Supplementary Information

Composition and state prediction of lithium-ion cathode via convolutional neural network trained on scanning electron microscopy images

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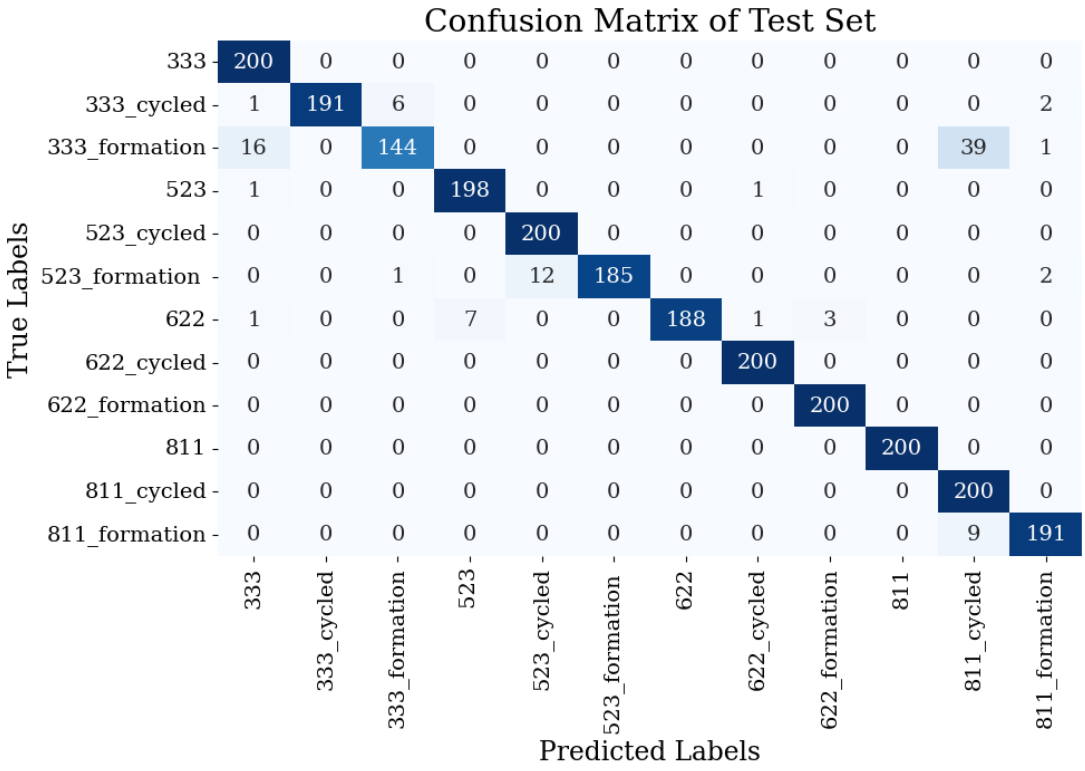
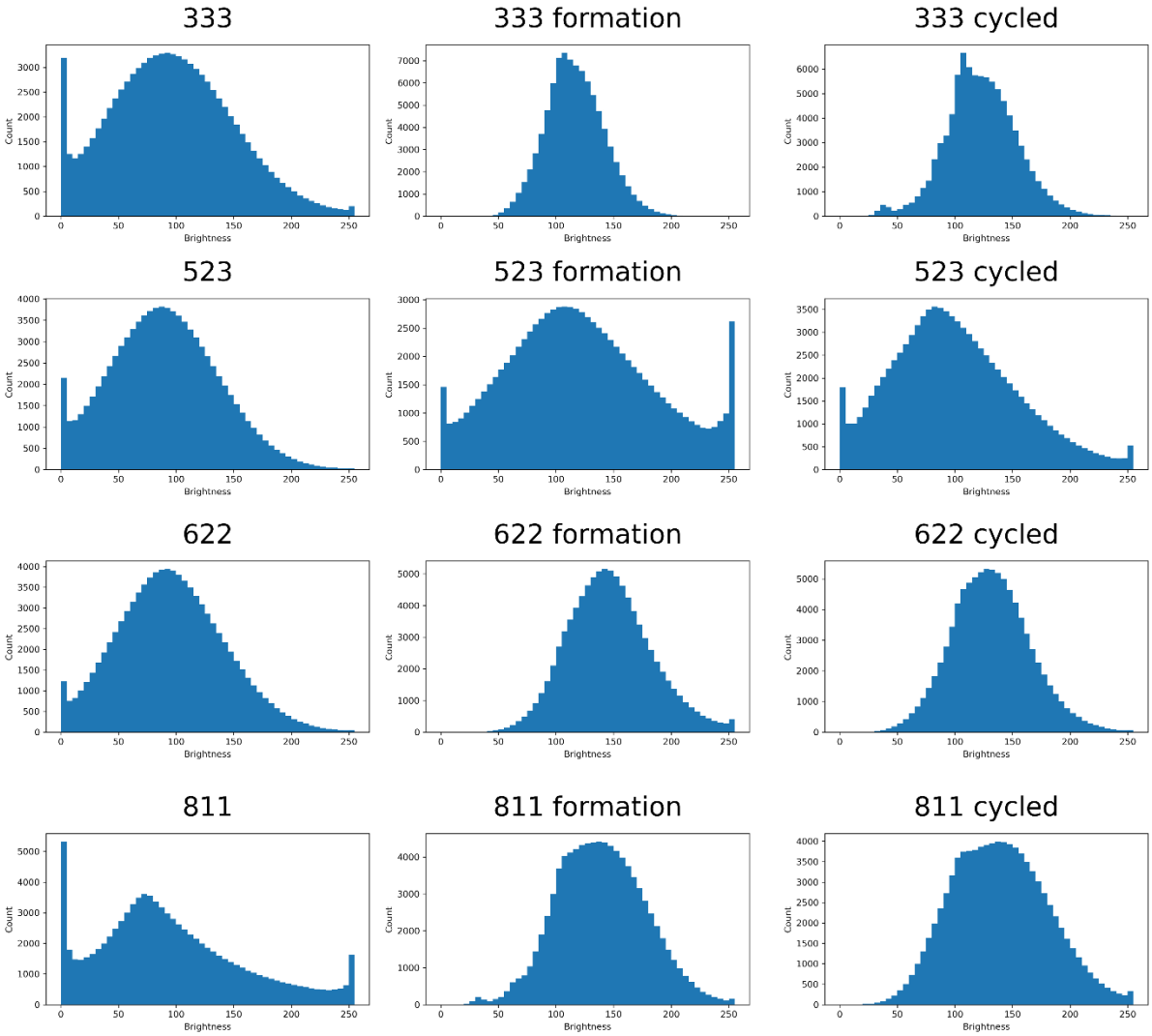


