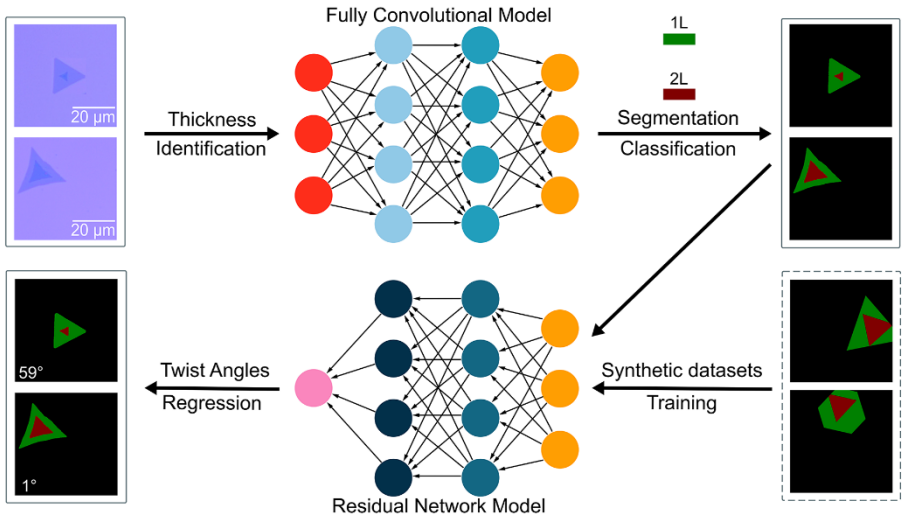
西安电子科技大学
XIDIAN UNIVERSITY

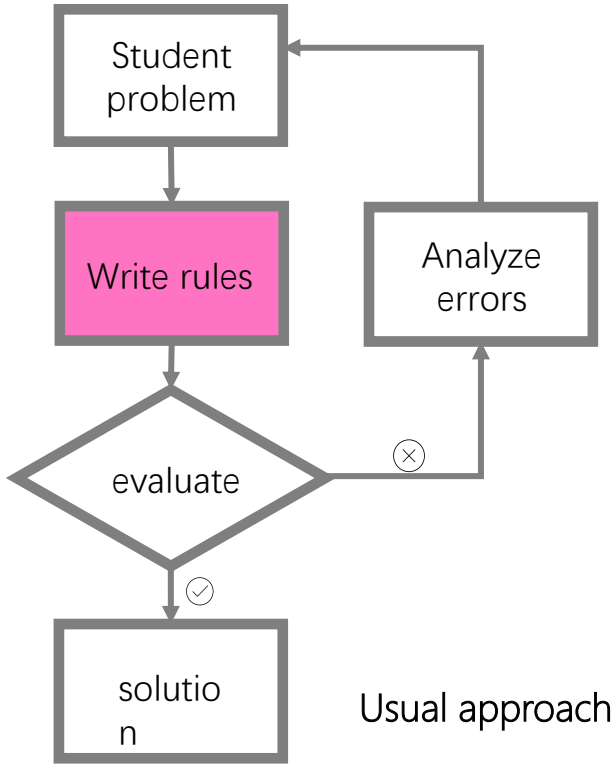
深度学习识别转角双层二维材料

谢涌
宽带隙半导体全国重点实验室，西安电子科技大学
yxie@xidian.edu.cn

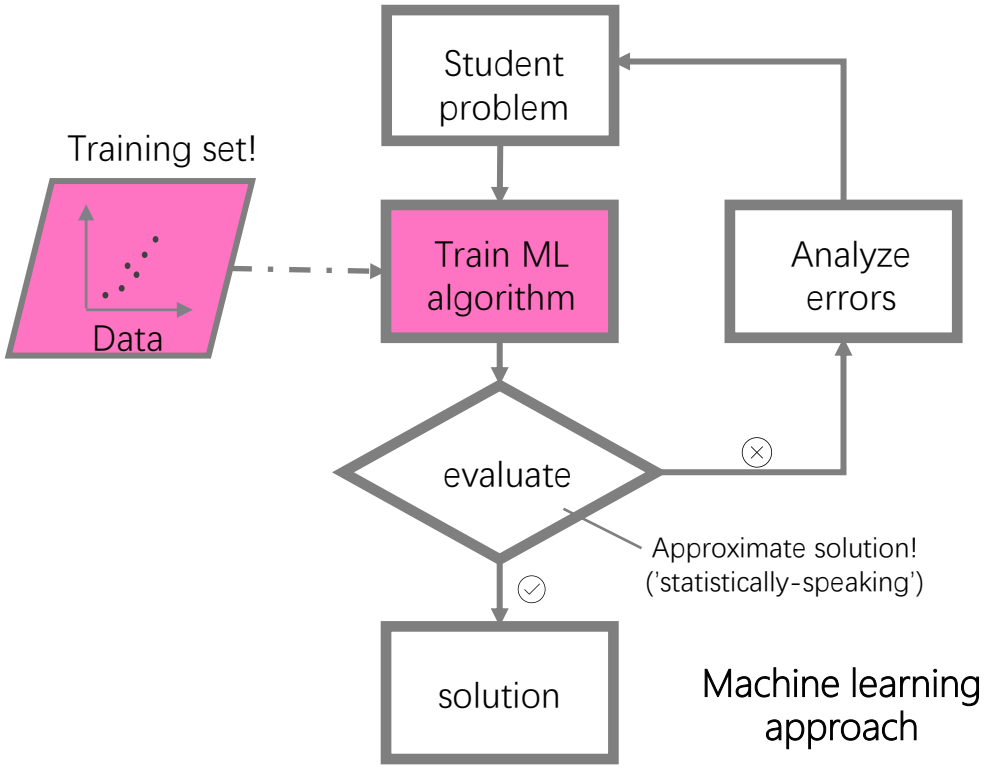


- Motivation
- Data Preparation and preprocessing
- Deep Learning to Identify Thickness
- OpenCV to Identify Twist Angles
- Deep Learning to Predict Twist Angles

Conventional vs "machine learning" approaches



Usual approach



Machine learning approach

MITx MicroMasters Programs

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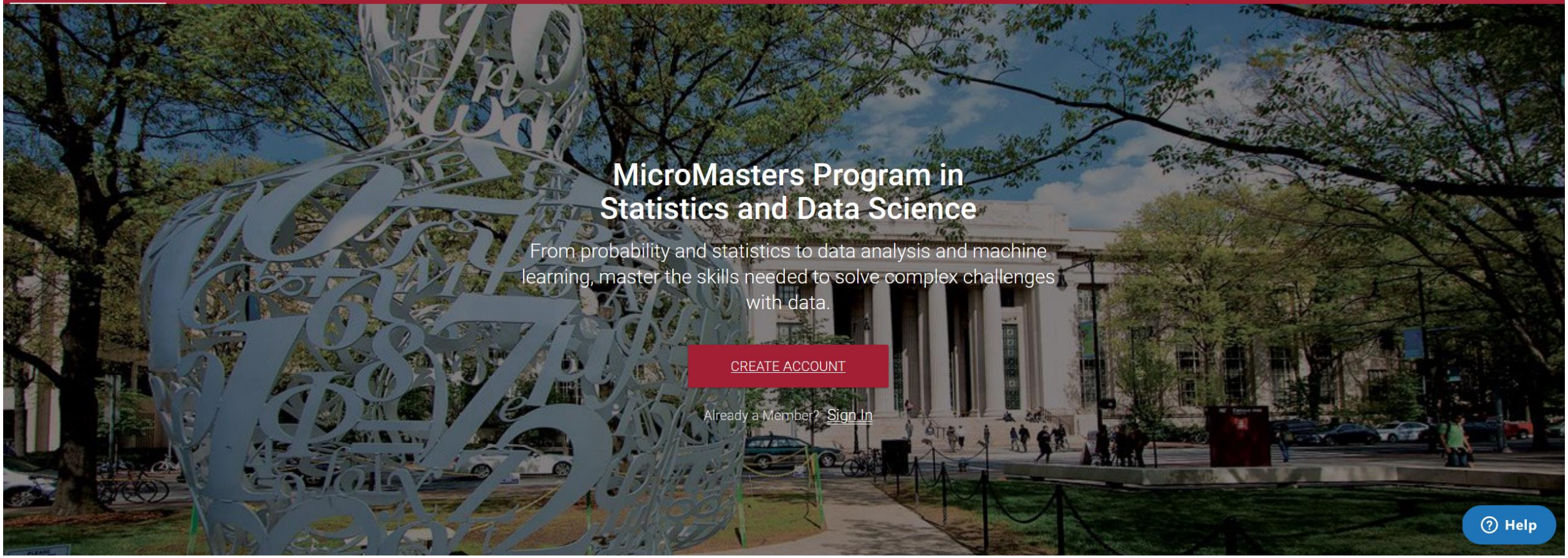

