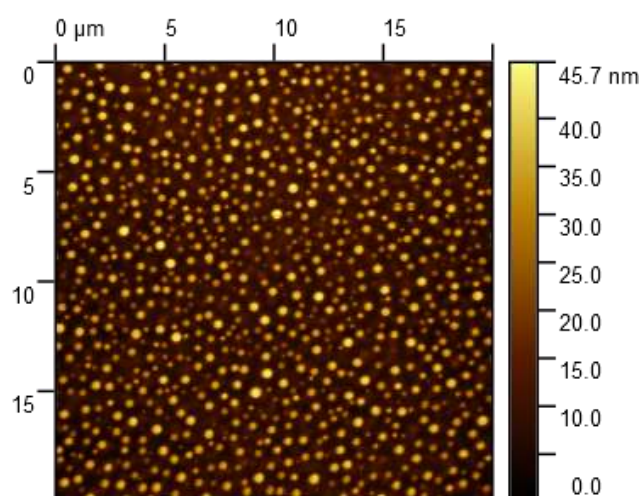
Sample: 3 (Morphology: Hole)

1. Area fraction of PMMA (%): 53.07
2. Average morphology diameter (nm): 1578
3. Average morphology height (nm): 30.77
4. Aspect ratio: 51.28



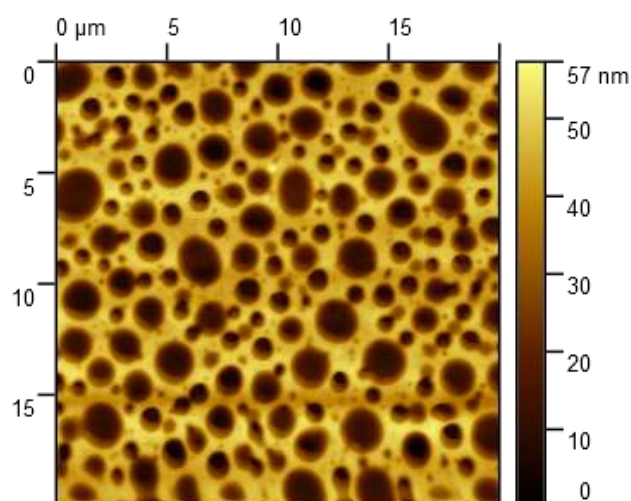
Sample: 4 (Morphology: Column)

1. Area fraction of PMMA (%): 12.6
2. Average morphology diameter (nm): 230.2
3. Average morphology height (nm): 19.46
4. Aspect ratio: 11.83



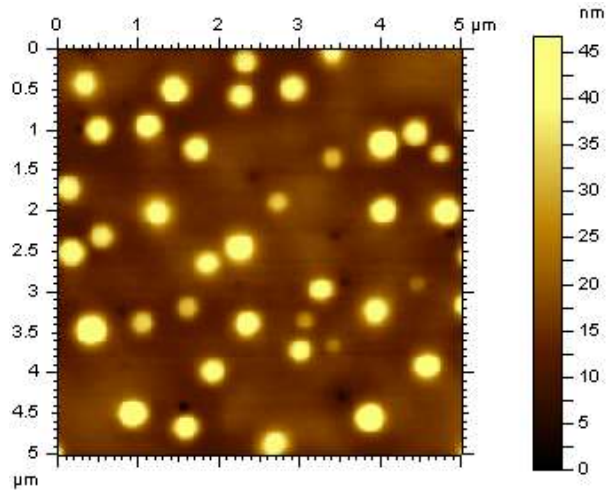
Sample: 5 (Morphology: Column)

1. Area fraction of PMMA (%): 20.4
2. Average morphology diameter (nm): 260.4
3. Average morphology height (nm): 39.2
4. Aspect ratio: 6.64



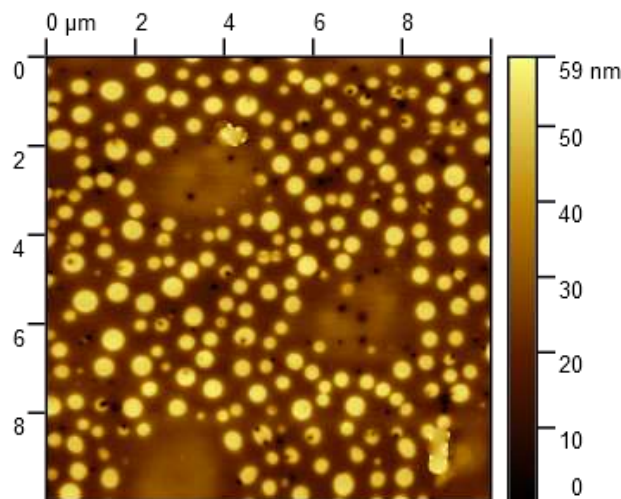
Sample: 6 (Morphology: Hole)

1. Area fraction of PMMA (%): 57.69
2. Average morphology diameter (nm): 1026
3. Average morphology height (nm): 42.15
4. Aspect ratio: 24.34



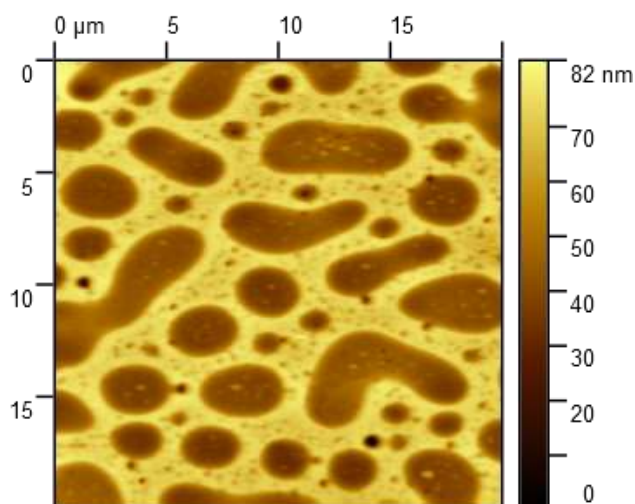
Sample: 7 (Morphology: Column)

1. Area fraction of PMMA (%): 16.9
2. Average morphology diameter (nm): 372.9
3. Average morphology height (nm): 37.24
4. Aspect ratio: 10.01



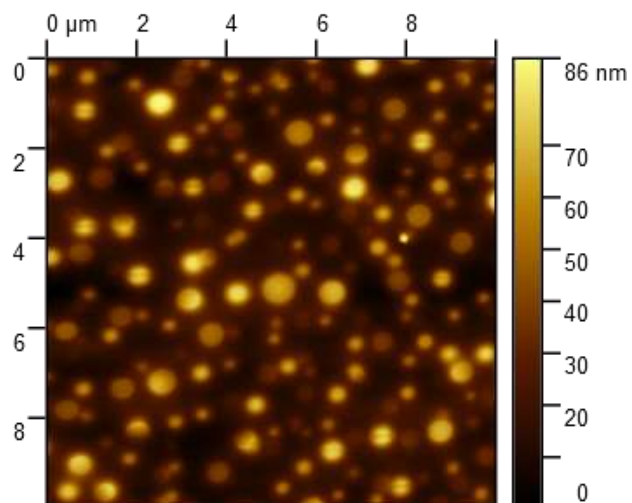
Sample: 8 (Morphology: Column)

1. Area fraction of PMMA (%): 24.52
2. Average morphology diameter (nm): 300.9
3. Average morphology height (nm): 47.82
4. Aspect ratio: 6.29



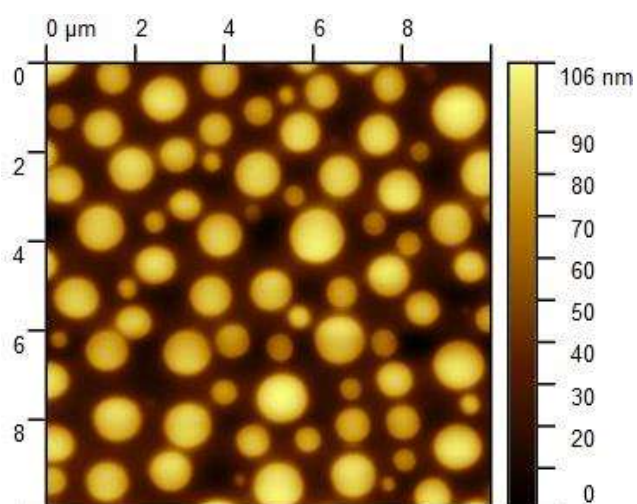
Sample: 9 (Morphology: Hole)

1. Area fraction of PMMA (%): 59.2
2. Average morphology diameter (nm): 2212
3. Average morphology height (nm): 41.64
4. Aspect ratio: 53.12



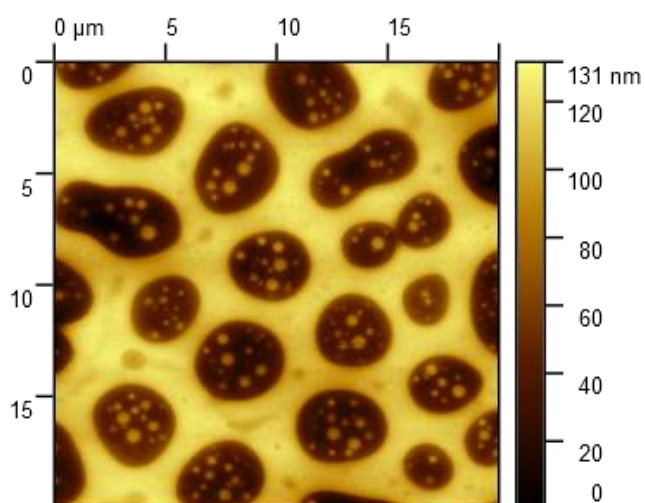
Sample: 10 (Morphology: Column)

1. Area fraction of PMMA (%): 13.51
2. Average morphology diameter (nm): 299.9
3. Average morphology height (nm): 52.62
4. Aspect ratio: 5.7



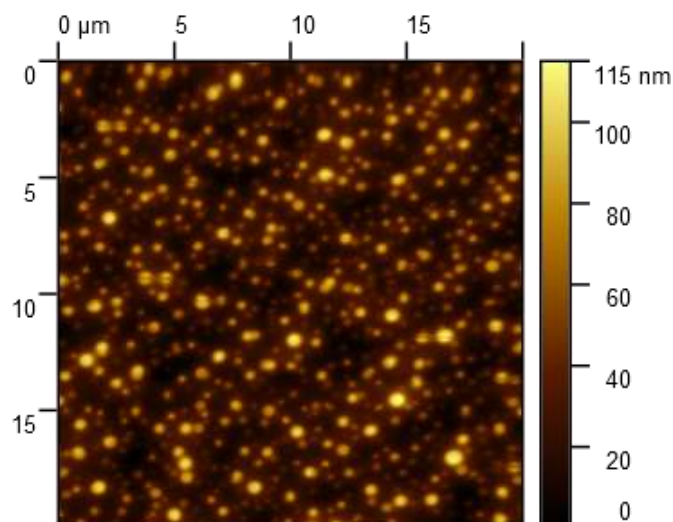
Sample: 11 (Morphology: Column)

1. Area fraction of PMMA (%): 40.03
2. Average morphology diameter (nm): 672.1
3. Average morphology height (nm): 79.2
4. Aspect ratio: 8.49



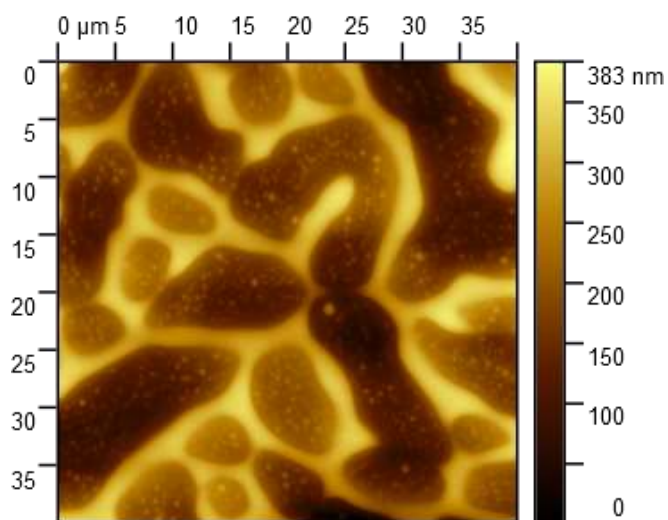
Sample: 12 (Morphology: Hole)

1. Area fraction of PMMA (%): 59.66
2. Average morphology diameter (nm): 2902
3. Average morphology height (nm): 63.84
4. Aspect ratio: 45.46



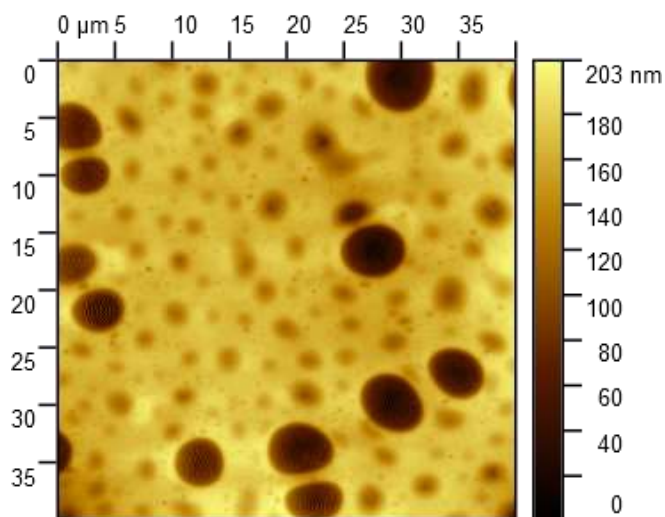
Sample: 13 (Morphology: Column)

1. Area fraction of PMMA (%): 10.35
2. Average morphology diameter (nm): 269.5
3. Average morphology height (nm): 85
4. Aspect ratio: 3.17