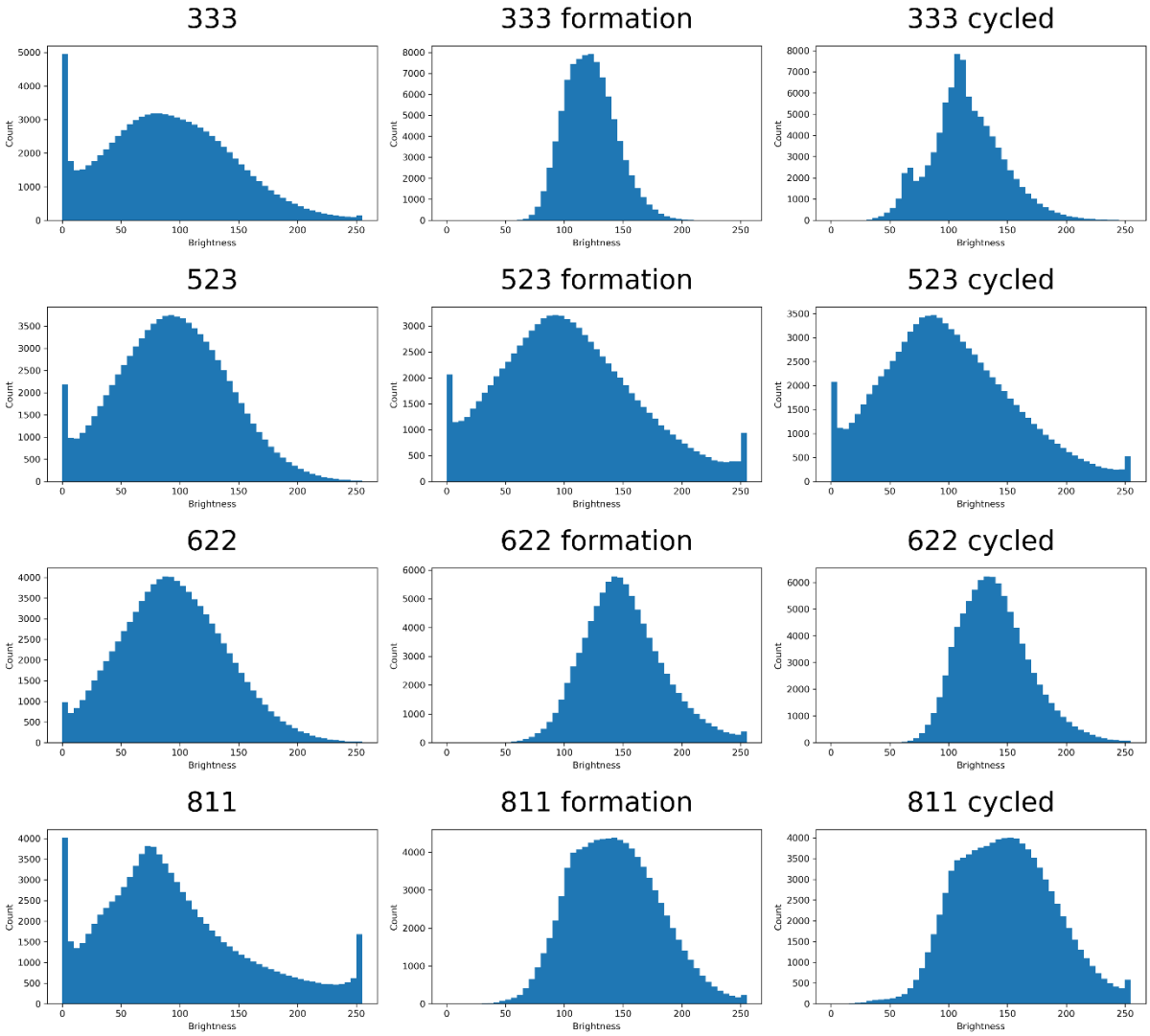
Supplementary Figure 1. Confusion matrix in the test set of the trained model.