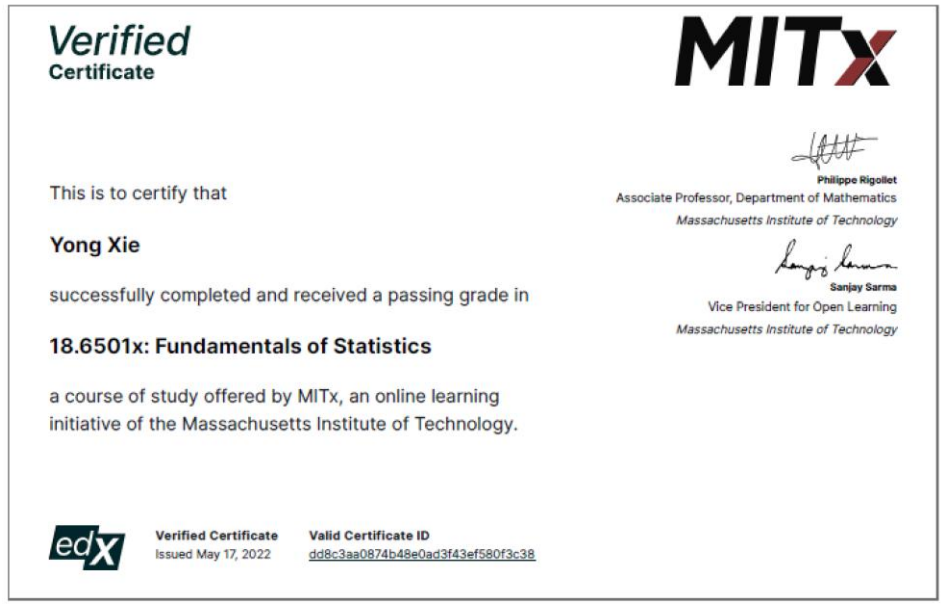

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Massachusetts Institute of Technology

Sanjay Sarma
Vice President for Open Learning
Massachusetts Institute of Technology

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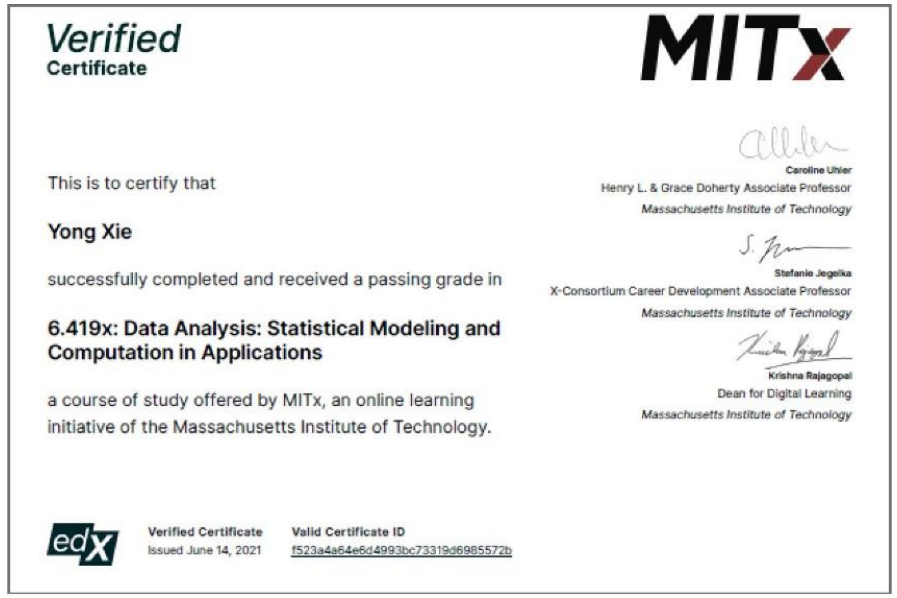

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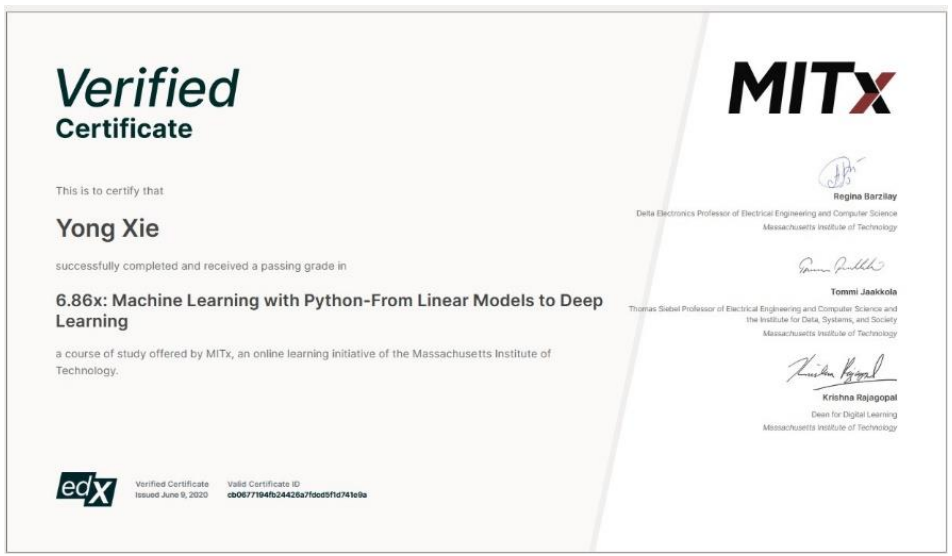

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Massachusetts Institute of Technology

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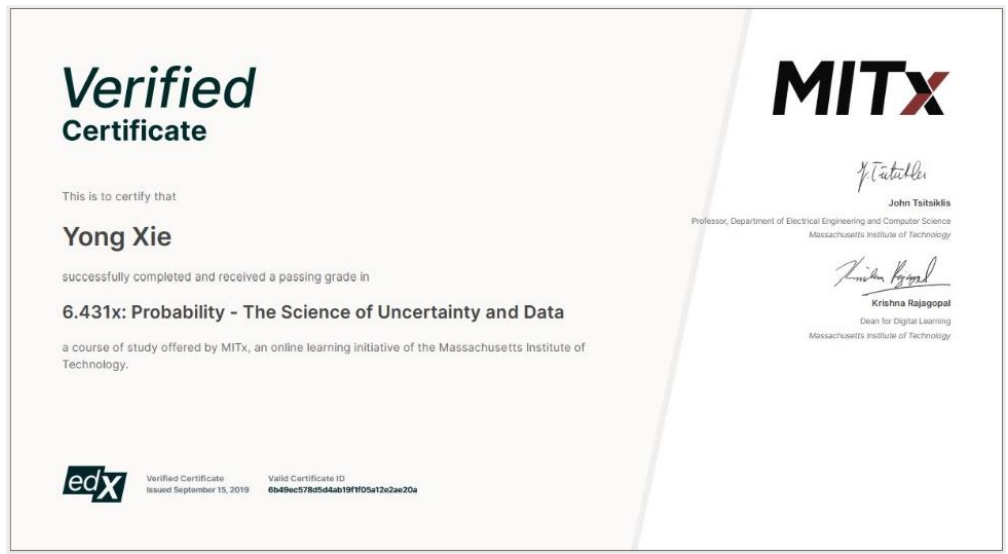

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Professor, Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology