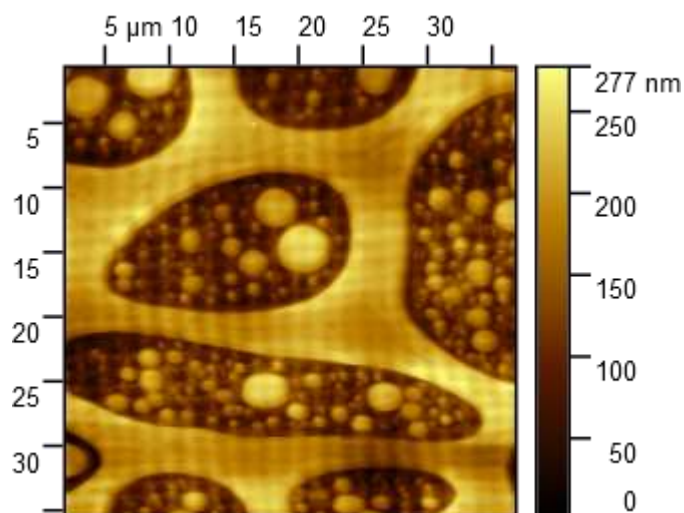
Sample: 14 (Morphology: Hole)

1. Area fraction of PMMA (%): 53.14
2. Average morphology diameter (nm): 4574
3. Average morphology height (nm): 92.1
4. Aspect ratio: 49.66



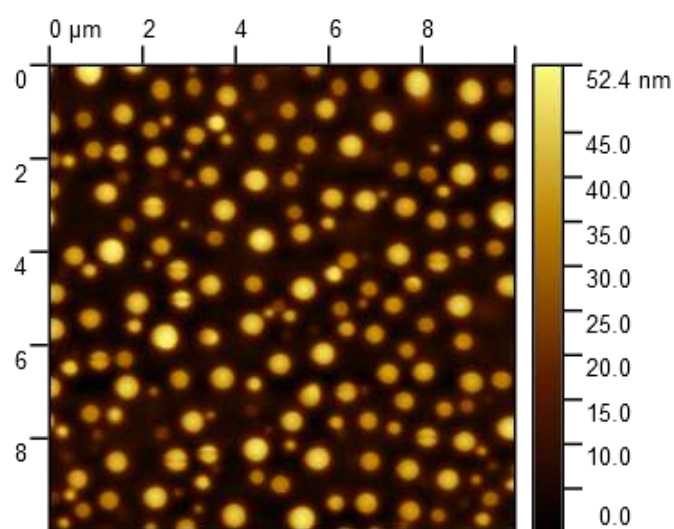
Sample: 15 (Morphology: Hole)

1. Area fraction of PMMA (%): 77.75
2. Average morphology diameter (nm): 1581
3. Average morphology height (nm): 108.9
4. Aspect ratio: 14.52



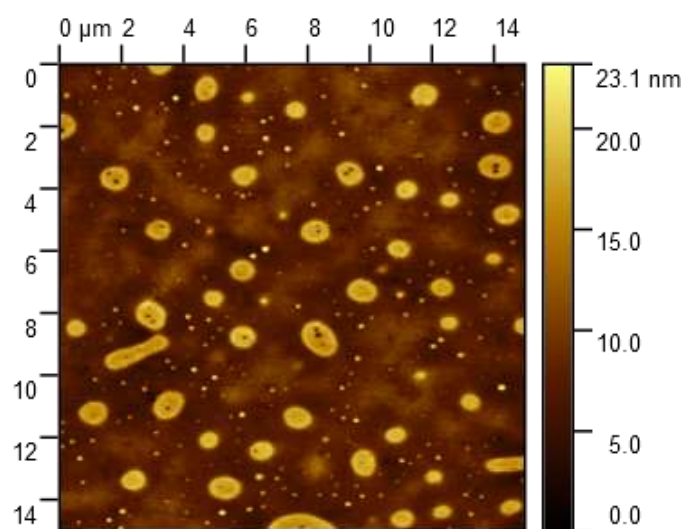
Sample: 16 (Morphology: Hole)

1. Area fraction of PMMA (%): 55.45
2. Average morphology diameter (nm): 5022
3. Average morphology height (nm): 83.7
4. Aspect ratio: 60



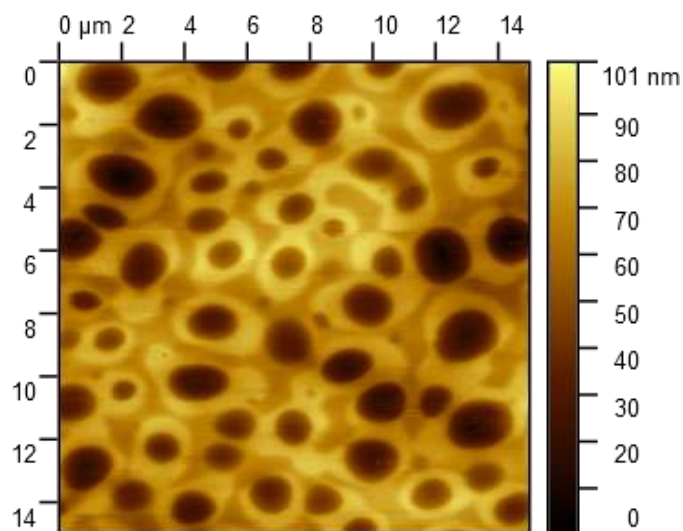
Sample: 17 (Morphology: Column)

1. Area fraction of PMMA (%): 14.2
2. Average morphology diameter (nm): 303.8
3. Average morphology height (nm): 40.48
4. Aspect ratio: 7.5



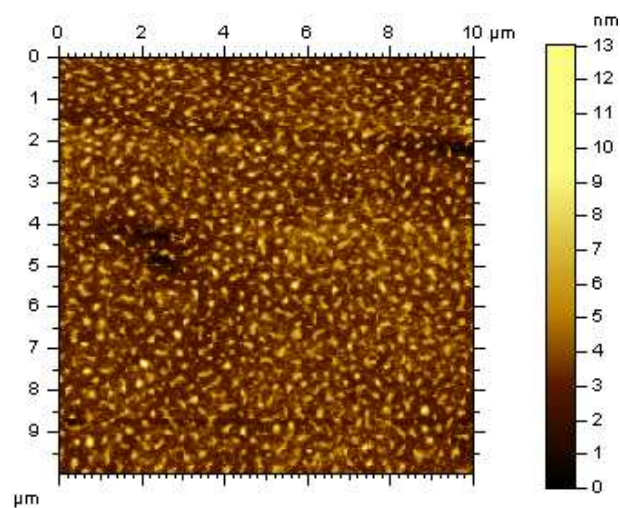
Sample: 18 (Morphology: Island)

1. Area fraction of PMMA (%): 11.47
2. Average morphology diameter (nm): 642.3
3. Average morphology height (nm): 18.42
4. Aspect ratio: 34.87



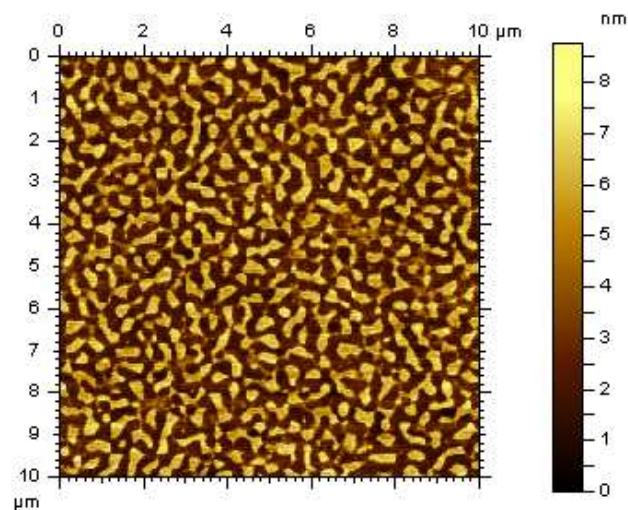
Sample: 19 (Morphology: Hole)

1. Area fraction of PMMA (%): 66.79
2. Average morphology diameter (nm): 319.8
3. Average morphology height (nm): 35.93
4. Aspect ratio: 8.9



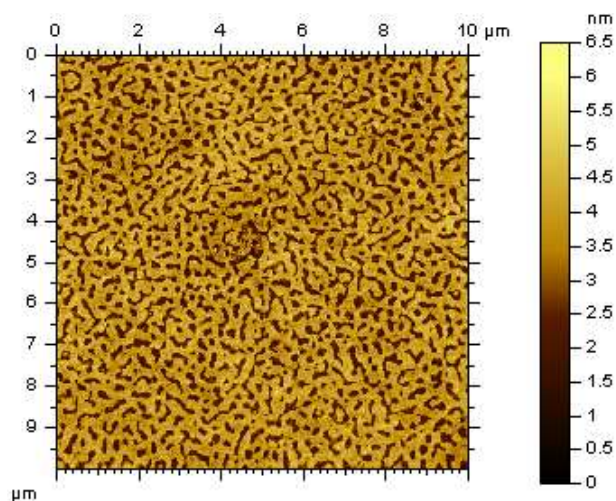
Sample: 20 (Morphology: Column)

1. Area fraction of PMMA (%): 19.01
2. Average morphology diameter (nm): 63
3. Average morphology height (nm): 10.22
4. Aspect ratio: 6.16



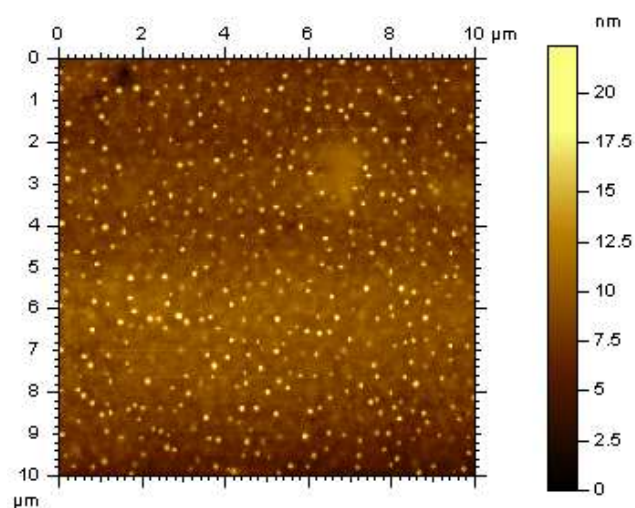
Sample: 21 (Morphology: Island)

1. Area fraction of PMMA (%): 41.3
2. Average morphology diameter (nm): 813
3. Average morphology height (nm): 4.77
4. Aspect ratio: 170.44



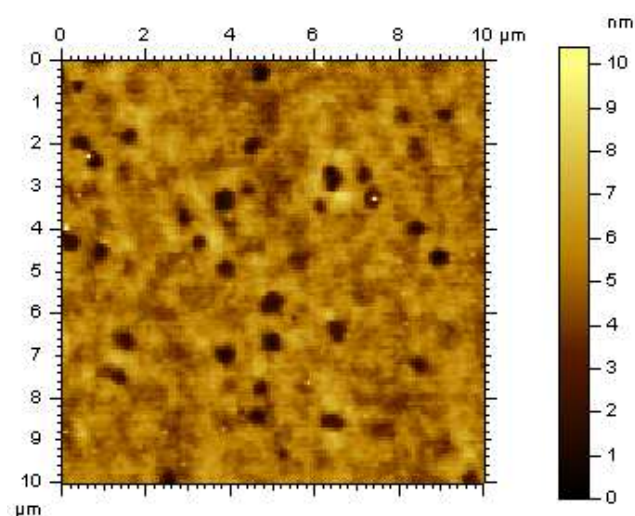
Sample: 22 (Morphology: Hole)

1. Area fraction of PMMA (%): 79.5
2. Average morphology diameter (nm): 101
3. Average morphology height (nm): 2.6
4. Aspect ratio: 38.85



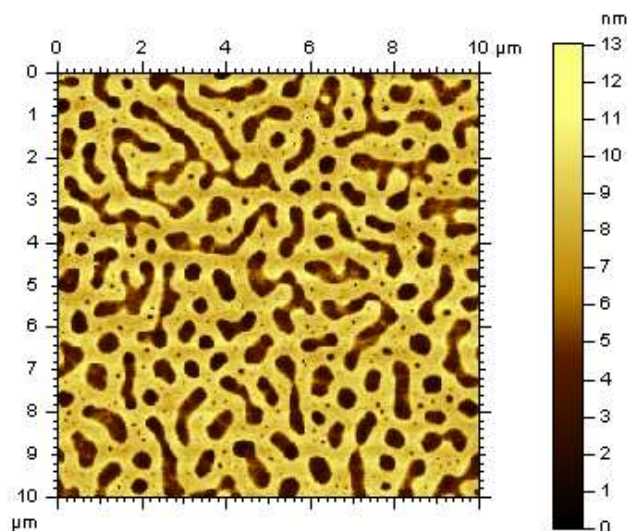
Sample: 23 (Morphology: Column)

1. Area fraction of PMMA (%): 6.35
2. Average morphology diameter (nm): 55.27
3. Average morphology height (nm): 16.6
4. Aspect ratio: 3.33



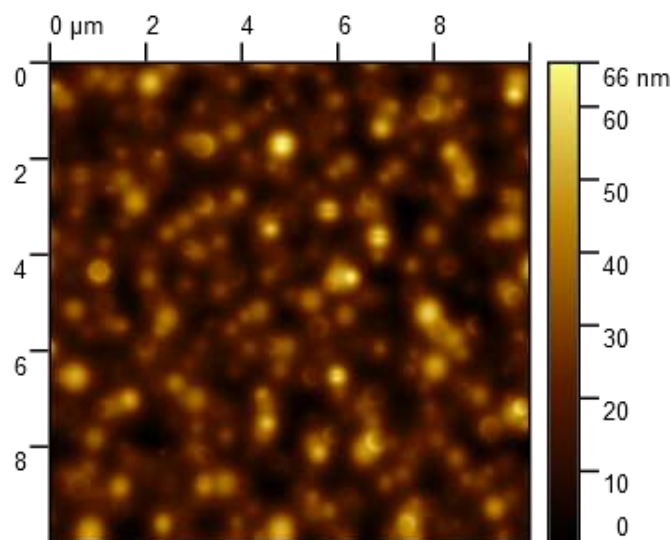
Sample: 24 (Morphology: Hole)