Supplementary Table 1. Classification report in the test set of the trained model.

NCM sample	Precision	Recall	F1-score	Support
333	0.91	1.00	0.95	200
333_cycled	1.00	0.95	0.98	200
333_formation	0.95	0.72	0.82	200
523	0.97	0.99	0.98	200
523_cycled	0.94	1.00	0.97	200
523_formation	1.00	0.93	0.96	200
622	1.00	0.94	0.97	200
622_cycled	0.99	1.00	1.00	200
622_formation	0.99	1.00	0.99	200
811	1.00	1.00	1.00	200
811_cycled	0.81	1.00	0.89	200
811_formation	0.97	0.95	0.96	200
Overall accuracy			0.96	2400



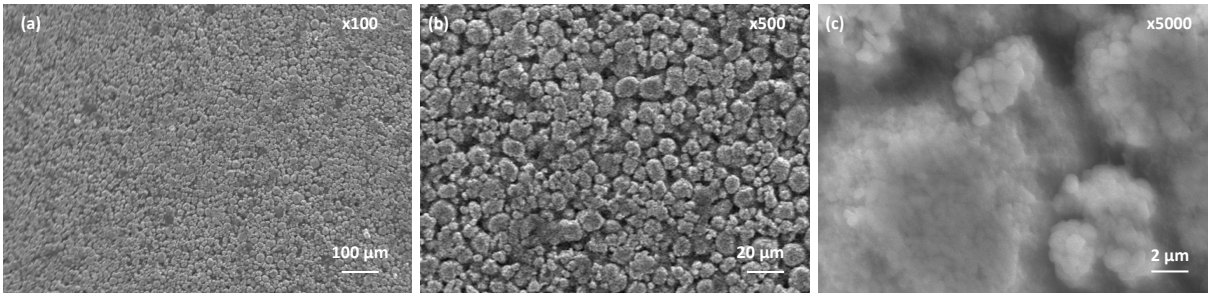
Supplementary Figure 2. Distribution of grayscale brightness value (0 ~ 255) in training image dataset containing pristine, formation, and cycled SEM images.



Supplementary Figure 3. Distribution of grayscale brightness value (0 ~ 255) in test image dataset containing pristine, formation, and cycled SEM images.