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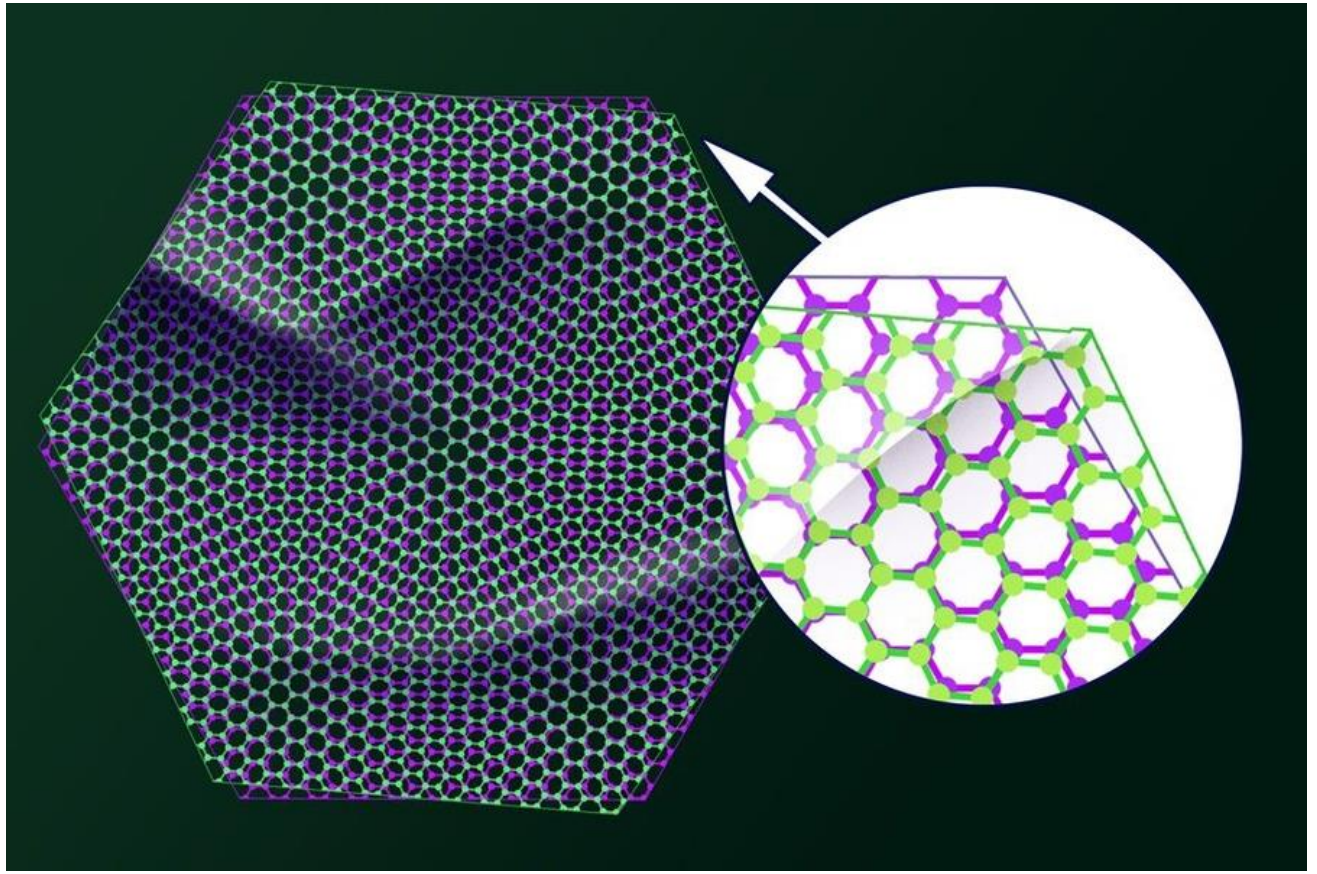
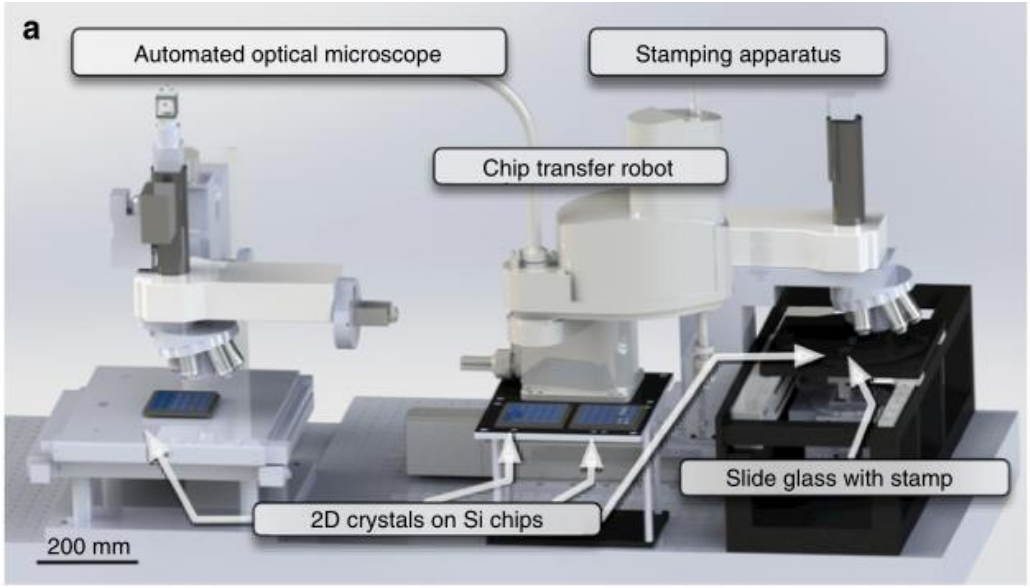
Ju Li MIT

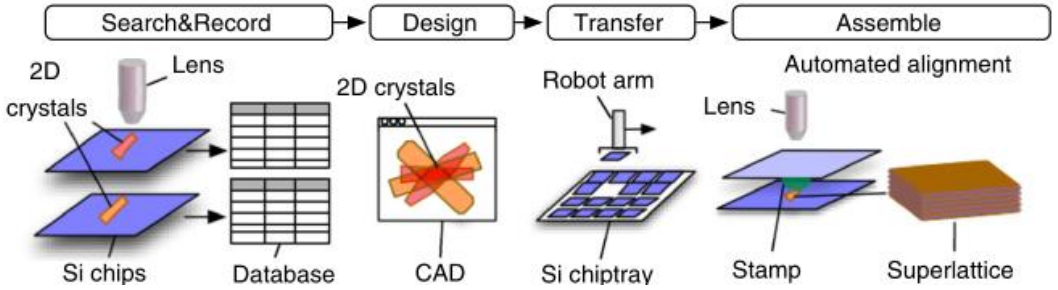
Motivation: twisted (Magic) angle

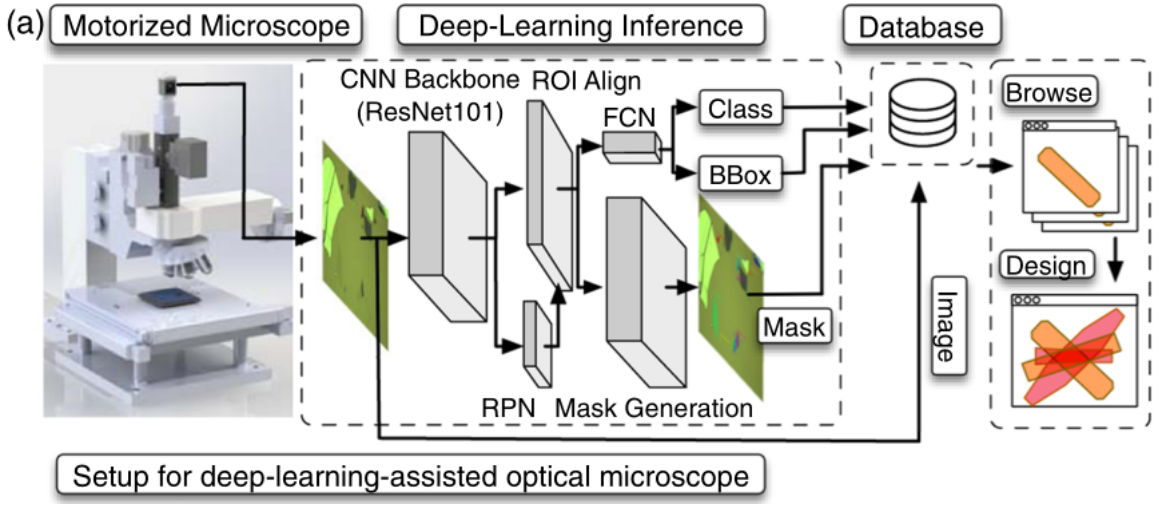


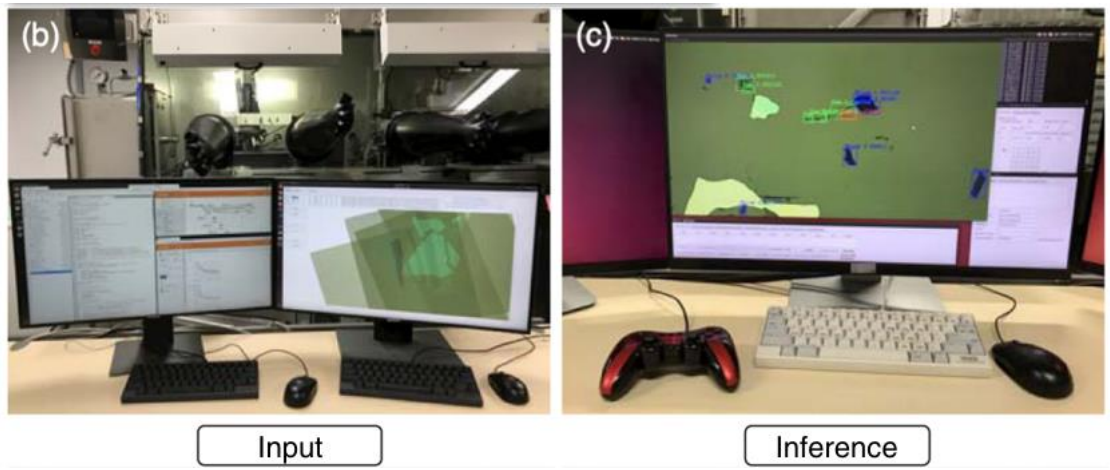
Pablo Jarillo-Herrero and Yuan Cao: **twistronics**, the study of electronic behavior in twisted graphene and other materials.

Motivation







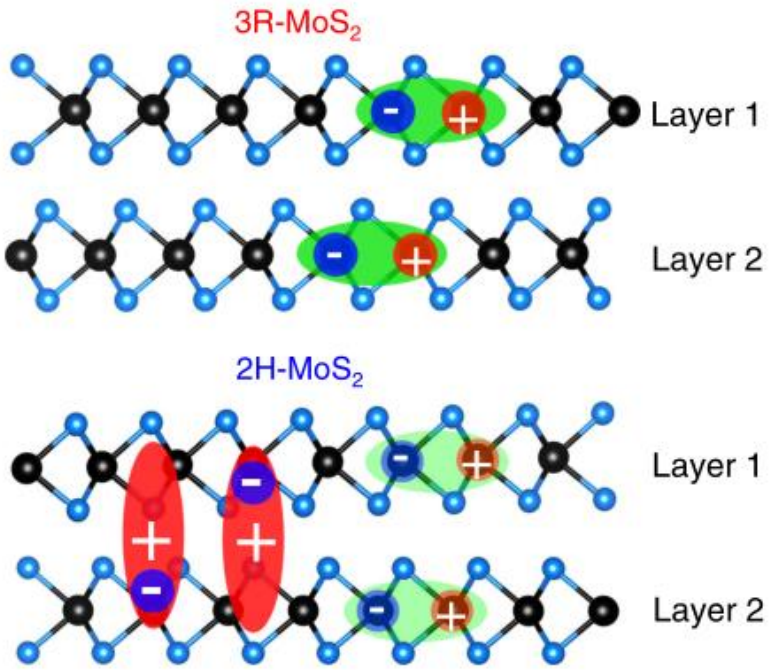


[1] *Nat Commun* **9**, 1413 (2018)