1. Area fraction of PMMA (%): 87.8
2. Average morphology diameter (nm): 152.9
3. Average morphology height (nm): 8.8
4. Aspect ratio: 17.38



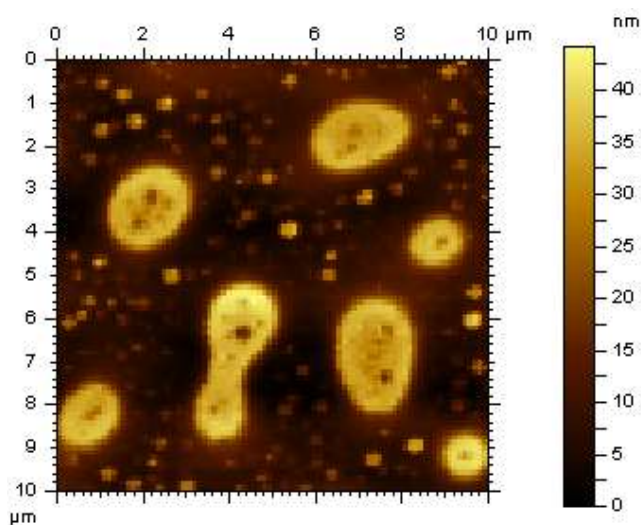
Sample: 25 (Morphology: Hole)

1. Area fraction of PMMA (%): 62.1
2. Average morphology diameter (nm): 127
3. Average morphology height (nm): 7.07
4. Aspect ratio: 17.96



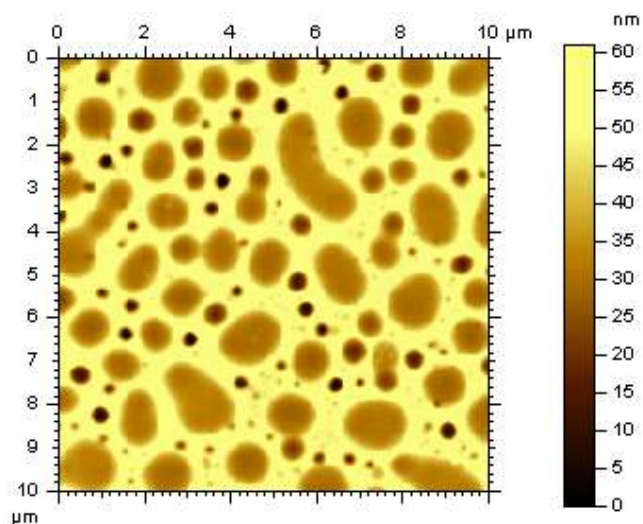
Sample: 26 (Morphology: Column)

1. Area fraction of PMMA (%): 28.96
2. Average morphology diameter (nm): 354.9
3. Average morphology height (nm): 30.58
4. Aspect ratio: 9.88



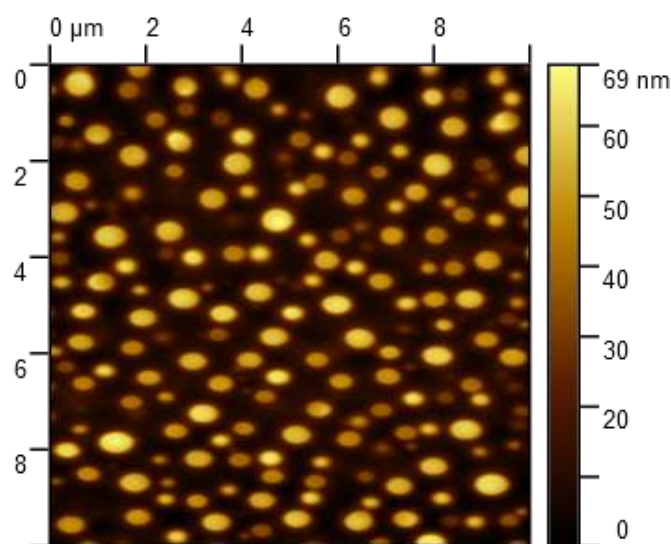
Sample: 27 (Morphology: Island)

1. Area fraction of PMMA (%): 24.9
2. Average morphology diameter (nm): 1025
3. Average morphology height (nm): 49.4
4. Aspect ratio: 20.75



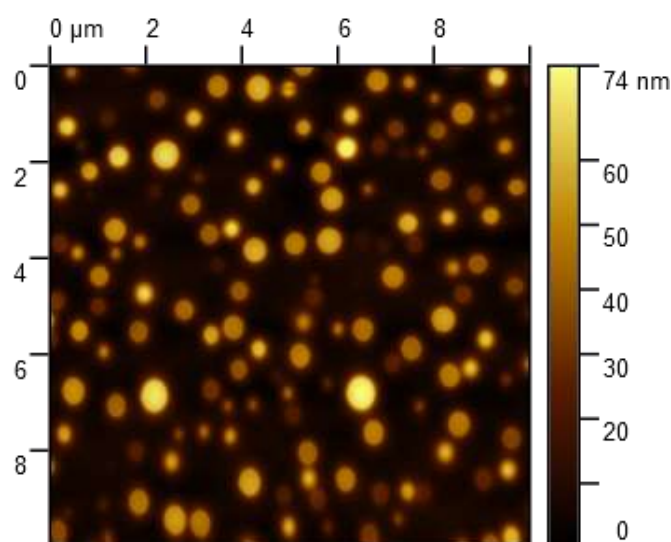
Sample: 28 (Morphology: Hole)

1. Area fraction of PMMA (%): 62.03
2. Average morphology diameter (nm): 381.9
3. Average morphology height (nm): 30.84
4. Aspect ratio: 12.38



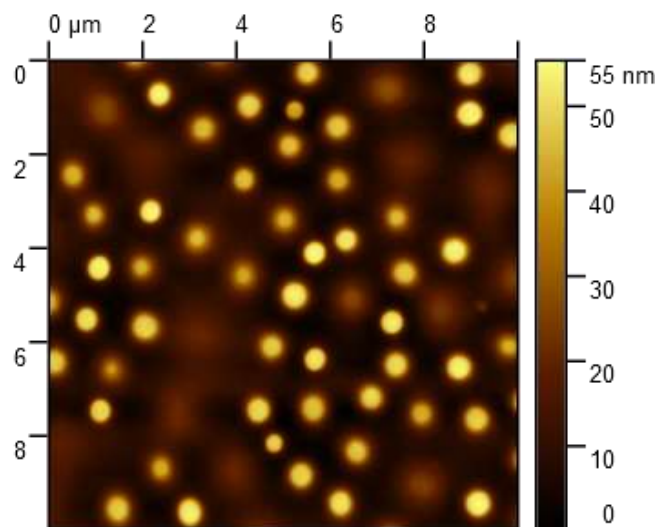
Sample: 29 (Morphology: Column)

1. Area fraction of PMMA (%): 21.62
2. Average morphology diameter (nm): 322.2
3. Average morphology height (nm): 44.84
4. Aspect ratio: 7.19



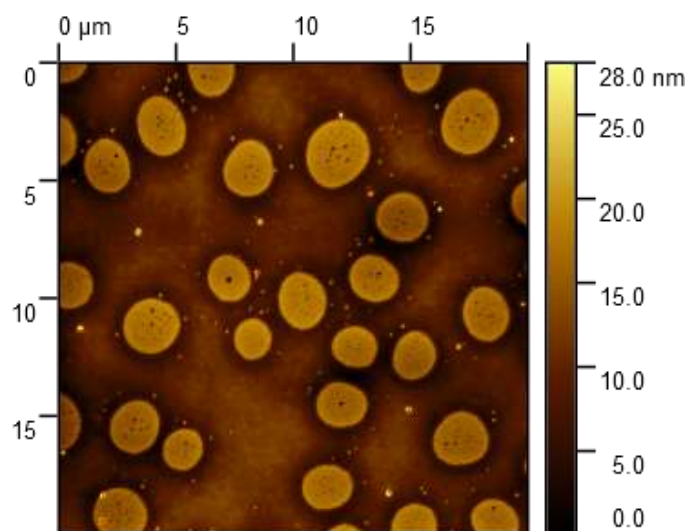
Sample: 30 (Morphology: Column)

1. Area fraction of PMMA (%): 11.33
2. Average morphology diameter (nm): 323.7
3. Average morphology height (nm): 55.18
4. Aspect ratio: 5.87



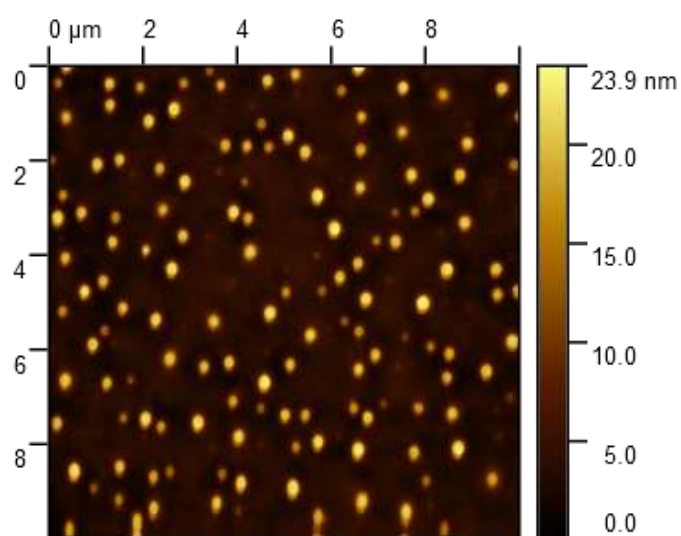
Sample: 31 (Morphology: Column)

1. Area fraction of PMMA (%): 14.04
2. Average morphology diameter (nm): 454.2
3. Average morphology height (nm): 51.33
4. Aspect ratio: 8.85



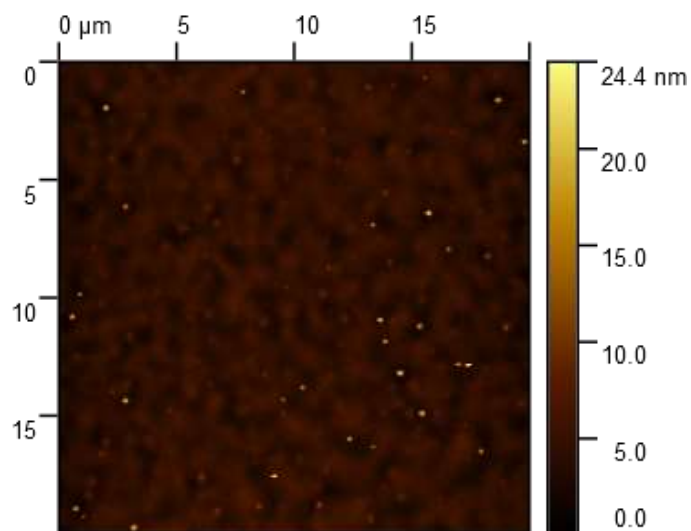
Sample: 32 (Morphology: Island)

1. Area fraction of PMMA (%): 22.9
2. Average morphology diameter (nm): 871.6
3. Average morphology height (nm): 24.37
4. Aspect ratio: 35.77



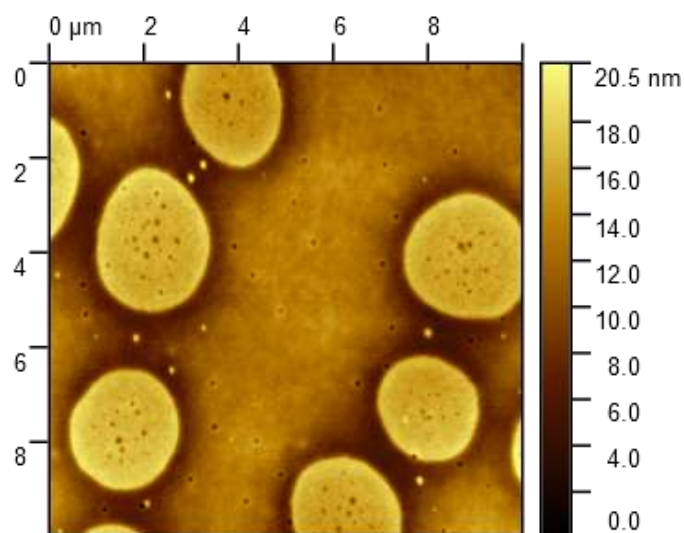
Sample: 33 (Morphology: Column)

1. Area fraction of PMMA (%): 9.27
2. Average morphology diameter (nm): 268.3
3. Average morphology height (nm): 18.35
4. Aspect ratio: 14.62



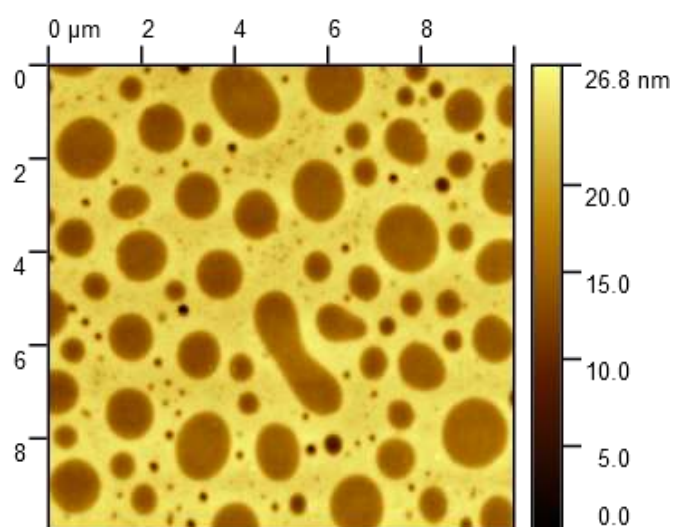
Sample: 34 (Morphology: Column)

1. Area fraction of PMMA (%): 0.58
2. Average morphology diameter (nm): 166.5
3. Average morphology height (nm): 9.4
4. Aspect ratio: 17.71