Supplementary Table 2. Average brightness and contrast value (0 ~ 255) of training and test SEM image datasets.

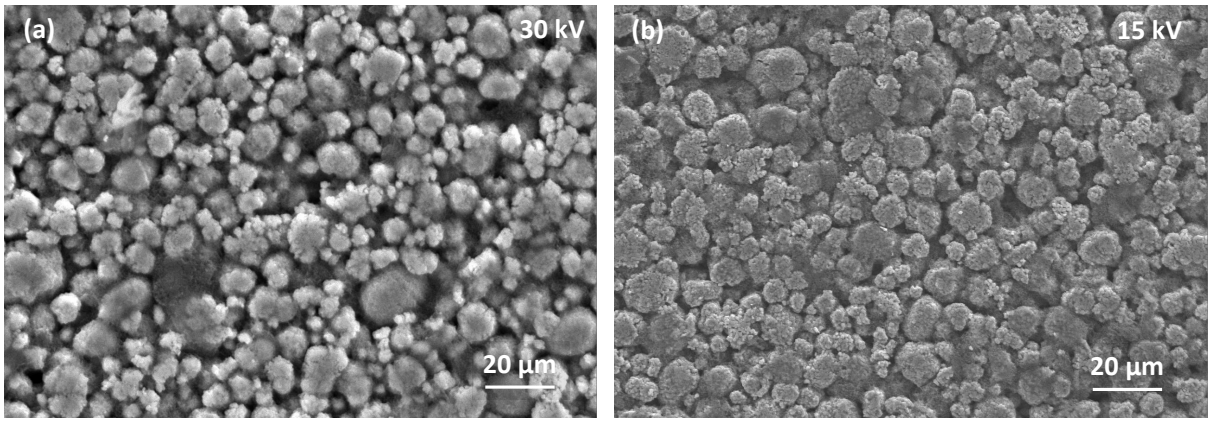
SEM Image Class	Training Dataset		Test Dataset	
	Average Brightness	Contrast (Std.)	Average Brightness	Contrast (Std.)
NCM333	96.05	52.50	89.70	53.11
NCM333 Formation	115.95	24.94	121.73	21.77
NCM333 Cycled	122.42	30.62	114.85	30.64
NCM523	89.76	45.94	93.74	46.27
NCM523 Formation	120.83	62.50	103.74	57.20
NCM523 Cycled	99.39	53.55	99.10	54.21
NCM622	95.34	45.50	94.53	44.52
NCM622 Formation	146.14	36.17	150.09	33.74
NCM622 Cycled	146.14	36.17	138.98	29.99
NCM811	94.72	62.37	94.11	60.98
NCM811 Formation	138.75	37.93	142.64	37.26
NCM811 Cycled	138.67	41.14	147.69	40.78



Supplementary Figure 4. SEM images of NCM622 pristine observed in (a) 100, (b) 500, and (c) 5000× magnification.

Supplementary Table 3. Accuracy prediction of the several nickel contents electrode samples as a function of magnification.