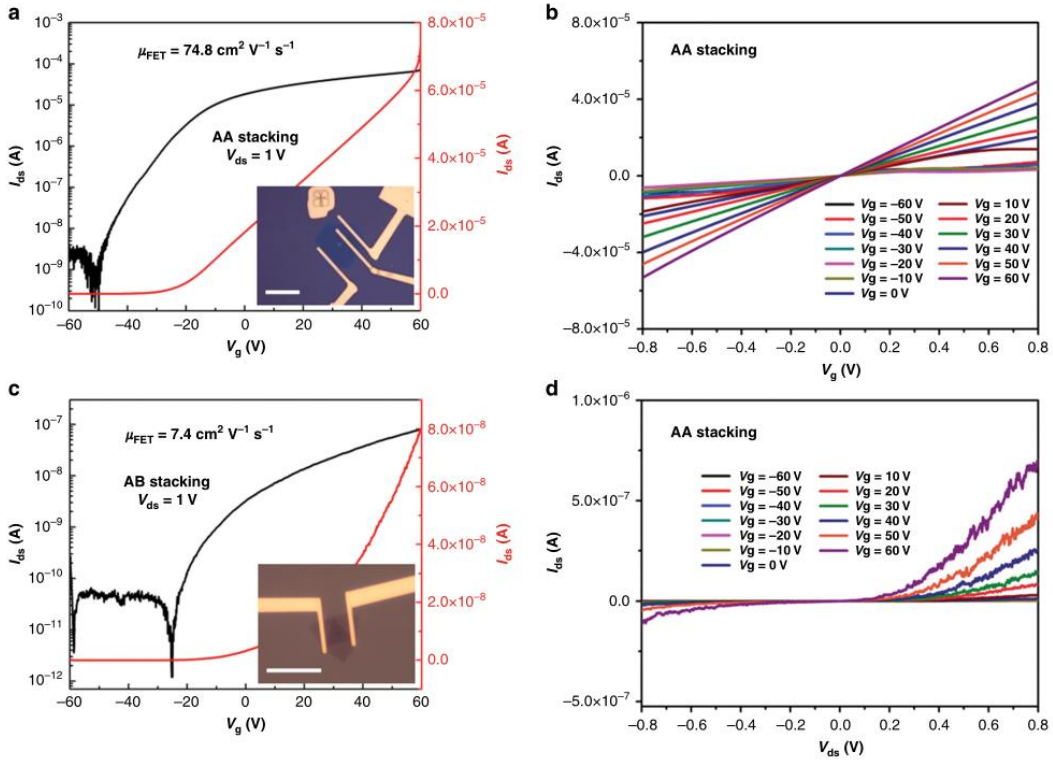
[2] *npj 2D Mater Appl* **4**, 3 (2020).

Motivation

The twist angle has a significant impact on the performance of TMDs



3R MoS_2 and 2H MoS_2 [1]



[1] *Nat Commun* **11**, 2391 (2020)

[2] *Nat Commun* **10**, 598 (2019)

[3] *Nat Commun* **5**, 4966 (2014)

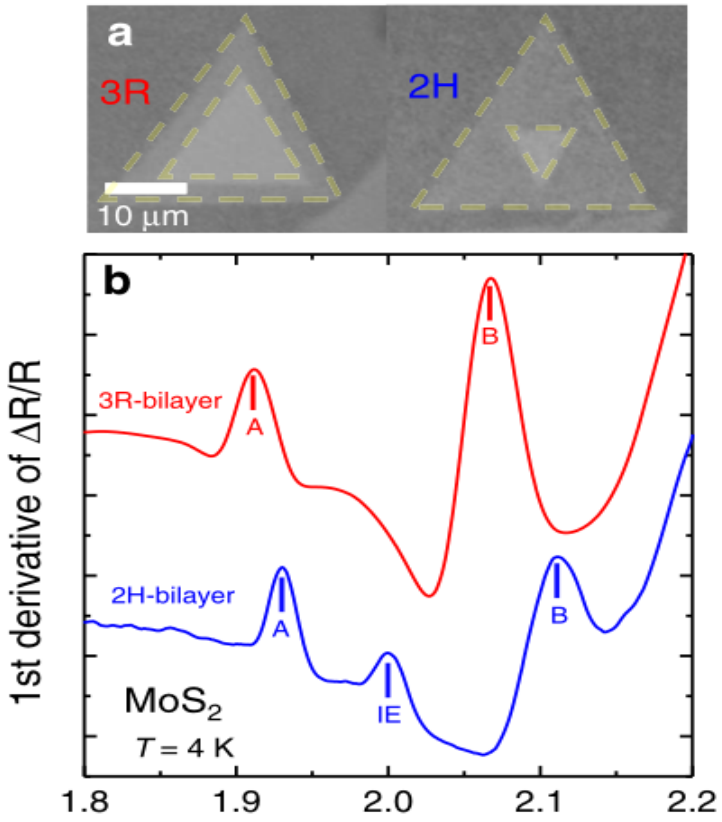
[4] *Chem Commun* **53**, 3054 (2017)

2H and 3R TMD's HER polarization curve[4]

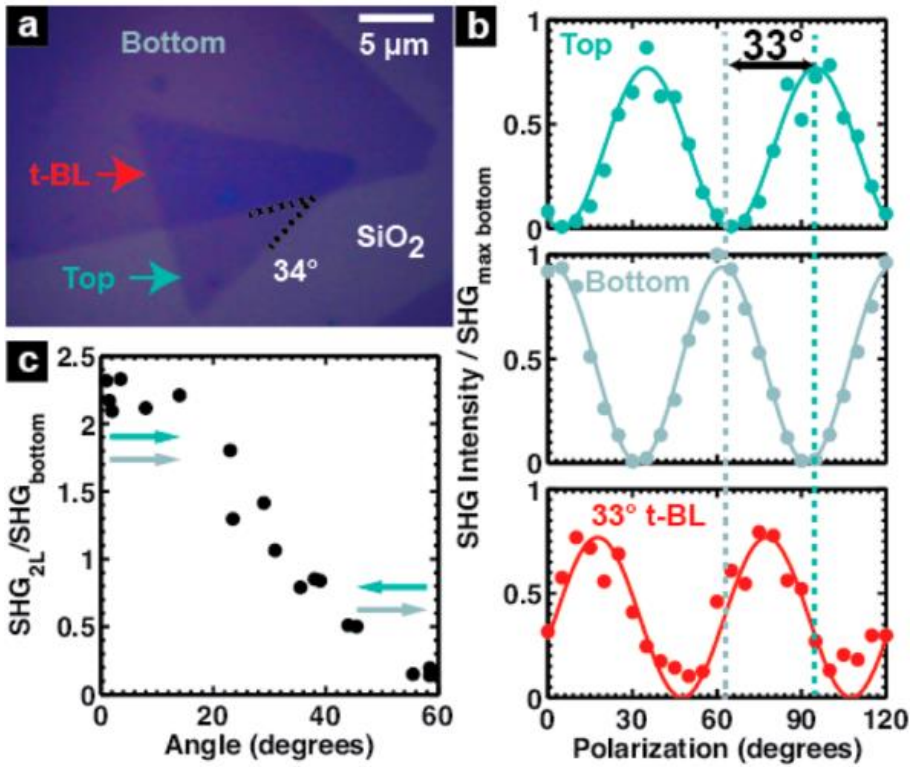
Transfer and output curve of AA and AB stacked MoS_2 FET devices[2]

Motivation

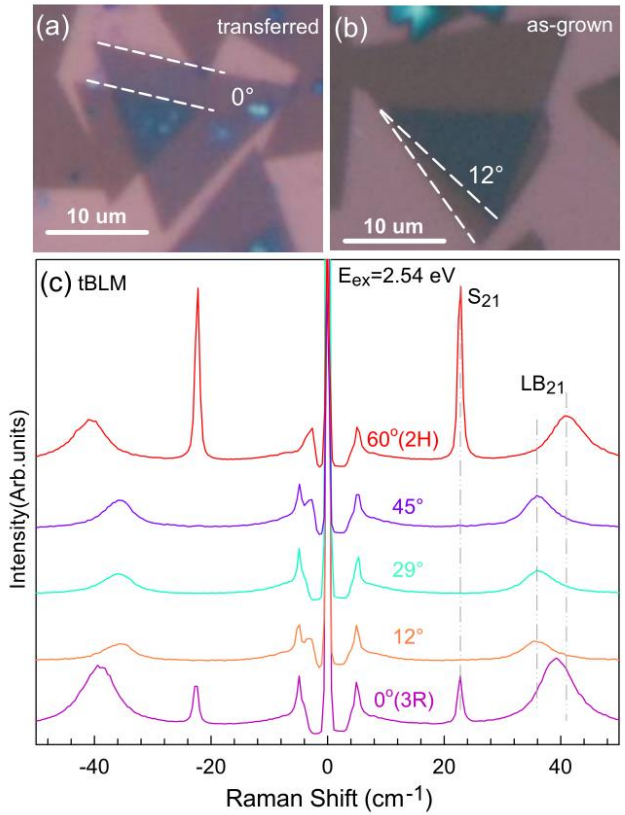
The current measurement methods for twist angles in TMDs



Differential Reflectance [1]



Generated through optical microscopy and second-harmonic generation [2]



Low wavenumber Raman spectra [3]