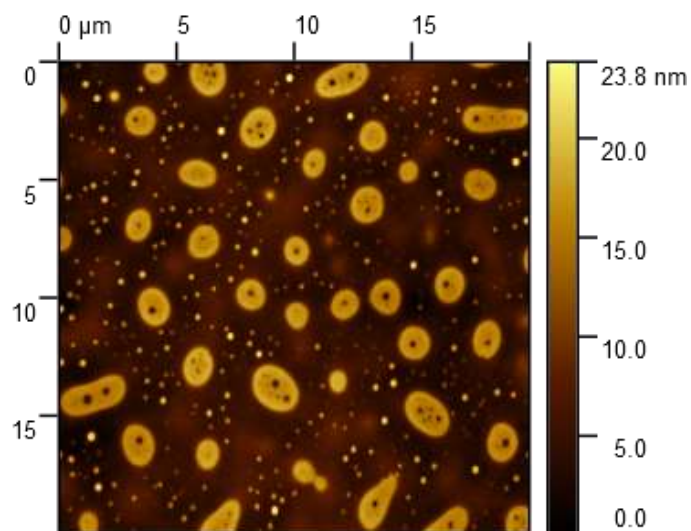
Sample: 35 (Morphology: Island)

1. Area fraction of PMMA (%): 14.94
2. Average morphology diameter (nm): 1058
3. Average morphology height (nm): 18.38
4. Aspect ratio: 57.56



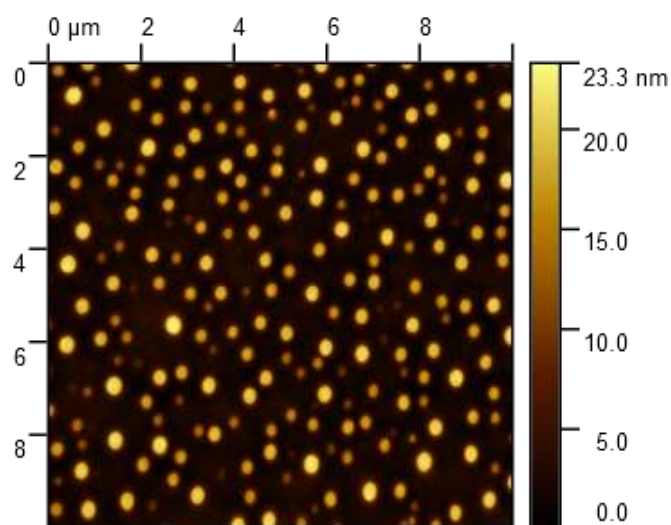
Sample: 36 (Morphology: Hole)

- Area fraction of PMMA (%): 67.63
- Average morphology diameter (nm): 497.2
- Average morphology height (nm): 13.82
- Aspect ratio: 35.98



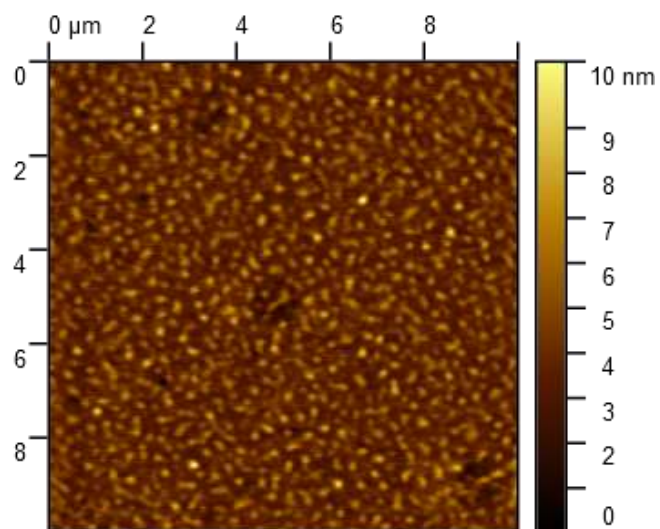
Sample: 37 (Morphology: Island)

1. Area fraction of PMMA (%): 14.21
2. Average morphology diameter (nm): 758.6
3. Average morphology height (nm): 16.46
4. Aspect ratio: 46.09



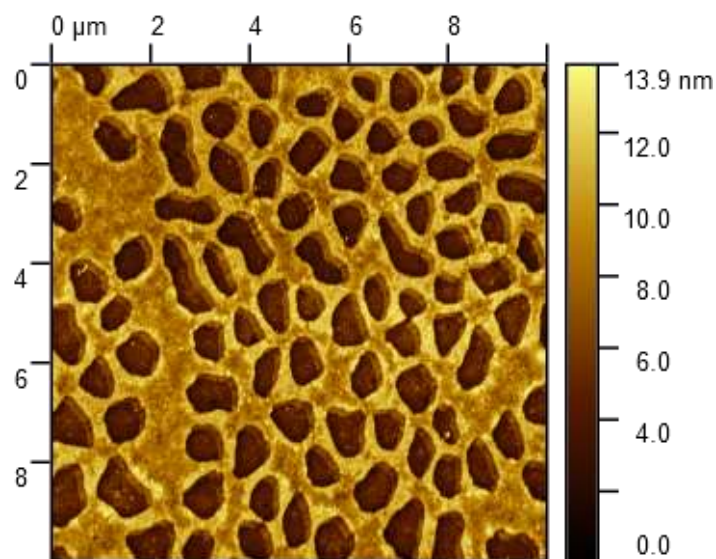
Sample: 38 (Morphology: Column)

1. Area fraction of PMMA (%): 15.79
2. Average morphology diameter (nm): 254.4
3. Average morphology height (nm): 14.58
4. Aspect ratio: 17.45



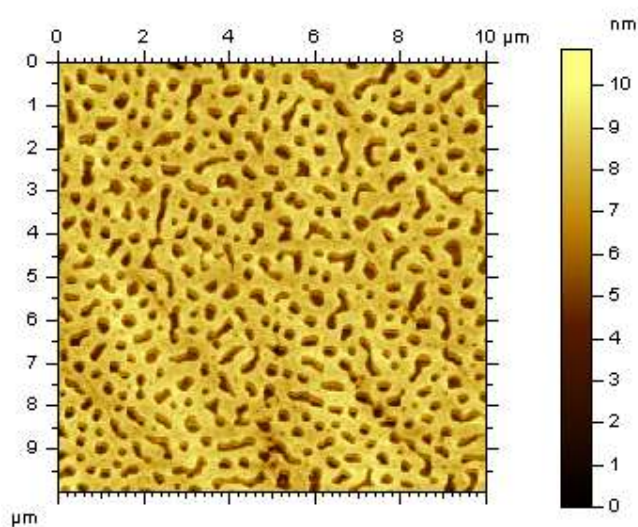
Sample: 39 (Morphology: Column)

1. Area fraction of PMMA (%): 12.87
2. Average morphology diameter (nm): 121.3
3. Average morphology height (nm): 5.36
4. Aspect ratio: 22.63



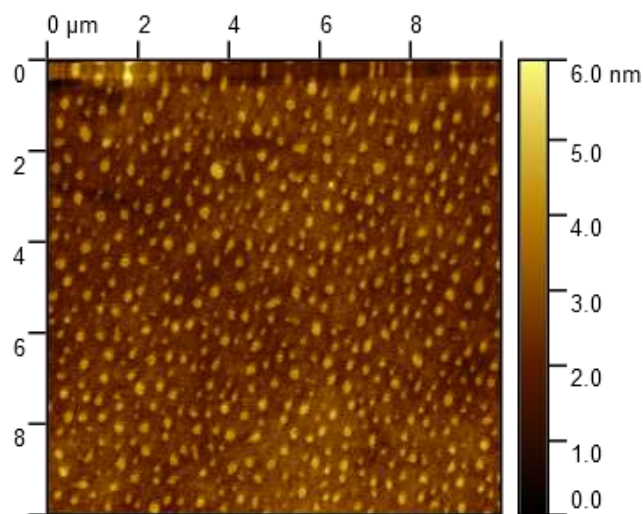
Sample: 40 (Morphology: Hole)

1. Area fraction of PMMA (%): 65.47
2. Average morphology diameter (nm): 345.8
3. Average morphology height (nm): 4.05
4. Aspect ratio: 85.36



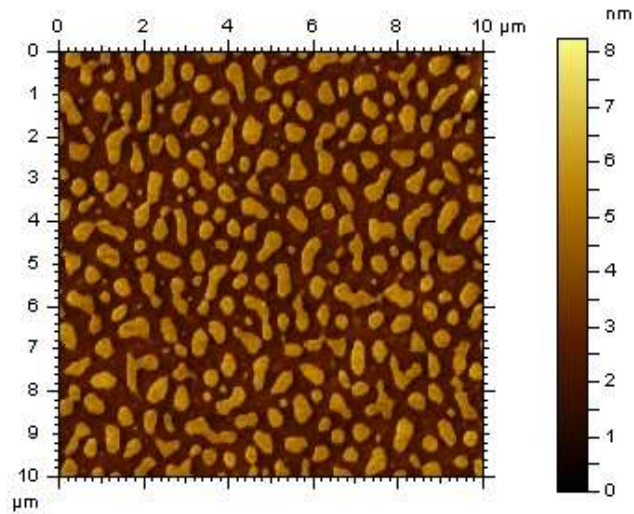
Sample: 41 (Morphology: Hole)

1. Area fraction of PMMA (%): 69.2
2. Average morphology diameter (nm): 221.1
3. Average morphology height (nm): 5.49
4. Aspect ratio: 40.27



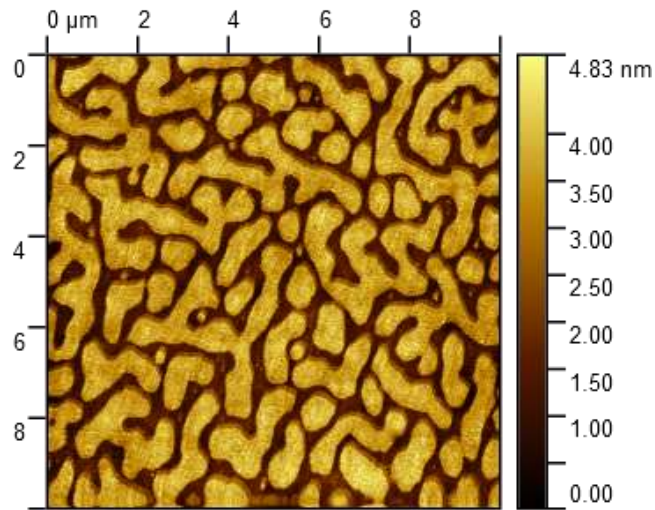
Sample: 42 (Morphology: Column)

1. Area fraction of PMMA (%): 15.5
2. Average morphology diameter (nm): 113.5
3. Average morphology height (nm): 5
4. Aspect ratio: 22.7



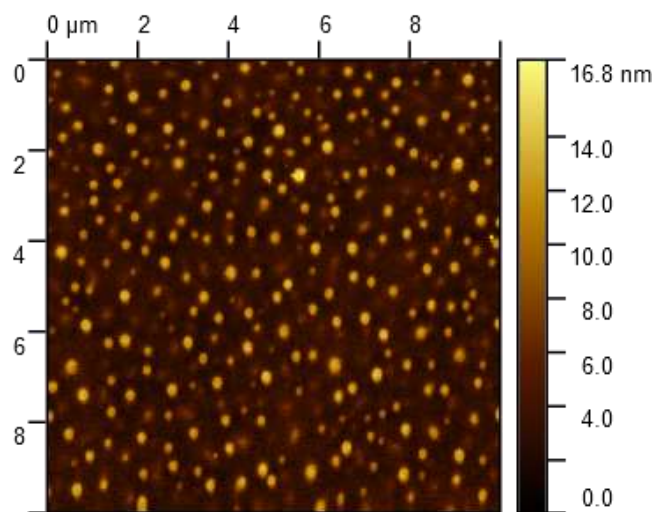
Sample: 43 (Morphology: Island)

1. Area fraction of PMMA (%): 36.68
2. Average morphology diameter (nm): 291.6
3. Average morphology height (nm): 4.8
4. Aspect ratio: 60.8



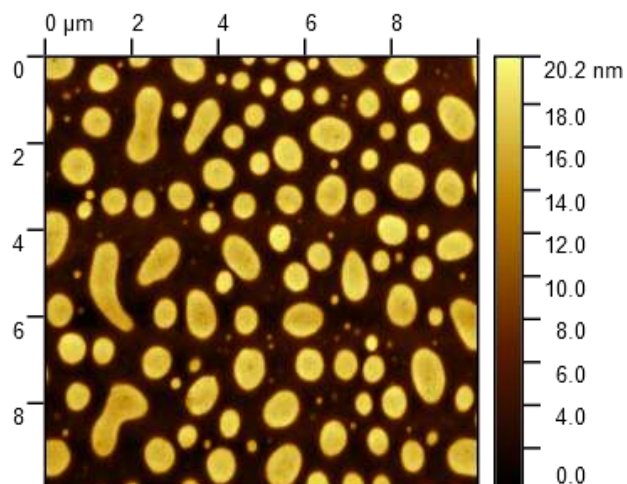
Sample: 44 (Morphology: Island)

1. Area fraction of PMMA (%): 60.32
2. Average morphology diameter (nm): 474
3. Average morphology height (nm): 3.59
4. Aspect ratio: 132.14



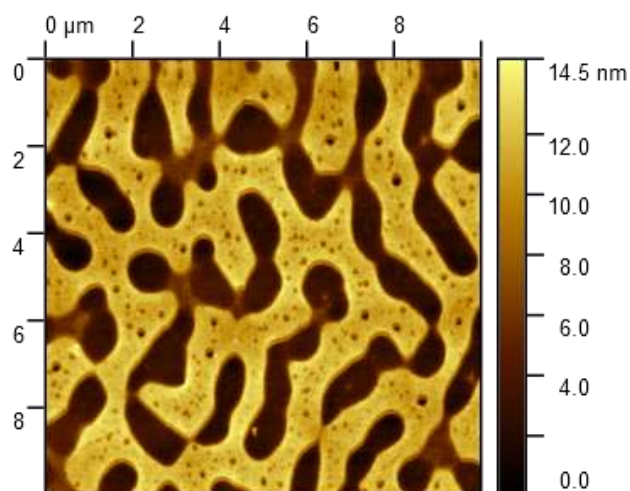
Sample: 45 (Morphology: Column)