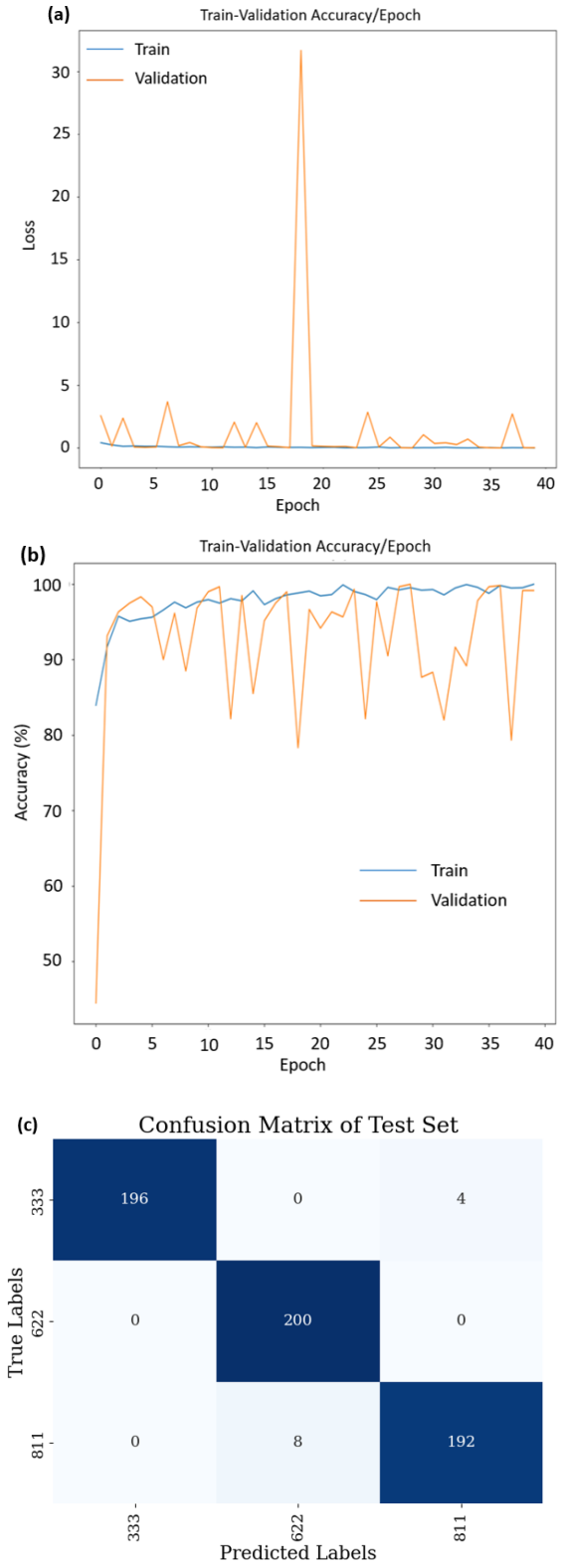
SEM Magnification	Accuracy (%)
100×	100.0
500×	99.6
5000×	100.0



Supplementary Figure 5. SEM images of NCM622 pristine observed with different accelerating voltages of (a) 30 kV, and (b) 15 kV.

Supplementary Table 4. Model accuracy of the pristine samples in the test set (magnification of 500 ×)

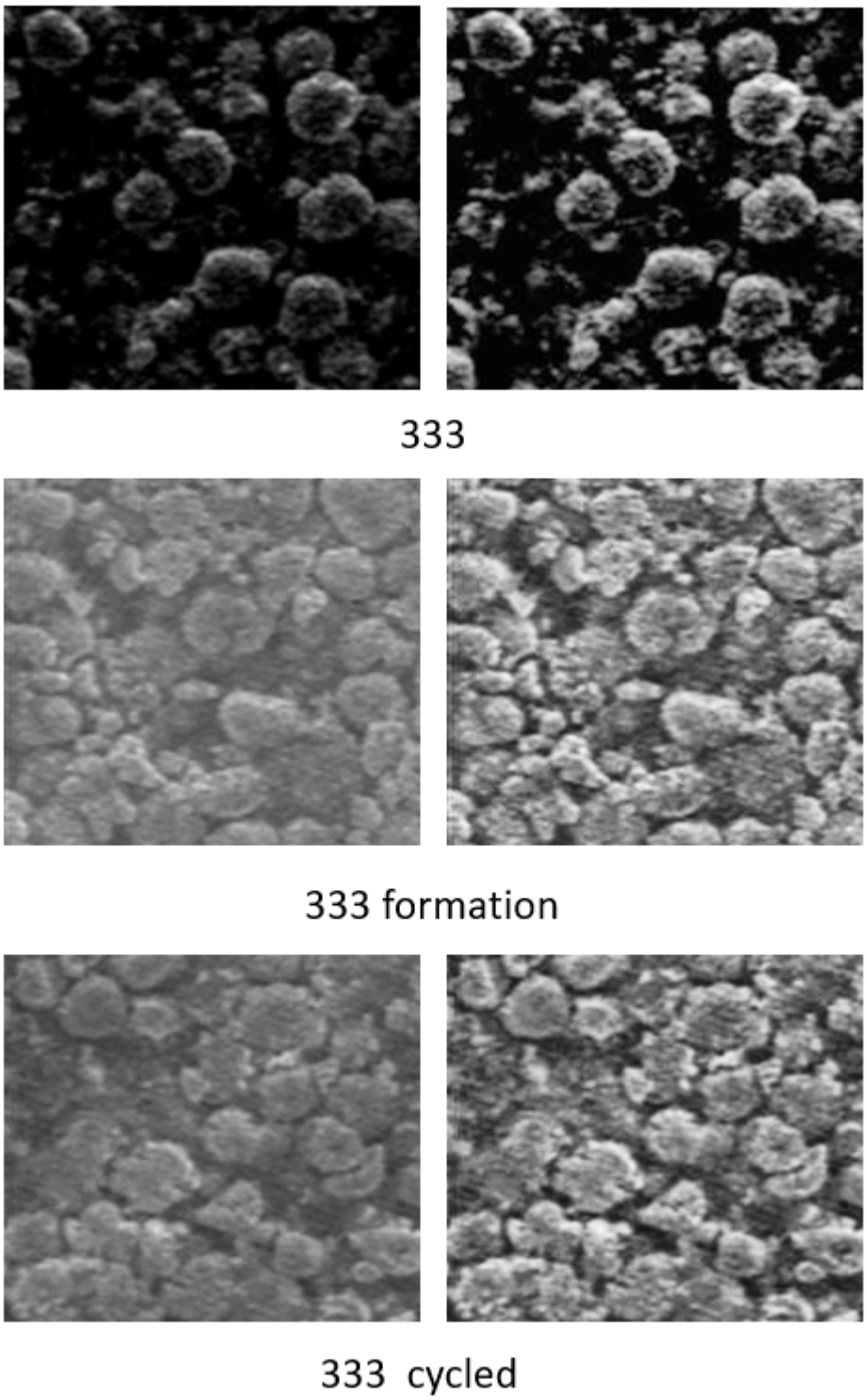
Accelerating voltage (kV)	Accuracy (%)
15	100
20	99.6
30	100