[1]*Nat Commun 11, 2391 (2020)*

[2] *Nano Lett. 2014 Jul 9;14(7):3869-75.*

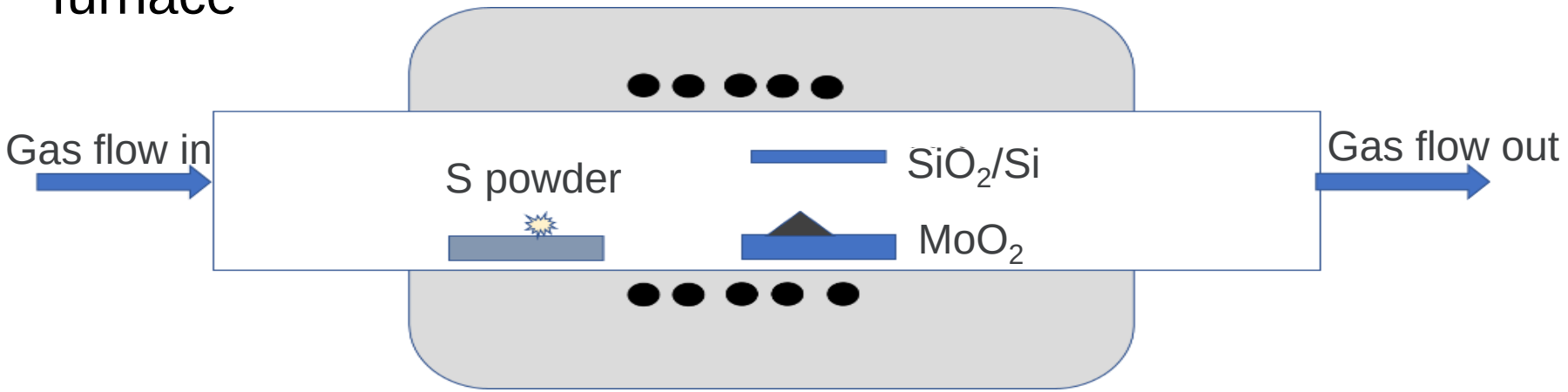
[3] *ACS Nano 2018, 12, 8, 8770–8780*

Data Preparation （CVD growth process）

Thermo Scientific
Single-zone tube furnace

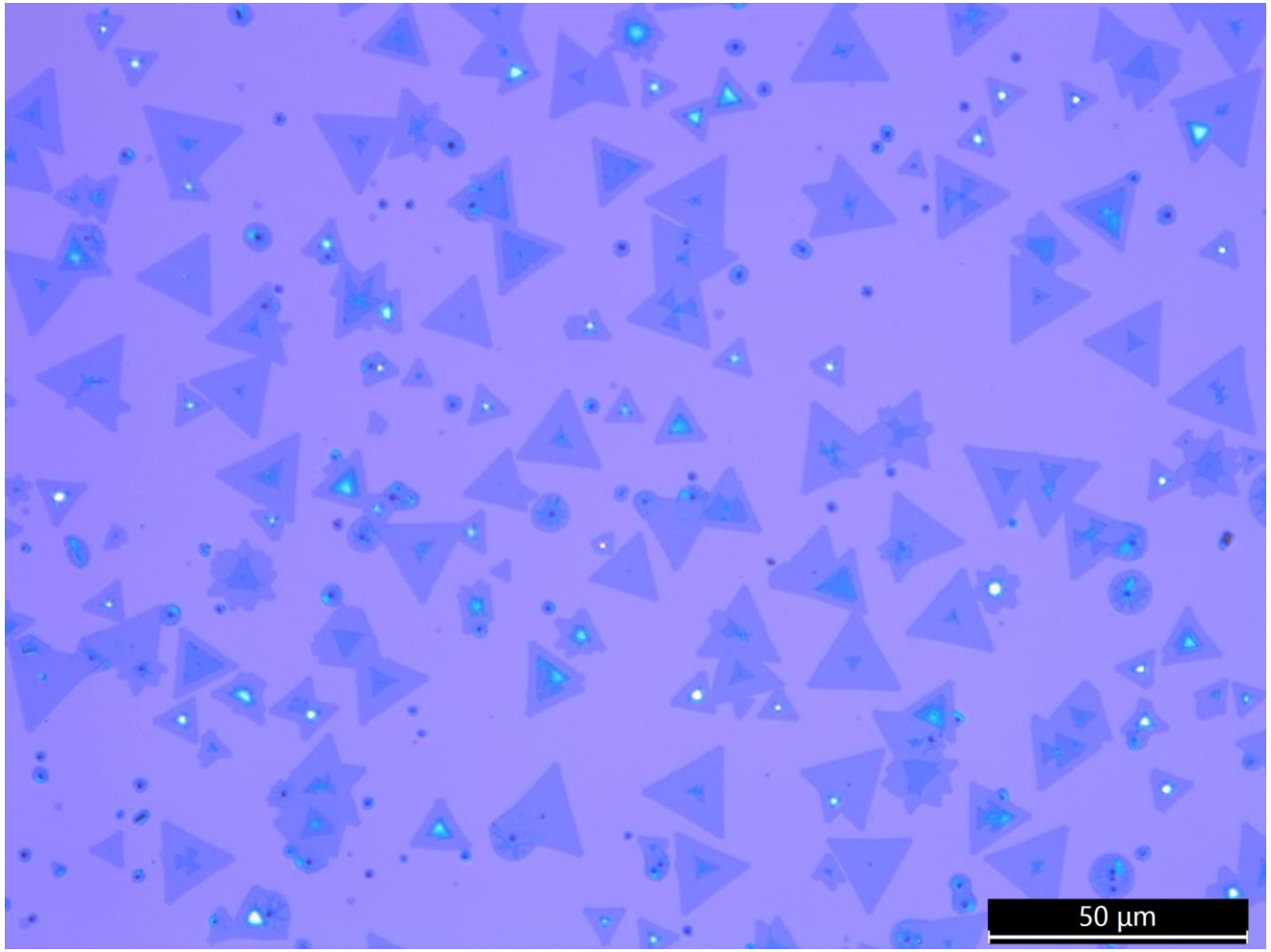
Alicat Scientific
Gas flow control valve