1. Area fraction of PMMA (%): 14.77
2. Average morphology diameter (nm): 180.6
3. Average morphology height (nm): 7.88
4. Aspect ratio: 22.92



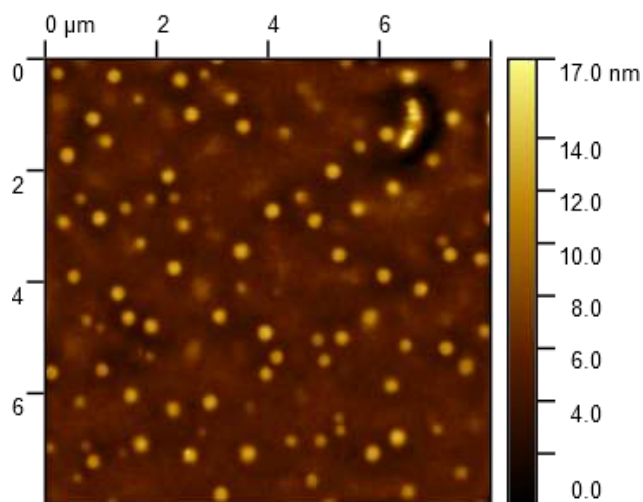
Sample: 46 (Morphology: Island)

1. Area fraction of PMMA (%): 31.59
2. Average morphology diameter (nm): 453.3
3. Average morphology height (nm): 14.72
4. Aspect ratio: 30.79



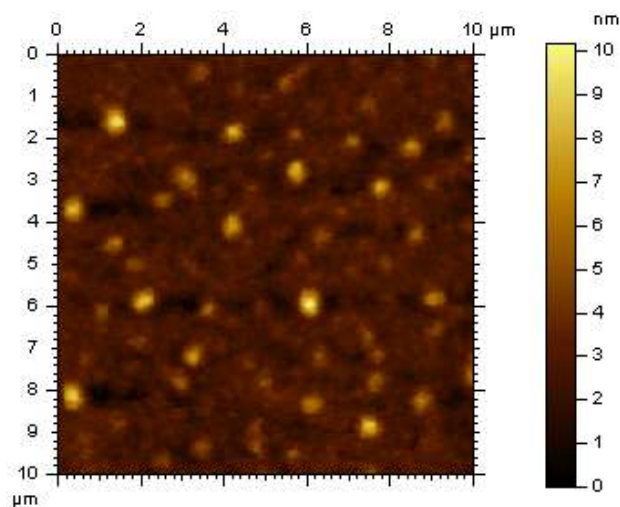
Sample: 47 (Morphology: Hole)

1. Area fraction of PMMA (%): 61.1
2. Average morphology diameter (nm): 399.4
3. Average morphology height (nm): 5.56
4. Aspect ratio: 71.82



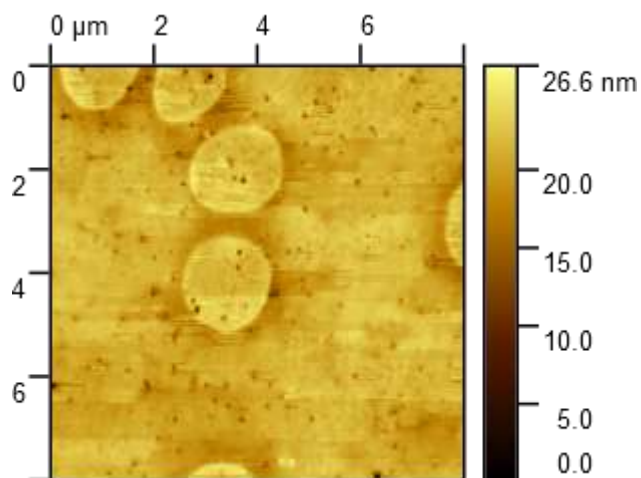
Sample: 48 (Morphology: Column)

1. Area fraction of PMMA (%): 6.22
2. Average morphology diameter (nm): 188.5
3. Average morphology height (nm): 13.62
4. Aspect ratio: 13.84



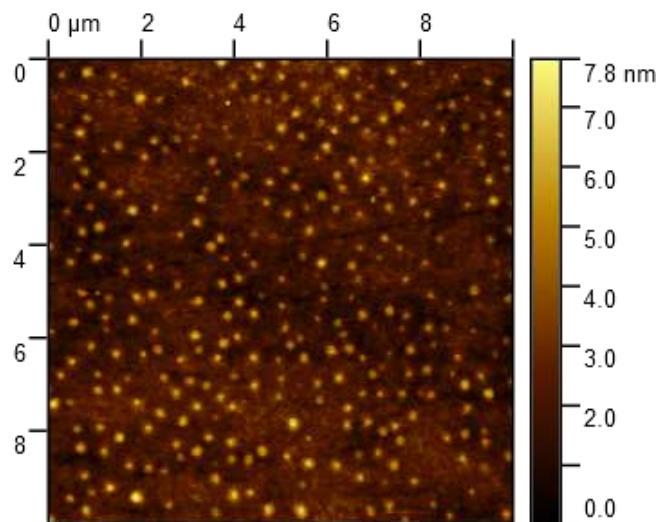
Sample: 49 (Morphology: Column)

1. Area fraction of PMMA (%): 1.48
2. Average morphology diameter (nm): 155.2
3. Average morphology height (nm): 9.67
4. Aspect ratio: 16.05



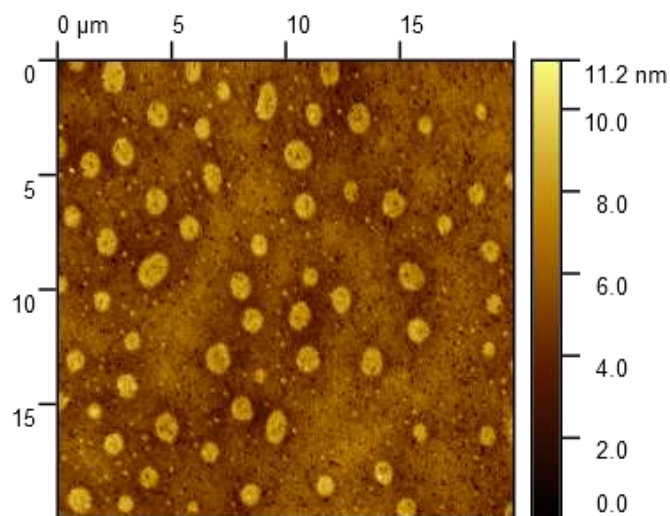
Sample: 50 (Morphology: Island)

1. Area fraction of PMMA (%): 2.37
2. Average morphology diameter (nm): 1189
3. Average morphology height (nm): 8.88
4. Aspect ratio: 133.9



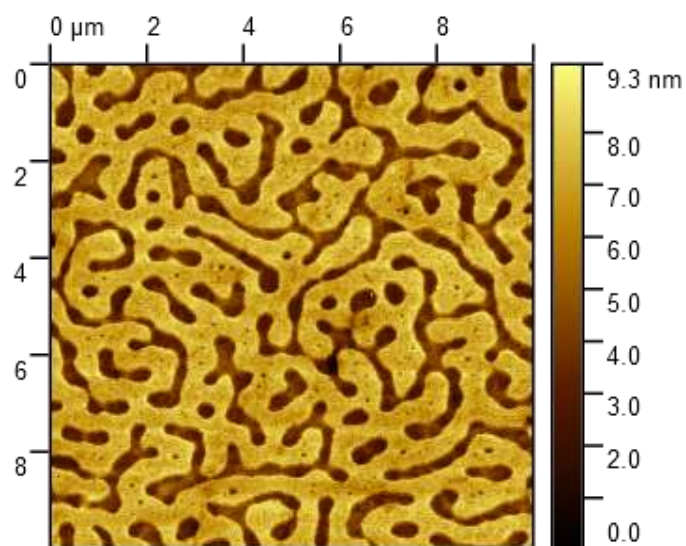
Sample: 51 (Morphology: Column)

1. Area fraction of PMMA (%): 6.79
2. Average morphology diameter (nm): 123.5
3. Average morphology height (nm): 4.87
4. Aspect ratio: 25.36



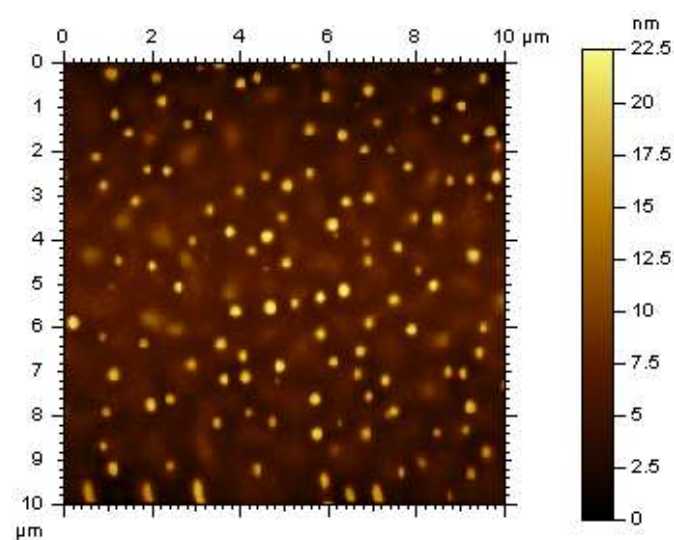
Sample: 52 (Morphology: Island)

1. Area fraction of PMMA (%): 8.44
2. Average morphology diameter (nm): 526.8
3. Average morphology height (nm): 5.64
4. Aspect ratio: 93.35



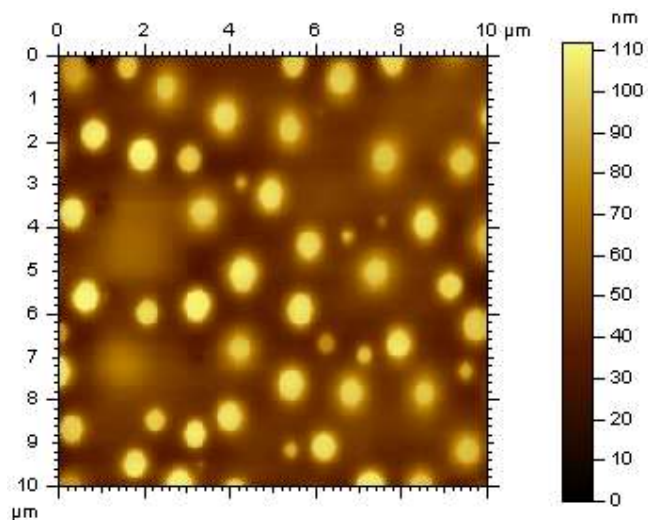
Sample: 53 (Morphology: Hole)

1. Area fraction of PMMA (%): 66.93
2. Average morphology diameter (nm): 362
3. Average morphology height (nm): 6.56
4. Aspect ratio: 55.18



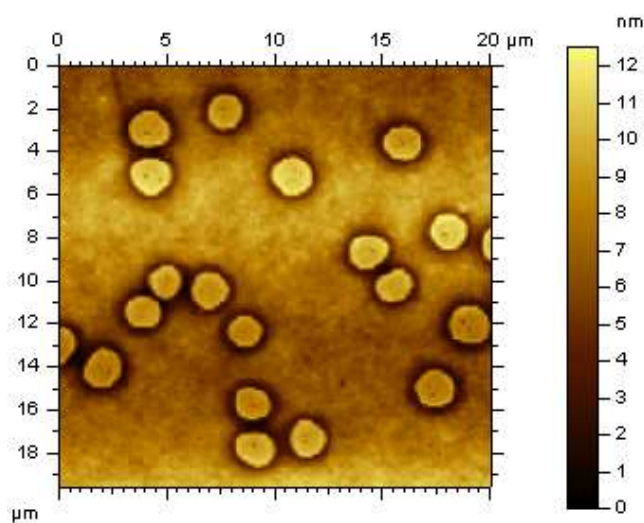
Sample: 54 (Morphology: Column)

1. Area fraction of PMMA (%): 4.33
2. Average morphology diameter (nm): 178.6
3. Average morphology height (nm): 13.27
4. Aspect ratio: 13.46



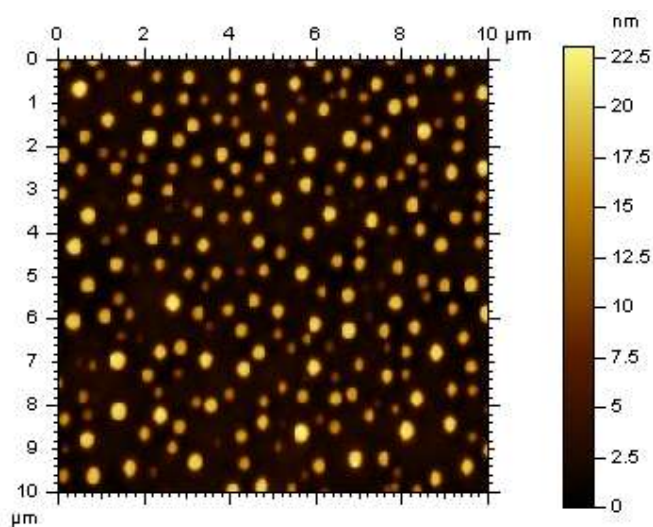
Sample: 55 (Morphology: Column)

1. Area fraction of PMMA (%): 40.59
2. Average morphology diameter (nm): 608.8
3. Average morphology height (nm): 76.3
4. Aspect ratio: 7.98