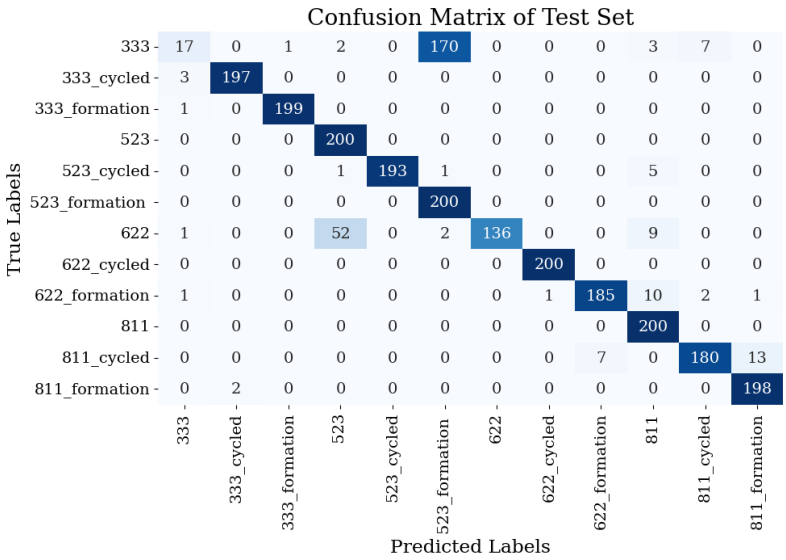
Supplementary Figure 6. (a) model loss, (b) model accuracy, and (c) confusion matrix of the model trained using OM images.

Supplementary Table 5. Classification report in the test for the model trained using OM images.

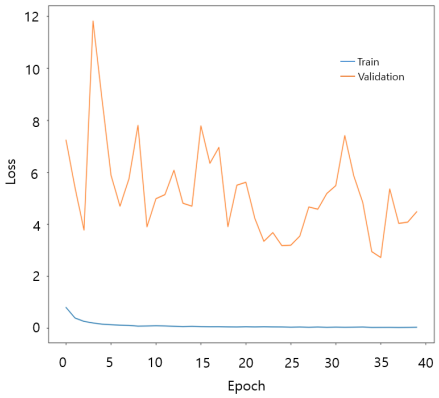
Pristine Sample	Precision	Recall	F1-score	Support
333	1.00	0.98	0.99	200
622	0.96	1.00	0.98	200
8111	0.98	0.96	0.97	200
Accuracy			0.98	600
Macro avg	0.98	0.98	0.98	600
Weighted avg	0.98	0.98	0.98	600