Ar Supply



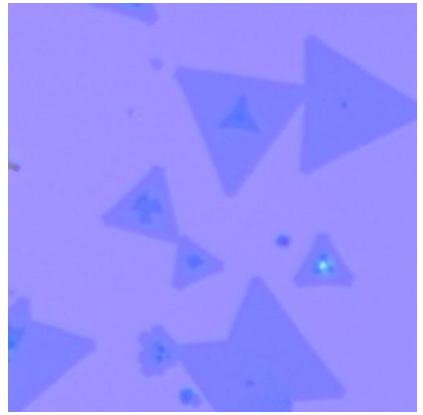
Data preprocessing

2592×1944

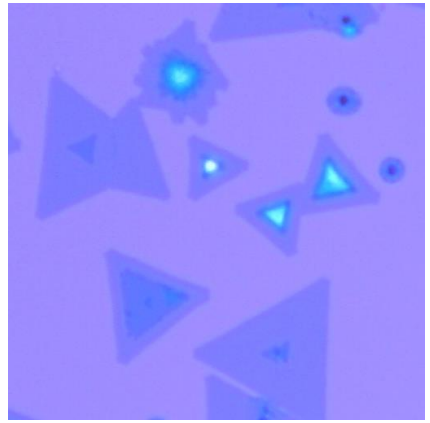


In total 1035 micrograph images

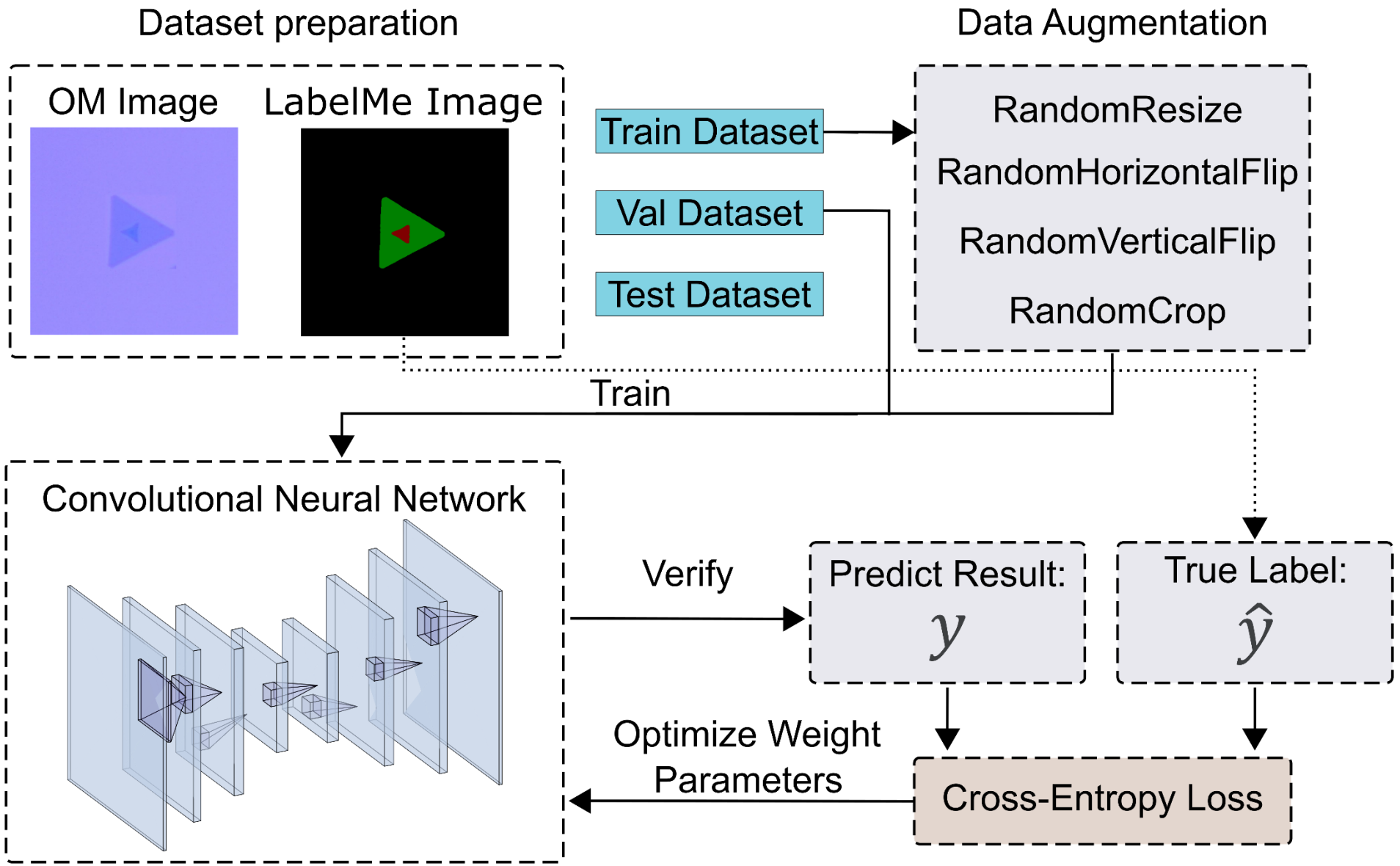
512x512
pixel images



Datasets

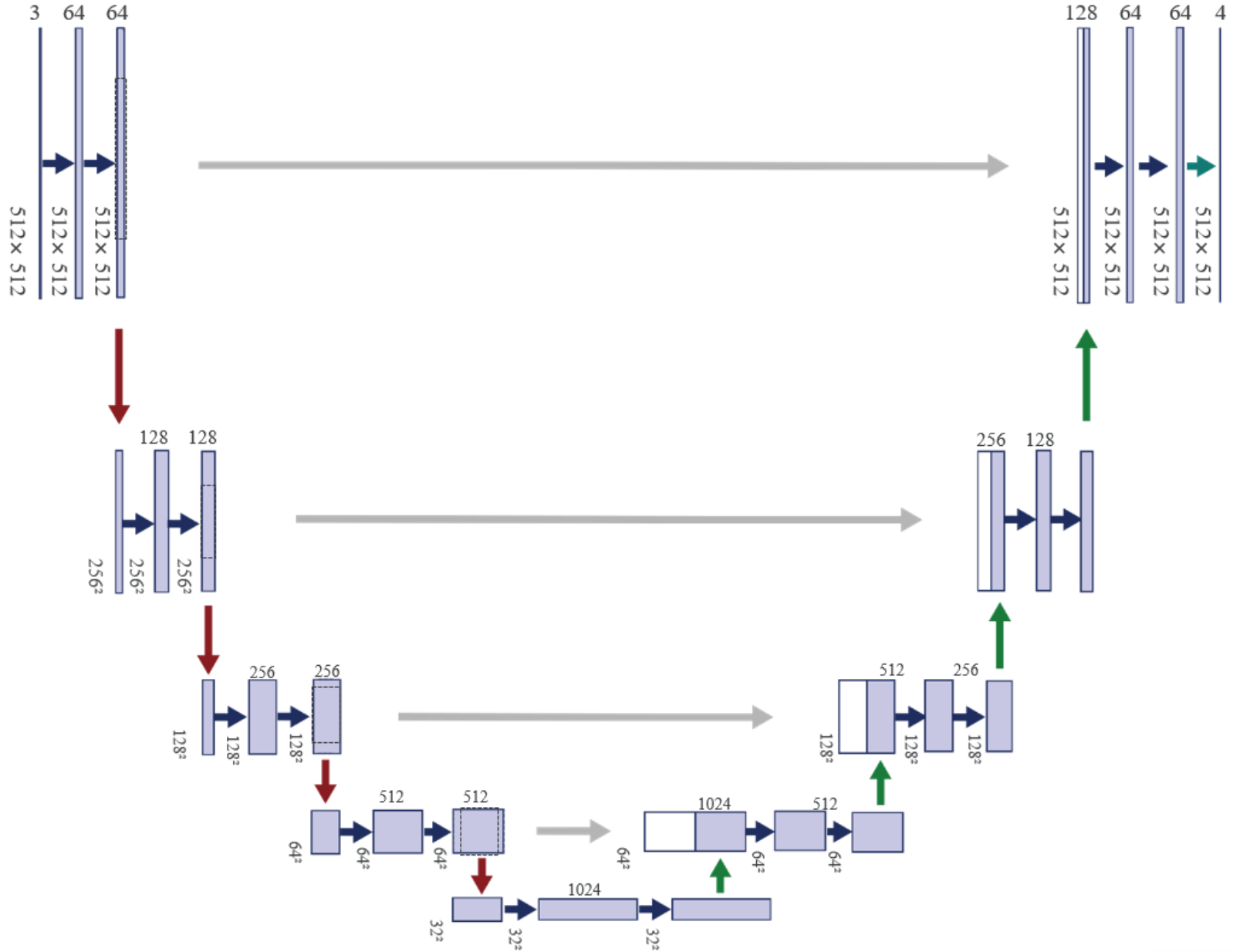


Deep Learning to Identify the Thickness of TMDs

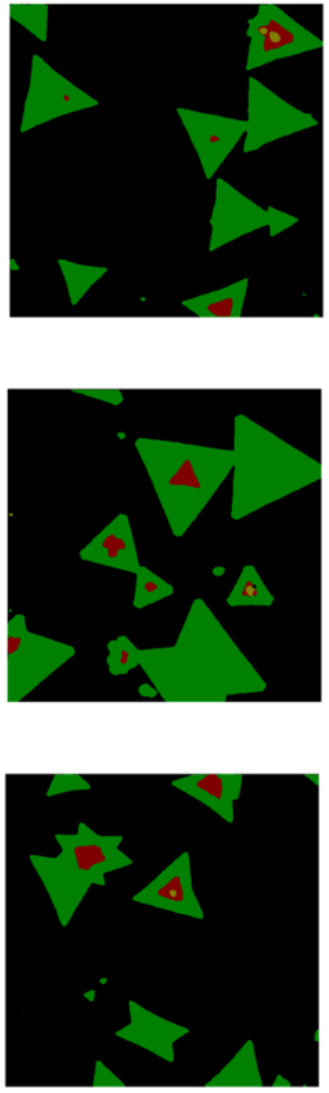


Deep Learning to Identify the Thickness of TMDs

Input Images

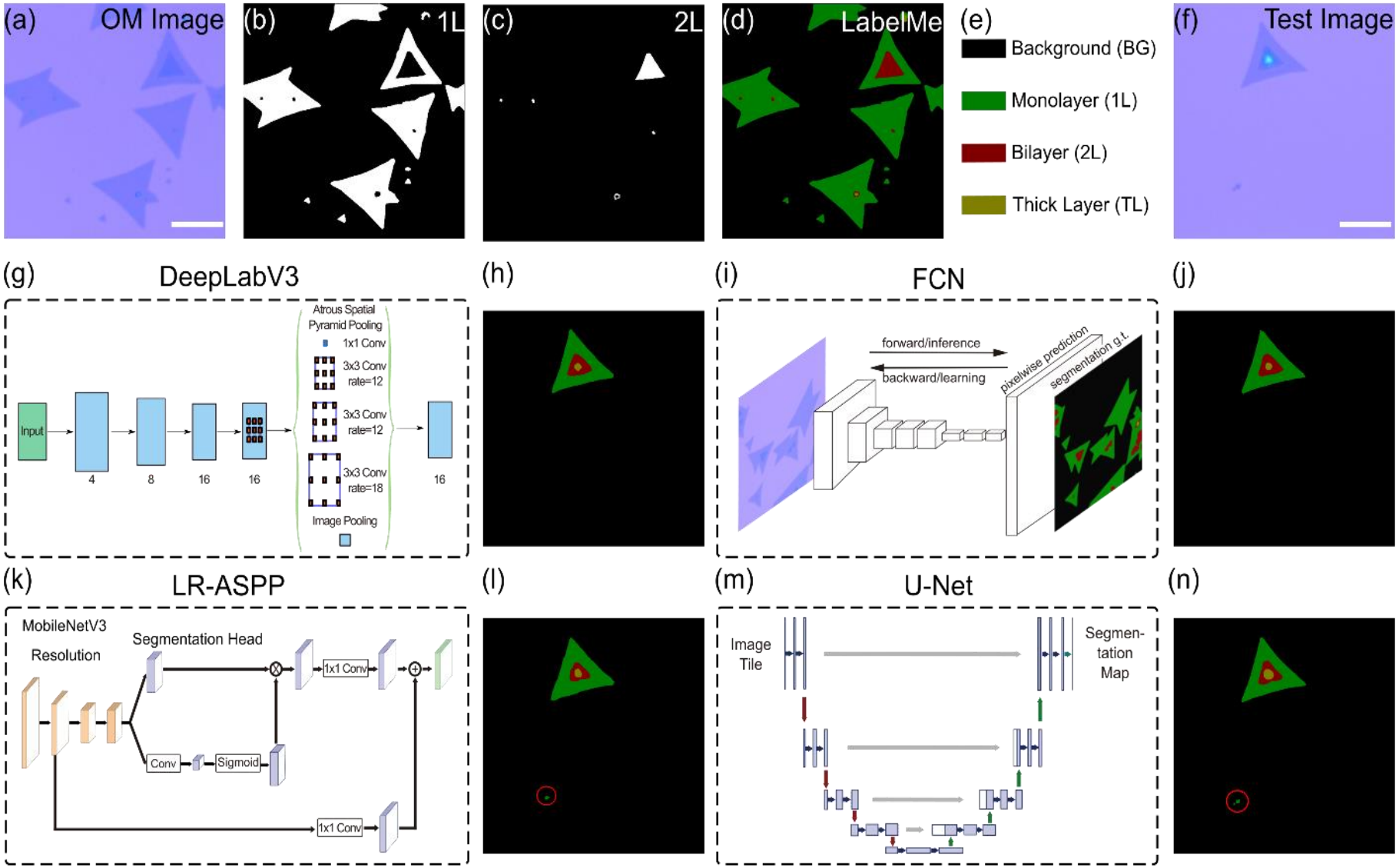


Output Images

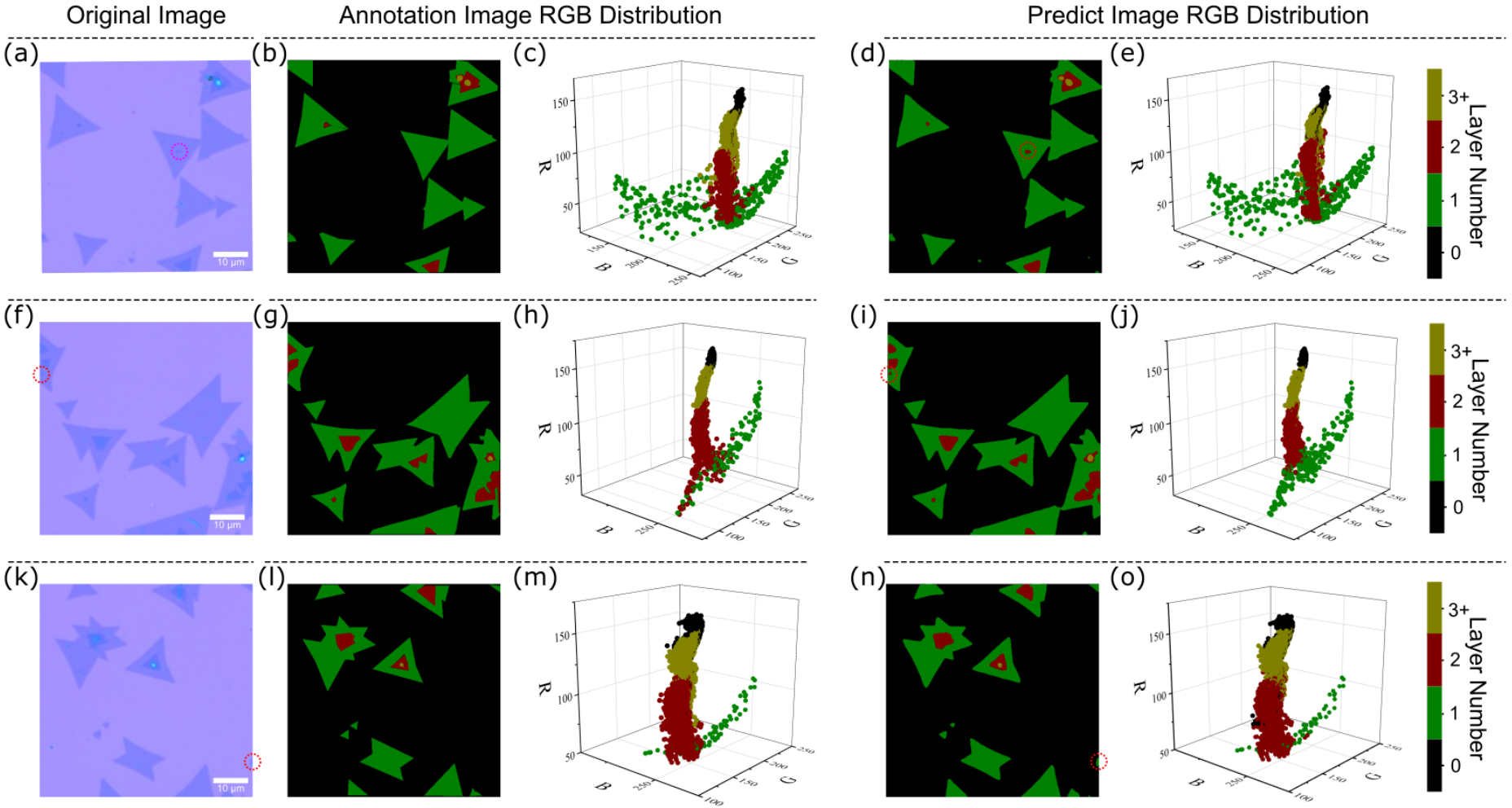