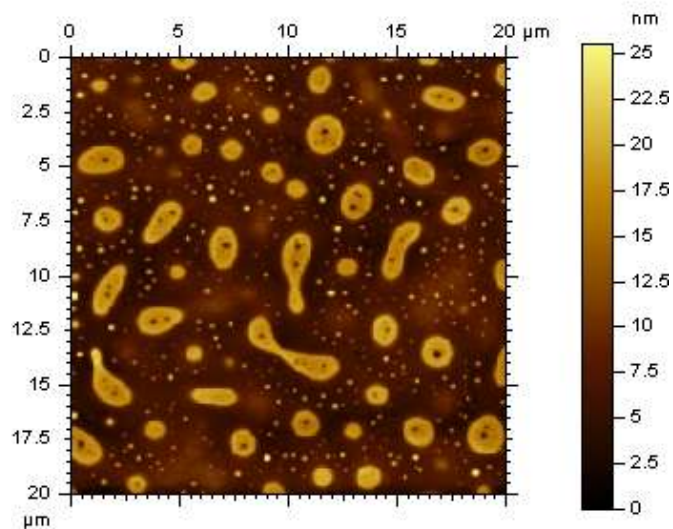
Sample: 56 (Morphology: Island)

1. Area fraction of PMMA (%): 9.2
2. Average morphology diameter (nm): 611.6
3. Average morphology height (nm): 10.23
4. Aspect ratio: 59.78



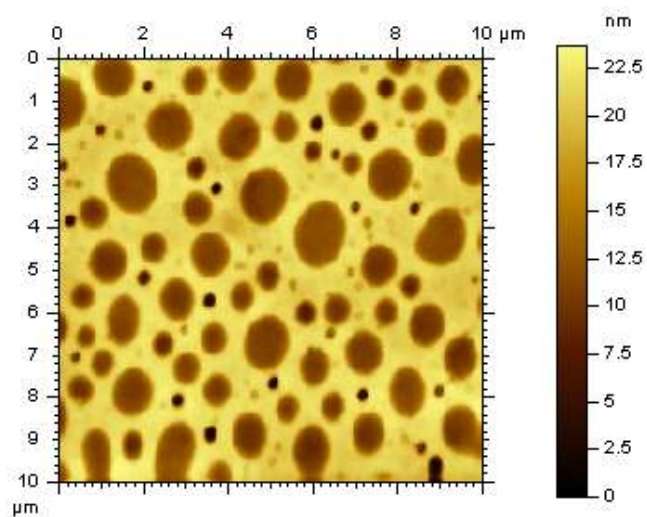
Sample: 57 (Morphology: Column)

1. Area fraction of PMMA (%): 9.57
2. Average morphology diameter (nm): 197.1
3. Average morphology height (nm): 111.8
4. Aspect ratio: 1.76



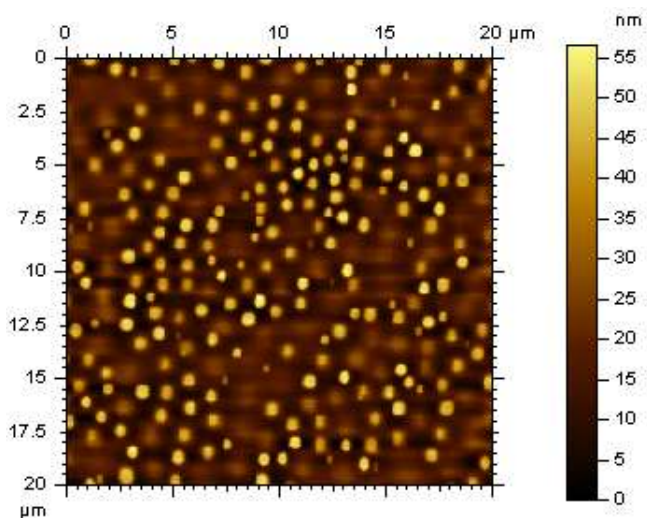
Sample: 58 (Morphology: Island)

1. Area fraction of PMMA (%): 20.63
2. Average morphology diameter (nm): 1081
3. Average morphology height (nm): 25.19
4. Aspect ratio: 42.91



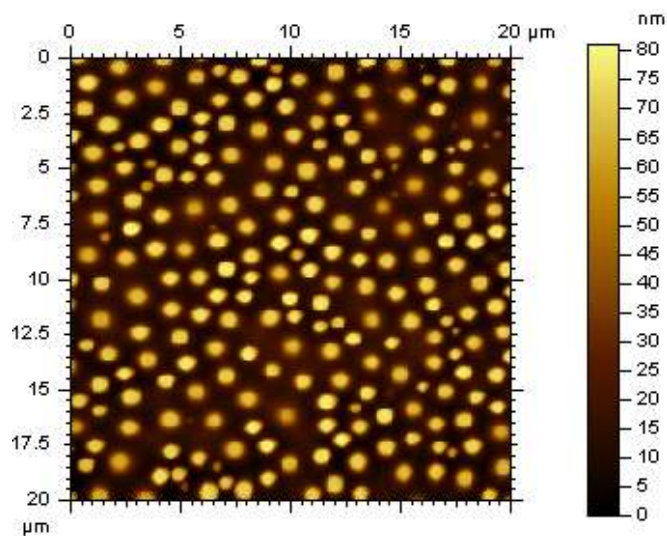
Sample: 59 (Morphology: Hole)

1. Area fraction of PMMA (%): 62.79
2. Average morphology diameter (nm): 475.7
3. Average morphology height (nm): 15.66
4. Aspect ratio: 30.38



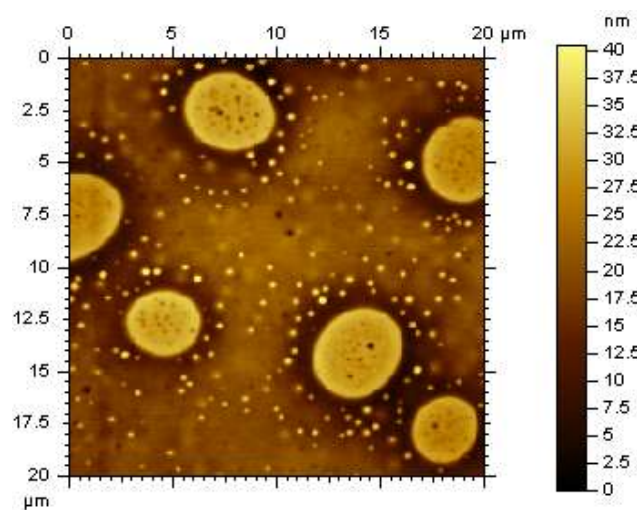
Sample: 60 (Morphology: Column)

1. Area fraction of PMMA (%): 9.56
2. Average morphology diameter (nm): 415
3. Average morphology height (nm): 41.84
4. Aspect ratio: 9.92



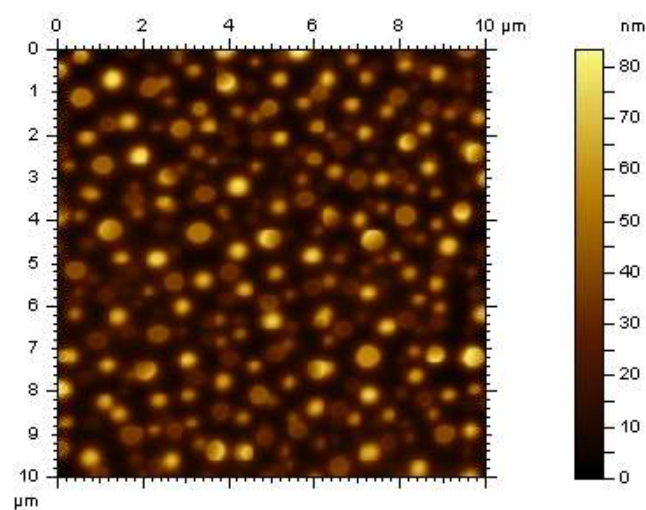
Sample: 61 (Morphology: Column)

1. Area fraction of PMMA (%): 23.64
2. Average morphology diameter (nm): 652.1
3. Average morphology height (nm): 86.3
4. Aspect ratio: 7.56



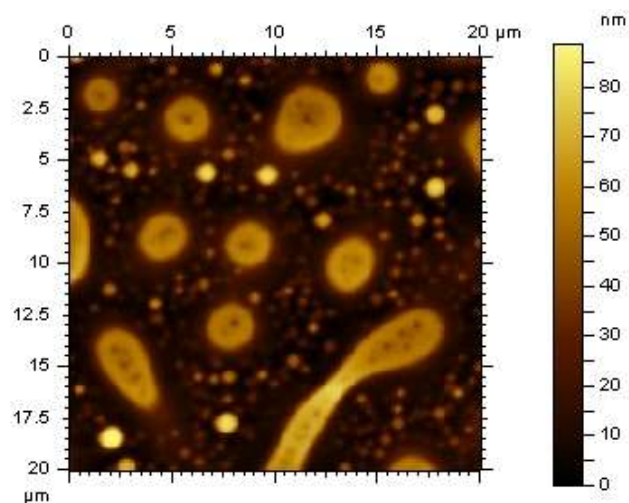
Sample: 62 (Morphology: Island)

1. Area fraction of PMMA (%): 11.93
2. Average morphology diameter (nm): 2594
3. Average morphology height (nm): 27.75
4. Aspect ratio: 93.48



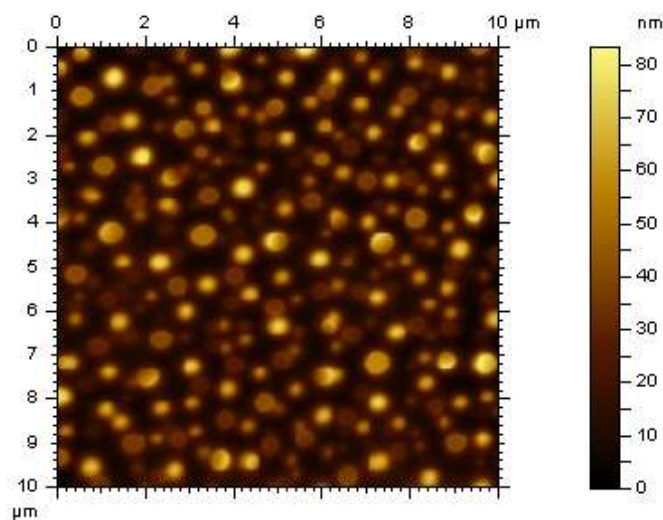
Sample: 63 (Morphology: Column)

1. Area fraction of PMMA (%): 14.28
2. Average morphology diameter (nm): 284.4
3. Average morphology height (nm): 38.68
4. Aspect ratio: 7.35



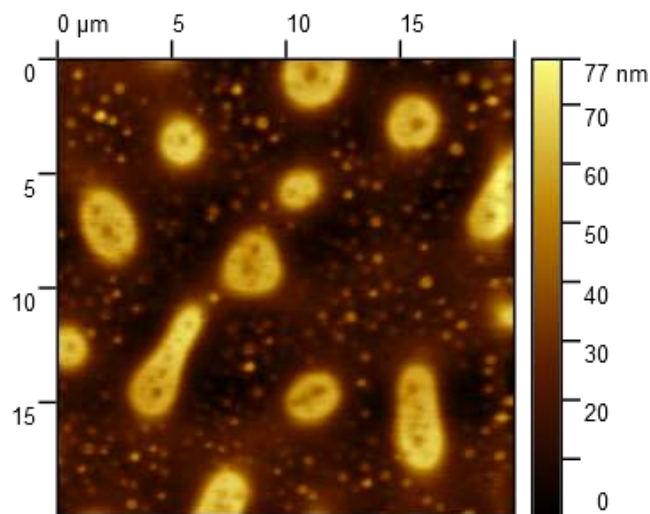
Sample: 64 (Morphology: Island)

1. Area fraction of PMMA (%): 26.89
2. Average morphology diameter (nm): 1415
3. Average morphology height (nm): 36.78
4. Aspect ratio: 38.47



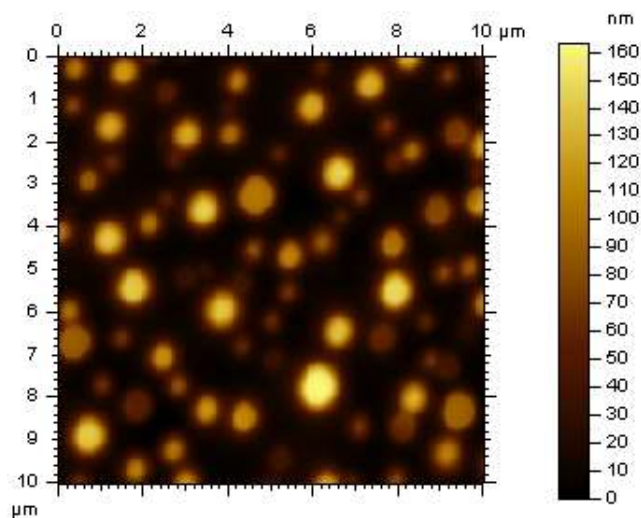
Sample: 65 (Morphology: Hole)

1. Area fraction of PMMA (%): 56.92
2. Average morphology diameter (nm): 984.3
3. Average morphology height (nm): 46.45
4. Aspect ratio: 21.19



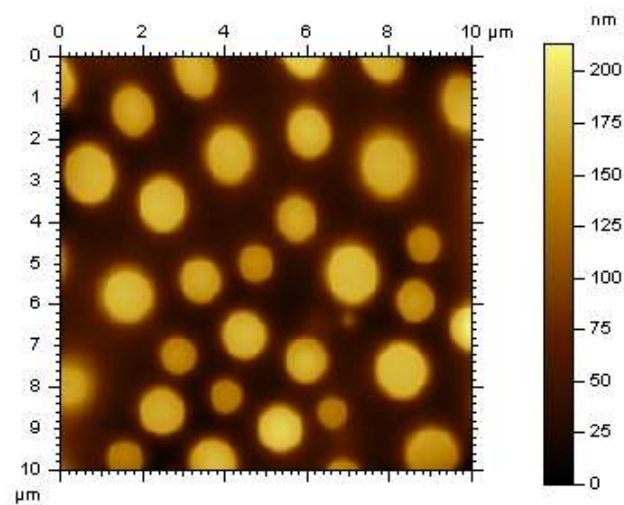
Sample: 66 (Morphology: Island)

1. Area fraction of PMMA (%): 22.27
2. Average morphology diameter (nm): 1811
3. Average morphology height (nm): 56.85
4. Aspect ratio: 31.86