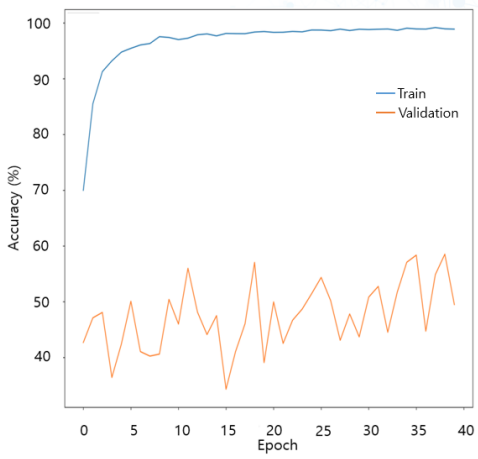
Supplementary Figure 7. The comparison of the SEM image samples without the CLAHE equalization technique (left) and with the CLAHE equalization technique (right).



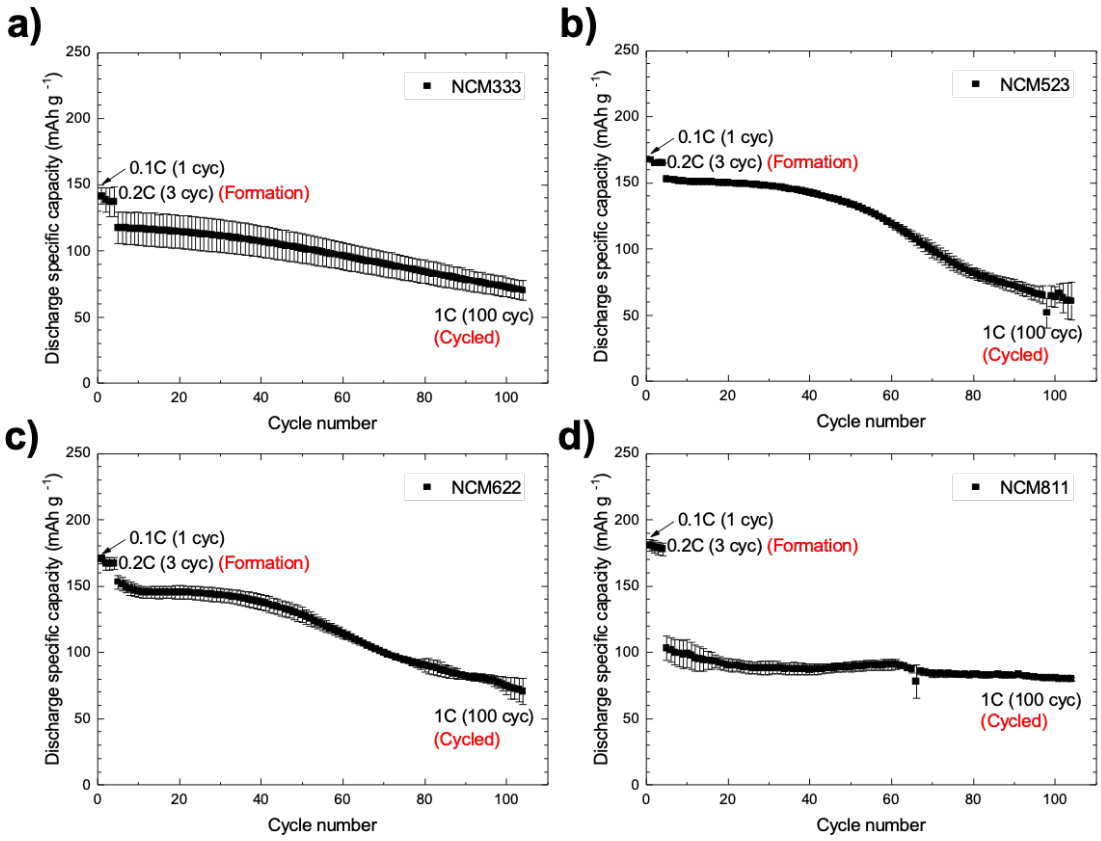
Supplementary Figure 8. The confusion matrix of the test of the images processed by CLAHE equalization.



Supplementary Figure 9. The loss of the model trained using images processed by CLAHE equalization.



Supplementary Figure 10. The accuracy of the model trained using images processed by CLAHE equalization.



Supplementary Figure 11. Cycle characteristics with formation (0.1C-rate 1 cycle + 0.2C-rate 3 cycles) and cycled (1C-rate 100 cycle) of a) NCM333, b) NCM523, c) NCM622 and d) NCM811.