Ronneberger O et al., Medical Image Computing and Computer-Assisted Intervention–MICCAI 2015: 18th International Conference, 234-241, 2015.

Deep Learning to Identify the Thickness of TMDs



Deep Learning to Identify Thickness of TMDs



Performance of the segmentation models using U-net.

(a), (f), and (k) Input optical micrographs from the CVD MoS_2.

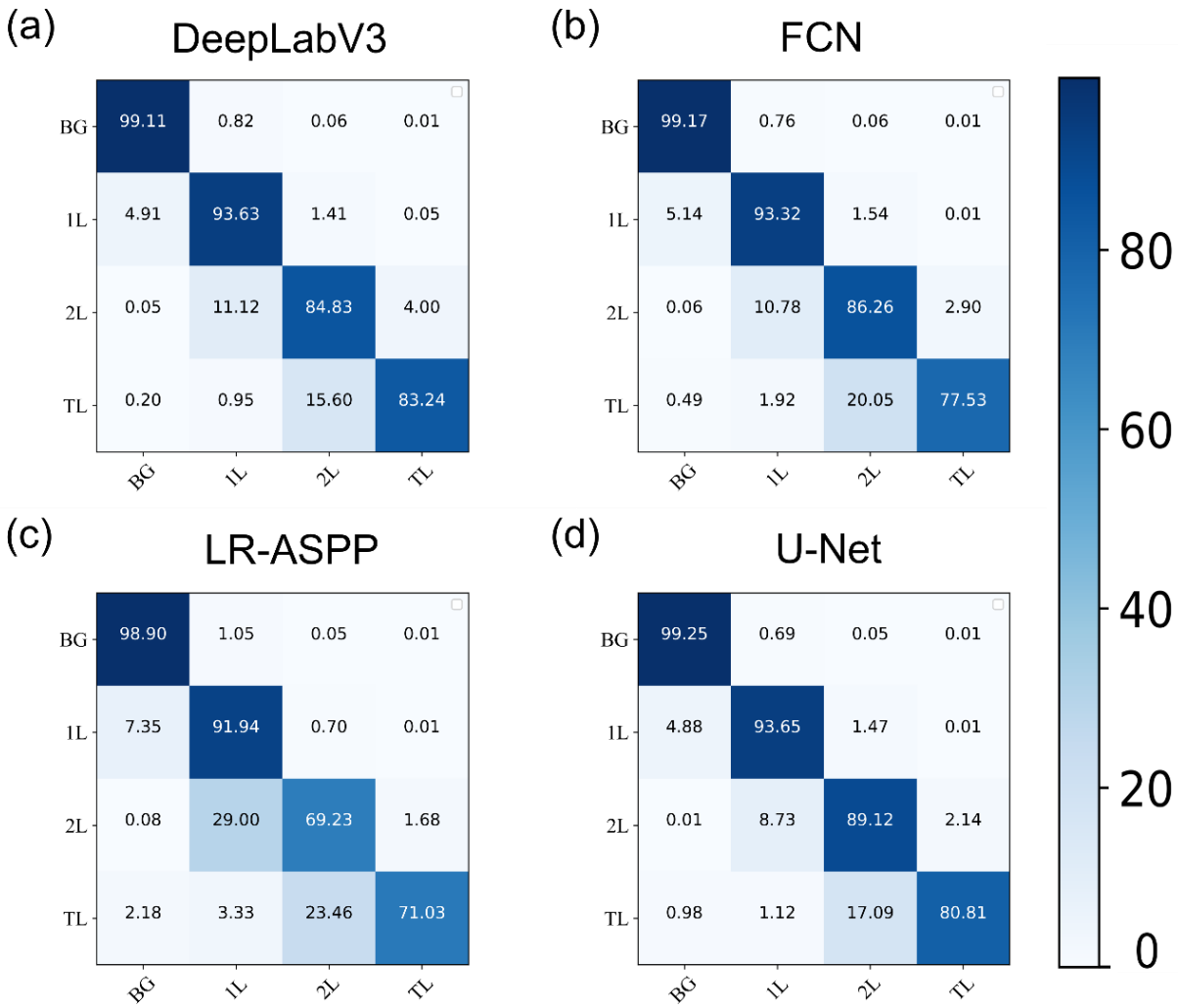
(b), (g), and (l) Manually annotated images.

(c), (h), and (m)The pixel value distribution of the annotated images.

(d), (i), and (n) Predicted images after segmentation .

(e), (j), and (o) Pixel value distribution of the segmented images.