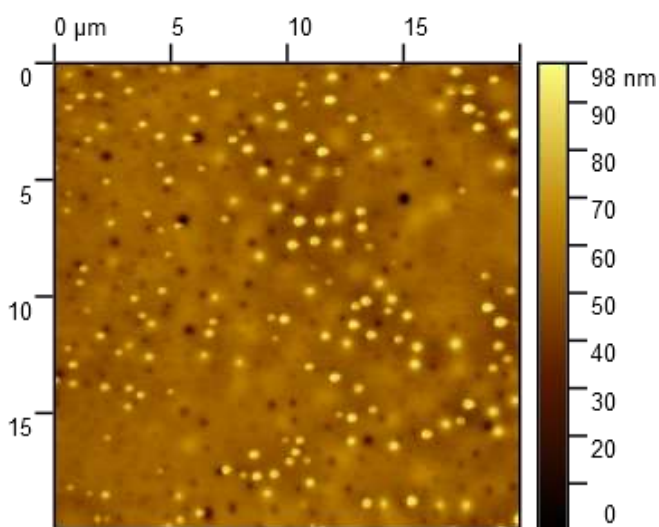
Sample: 67 (Morphology: Column)

1. Area fraction of PMMA (%): 9.88
2. Average morphology diameter (nm): 426.1
3. Average morphology height (nm): 105.2
4. Aspect ratio: 4.05



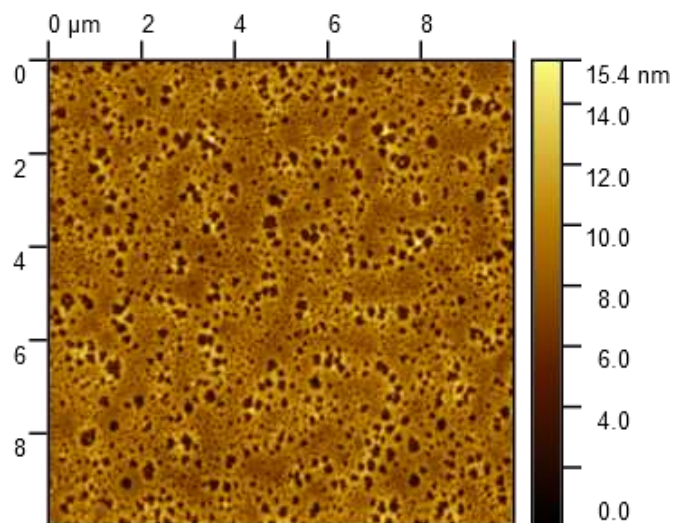
Sample: 68 (Morphology: Column)

1. Area fraction of PMMA (%): 36.1
2. Average morphology diameter (nm): 1056
3. Average morphology height (nm): 893.5
4. Aspect ratio: 1.18



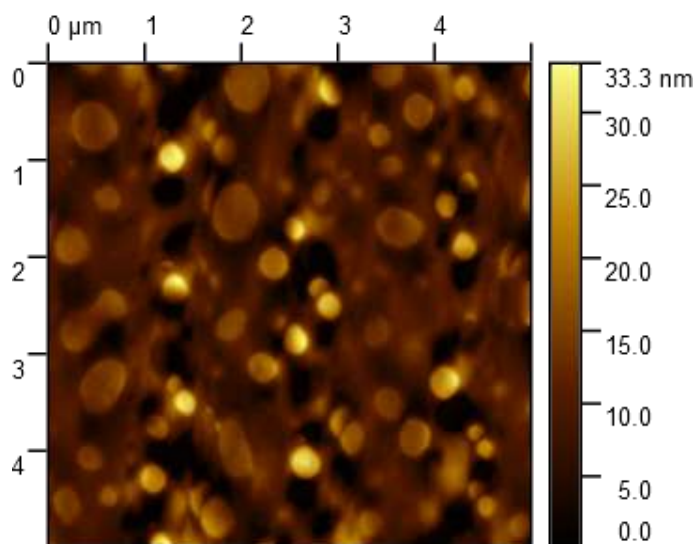
Sample: 69 (Morphology: Column)

1. Area fraction of PMMA (%): 3.35
2. Average morphology diameter (nm): 304.9
3. Average morphology height (nm): 80.67
4. Aspect ratio: 3.78



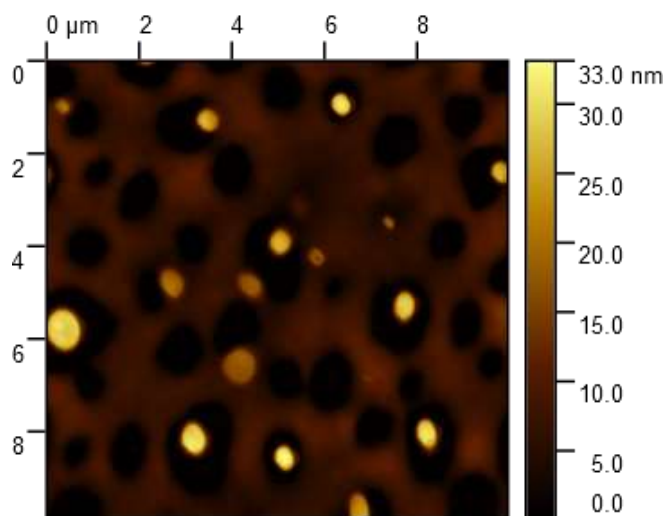
Sample: 70 (Morphology: Hole)

1. Area fraction of PMMA (%): 88.7
2. Average morphology diameter (nm): 63.8
3. Average morphology height (nm): 5.12
4. Aspect ratio: 12.45



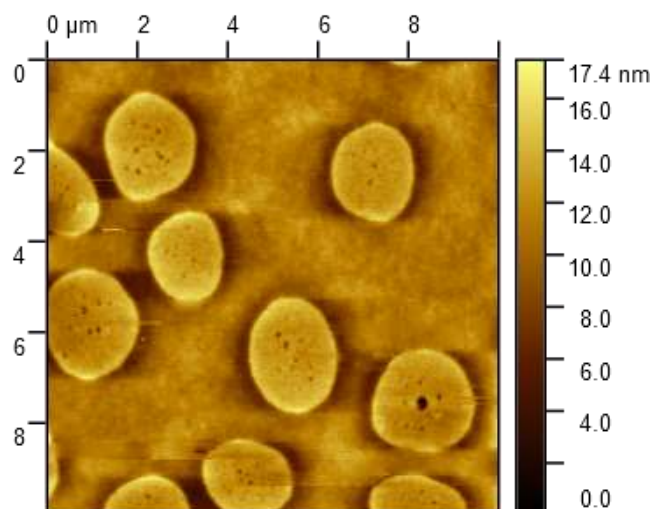
Sample: 71 (Morphology: Column)

1. Area fraction of PMMA (%): 39.42
2. Average morphology diameter (nm): 209.3
3. Average morphology height (nm): 29.42
4. Aspect ratio: 7.11



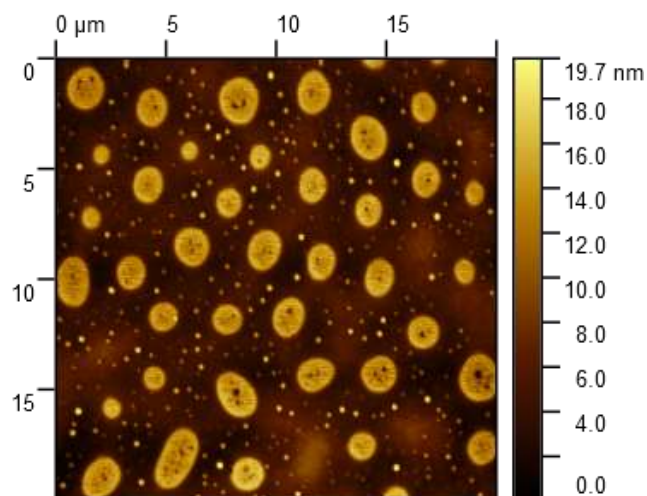
Sample: 72 (Morphology: Column)

1. Area fraction of PMMA (%): 3.52
2. Average morphology diameter (nm): 403.8
3. Average morphology height (nm): 29.23
4. Aspect ratio: 13.81



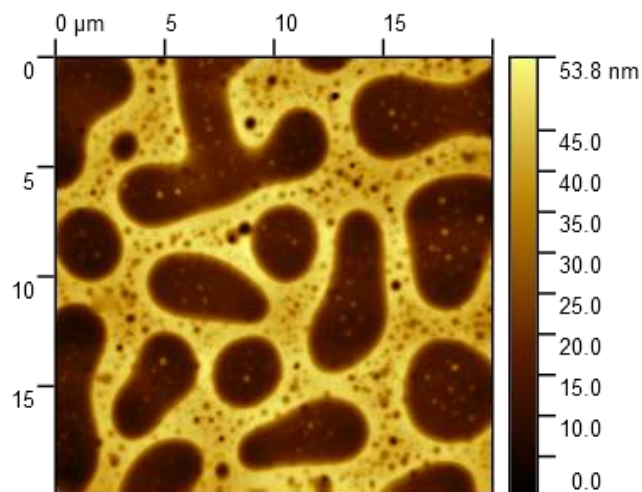
Sample: 73 (Morphology: Island)

1. Area fraction of PMMA (%): 30.8
2. Average morphology diameter (nm): 358.1
3. Average morphology height (nm): 12.98
4. Aspect ratio: 27.59



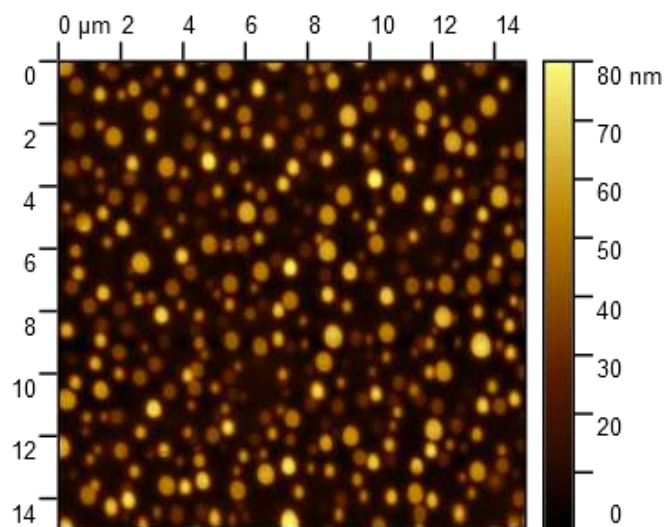
Sample: 74 (Morphology: Island)

1. Area fraction of PMMA (%): 19.38
2. Average morphology diameter (nm): 851.3
3. Average morphology height (nm): 12.7
4. Aspect ratio: 67.03



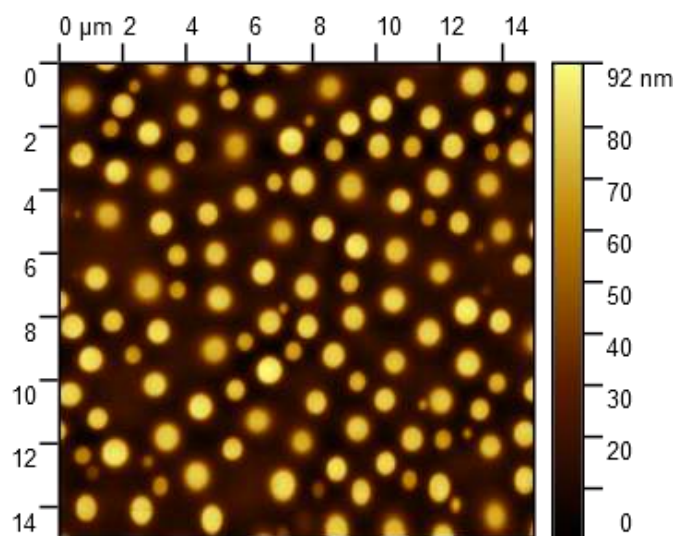
Sample: 75 (Morphology: Hole)

1. Area fraction of PMMA (%): 52.95
2. Average morphology diameter (nm): 824.4
3. Average morphology height (nm): 16.32
4. Aspect ratio: 50.51



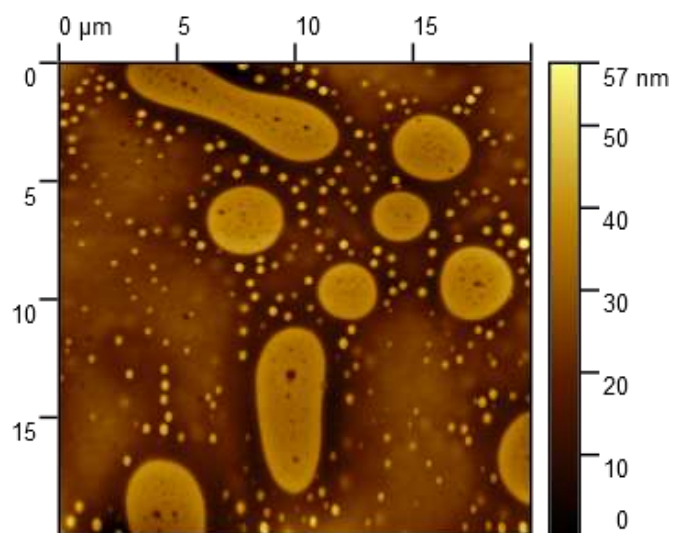
Sample: 76 (Morphology: Column)

1. Area fraction of PMMA (%): 18.14
2. Average morphology diameter (nm): 359.8
3. Average morphology height (nm): 46.74
4. Aspect ratio: 7.7



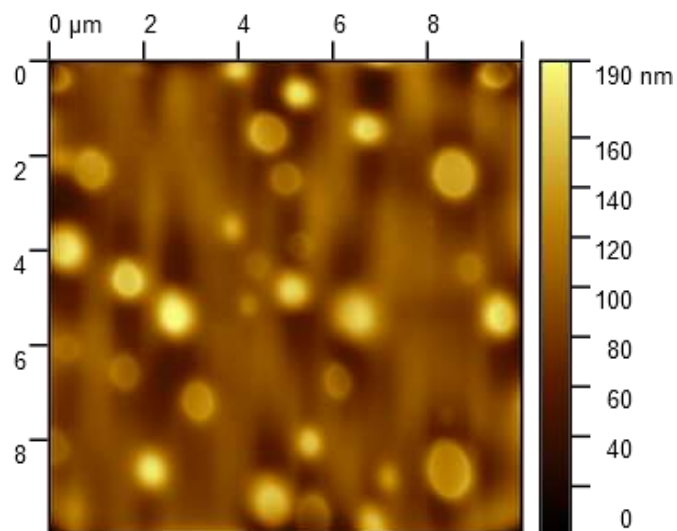
Sample: 77 (Morphology: Column)

1. Area fraction of PMMA (%): 19.86
2. Average morphology diameter (nm): 552.6
3. Average morphology height (nm): 71.5
4. Aspect ratio: 7.73



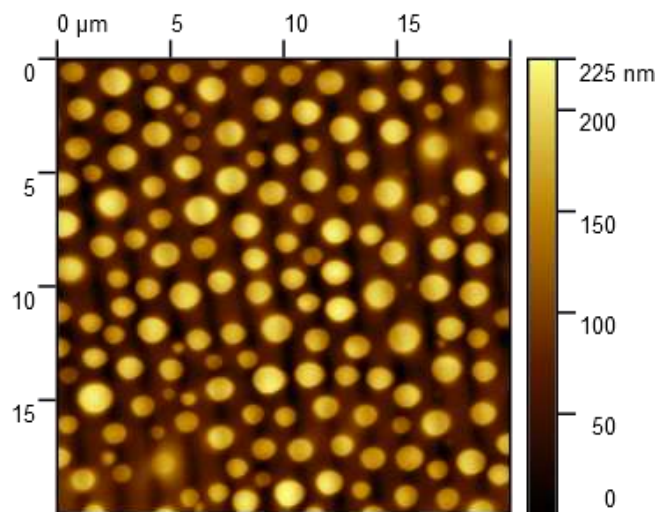
Sample: 78 (Morphology: Island)

1. Area fraction of PMMA (%): 20.37
2. Average morphology diameter (nm): 2051.9
3. Average morphology height (nm): 33.91
4. Aspect ratio: 60.51



Sample: 79 (Morphology: Column)

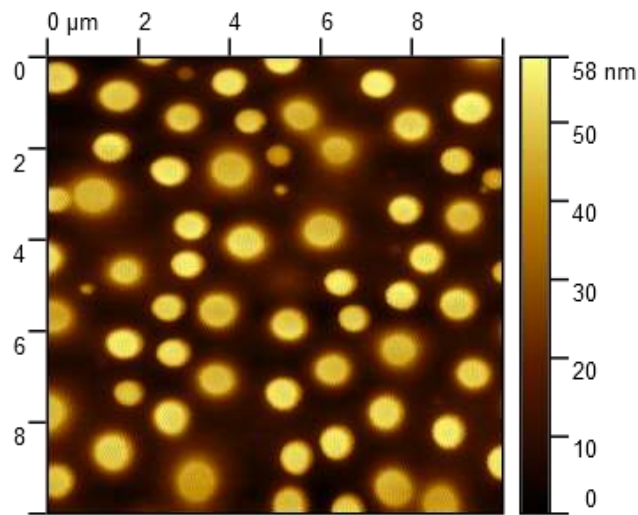
1. Area fraction of PMMA (%): 14.67
2. Average morphology diameter (nm): 515.9
3. Average morphology height (nm): 136.4
4. Aspect ratio: 3.78



Sample: 80 (Morphology: Column)

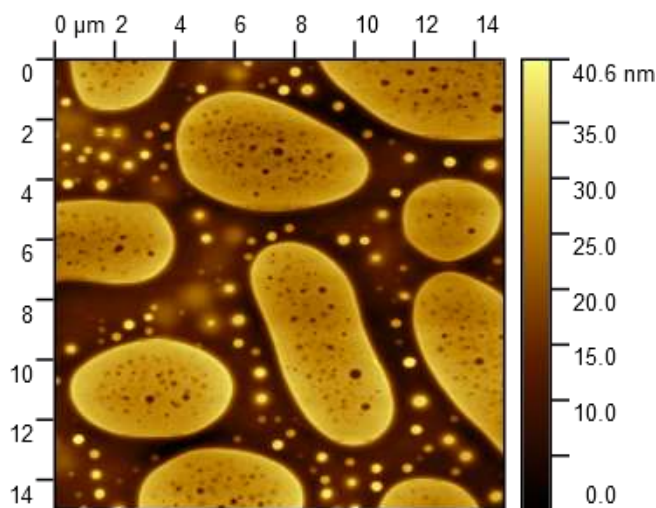
1. Area fraction of PMMA (%): 31.54
2. Average morphology diameter: 852.8
3. Average morphology height (nm): 162.2
4. Aspect ratio: 5.26

S2: AFM images used for model validation



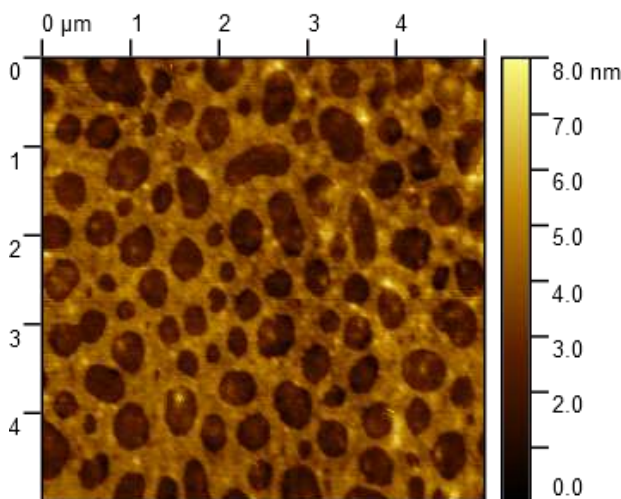
Validation: 1 (Morphology: Column)

1. Area fraction of PMMA (%): 21.53
2. Average morphology diameter: 562.5
3. Average morphology height (nm): 46.9
4. Aspect ratio: 11.99



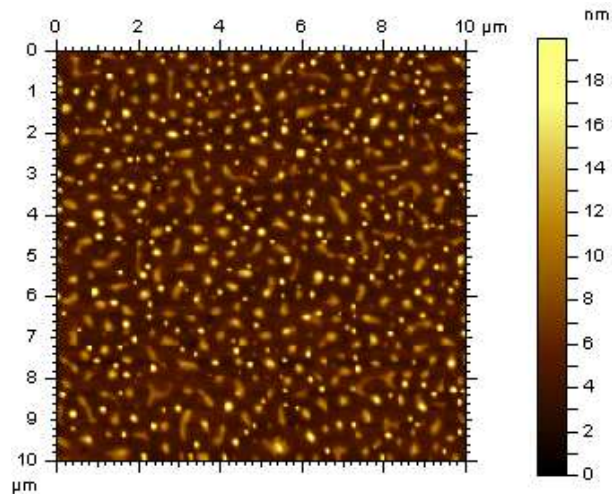
Validation: 2 (Morphology: Island)

1. Area fraction of PMMA (%): 46.33
2. Average morphology diameter: 1841
3. Average morphology height (nm): 28.04
4. Aspect ratio: 65.66



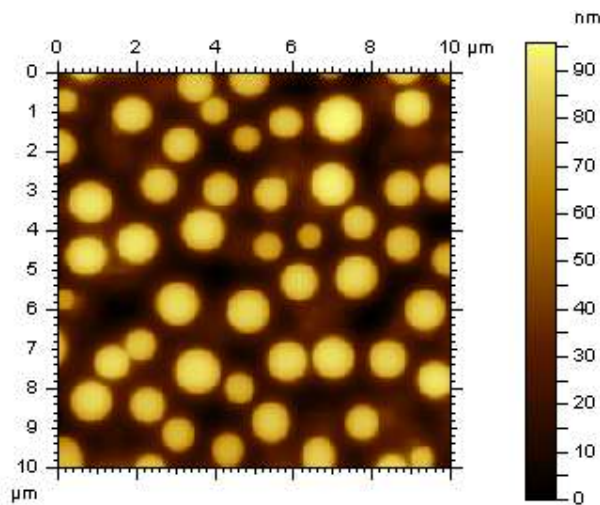
Validation: 3 (Morphology: Hole)

1. Area fraction of PMMA (%): 57.68
2. Average morphology diameter: 136
3. Average morphology height (nm): 3.2
4. Aspect ratio: 42.5



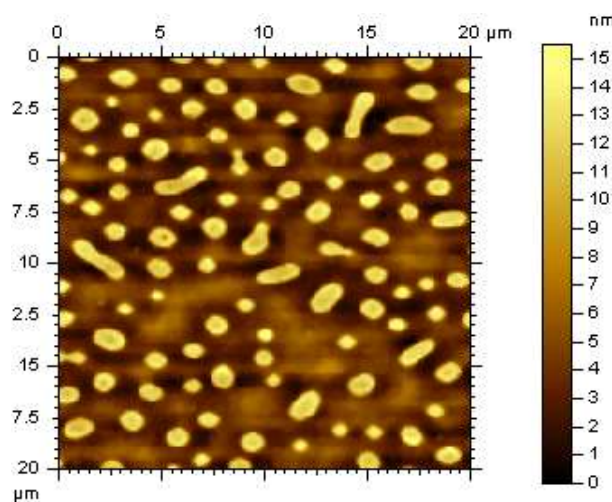
Validation: 4 (Morphology: Column)

1. Area fraction of PMMA (%): 16.64
2. Average morphology diameter: 104.05
3. Average morphology height (nm): 12.22
4. Aspect ratio: 8.51



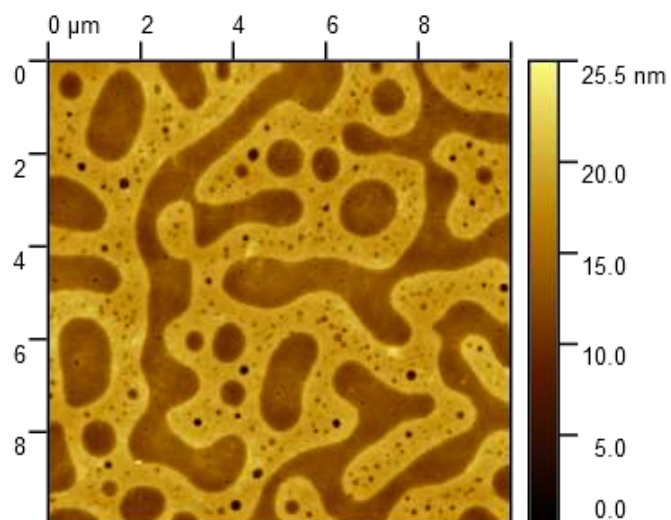
Validation: 5 (Morphology: Column)

1. Area fraction of PMMA (%): 31.39
2. Average morphology diameter: 419
3. Average morphology height (nm): 88
4. Aspect ratio: 4.76



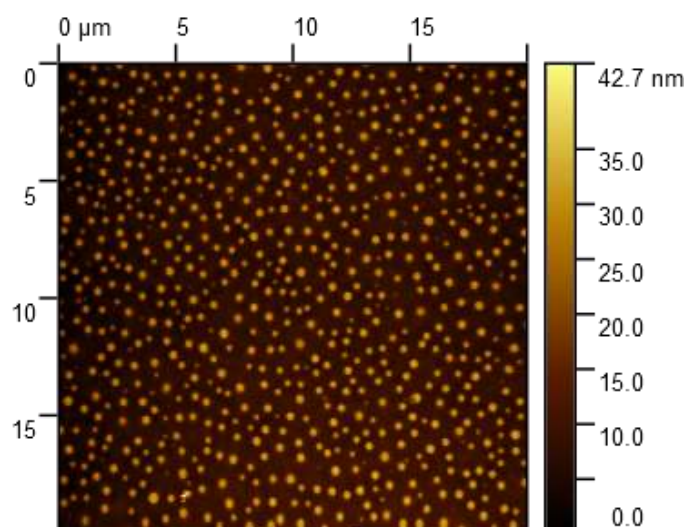
Validation: 6 (Morphology: Column)

1. Area fraction of PMMA (%): 36.7
2. Average morphology diameter: 595
3. Average morphology height (nm): 10.2
4. Aspect ratio: 58.33



Validation: 7 (Morphology: Hole)

1. Area fraction of PMMA (%): 56.11
2. Average morphology diameter: 353.9
3. Average morphology height (nm): 18.7
4. Aspect ratio: 18.93



Validation: 8 (Morphology: Column)

1. Area fraction of PMMA (%): 10.77
2. Average morphology diameter: 230.9
3. Average morphology height (nm): 26.04
4. Aspect ratio: 8.87

S3: Impact of substrate surface energy on model accuracy

To investigate the impact of substrate surface energy (γ_s) on the performance of the classification model, a 3-input model (i.e., excluding γ_s) was developed using the same 80 AFM images as explained in section 2.2 of the manuscript. The methodology used to develop the 3-input model is the same as that given in section 2.3 of the manuscript. Results obtained for the 3-input model is given in Table S1. It is clearly evident that the accuracy of the SVM-based classification model using 3-inputs (i.e., excluding γ_s) was only 75% as compared to 93.75% for the proposed 4-input model (i.e., including γ_s as given in Table 3 of the manuscript). Thus, γ_s indeed plays a pivotal role in accurately predicting the different morphologies for PS/PMMA blend thin films. Hence, this justifies the inclusion of γ_s as an input feature in the proposed multi-class classification model.

Table S1: Performance metrics and confusion matrix for the best SVM model with 3 inputs (i.e., excluding γ_s).

Performance metric		Value		
Accuracy		0.75		
Precision (Column, Hole, Island)		0.67, 1, 0		
Recall (Column, Hole, Island)		1, 1, 0		
Specificity (Column, Hole, Island)		0.5, 1, 1		
F1 Score (Column, Hole, Island)		0.8, 1, 0		
MCC		0.6455		
Confusion Matrix	Column	Hole	Island	
Column	8	0	0	
Hole	0	0	4	
Island	4	0	0	