Deep Learning to Identify Thickness of TMDs



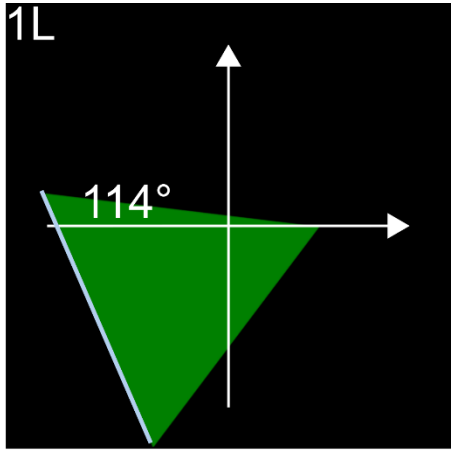
Confusion matrices of each class after the semantic segmentation network.

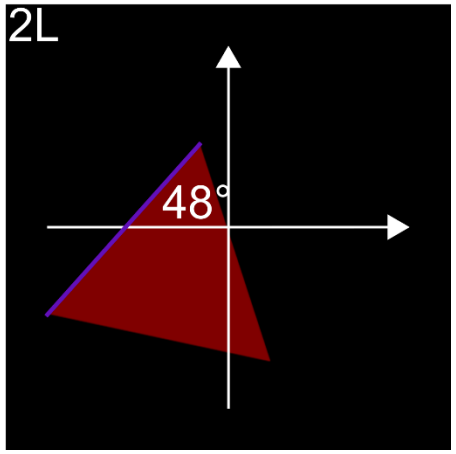
Deep Learning to identify Twist Angles

1.Find the leftmost side of each triangle.

2.Determine its rotation angle relative to the center of the image

3.Calculate the torsion angle based on the rotation angle of the leftmost side of the single and double layers.

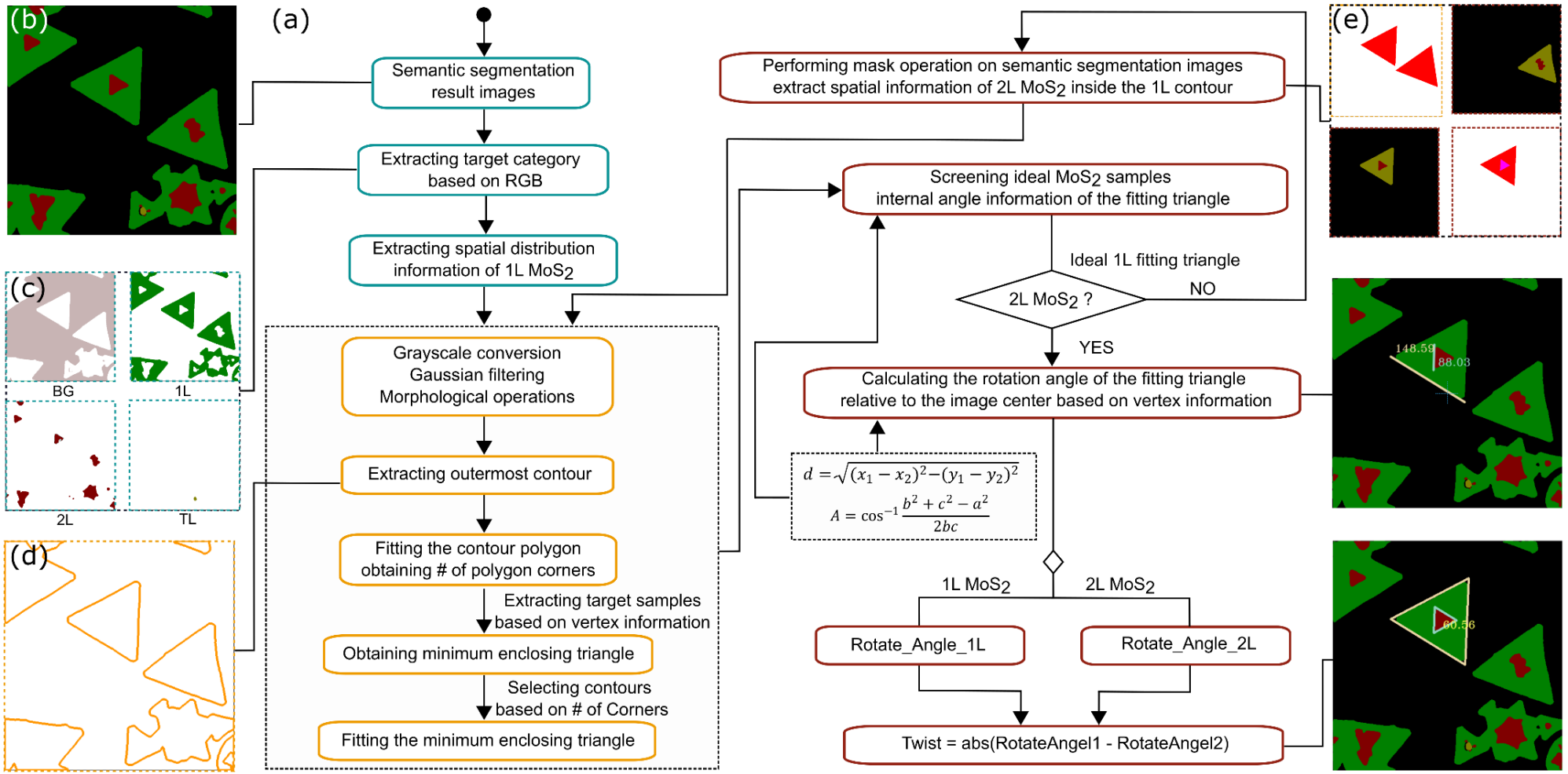




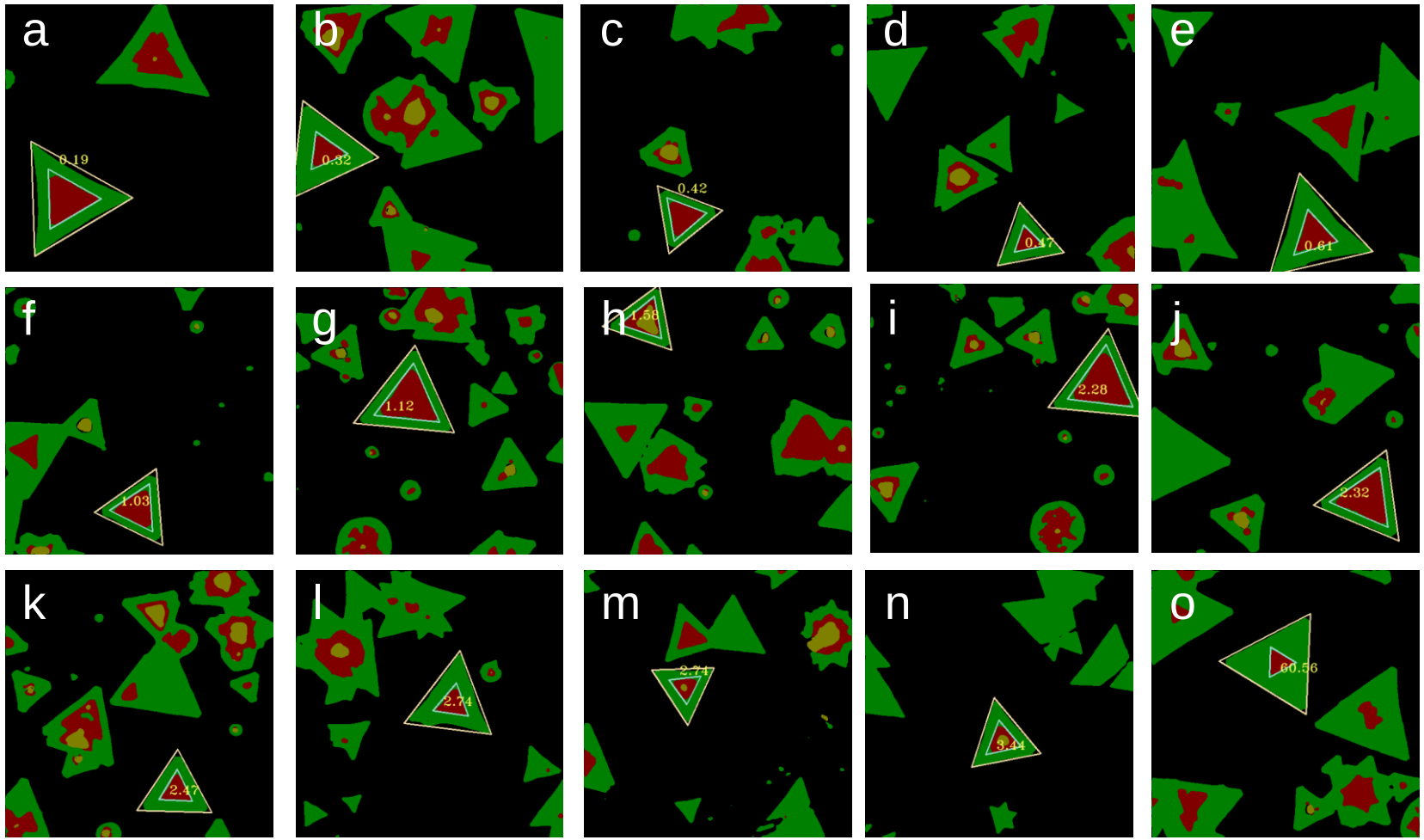
OpenCV to Identify Twisted Angles of TMDs

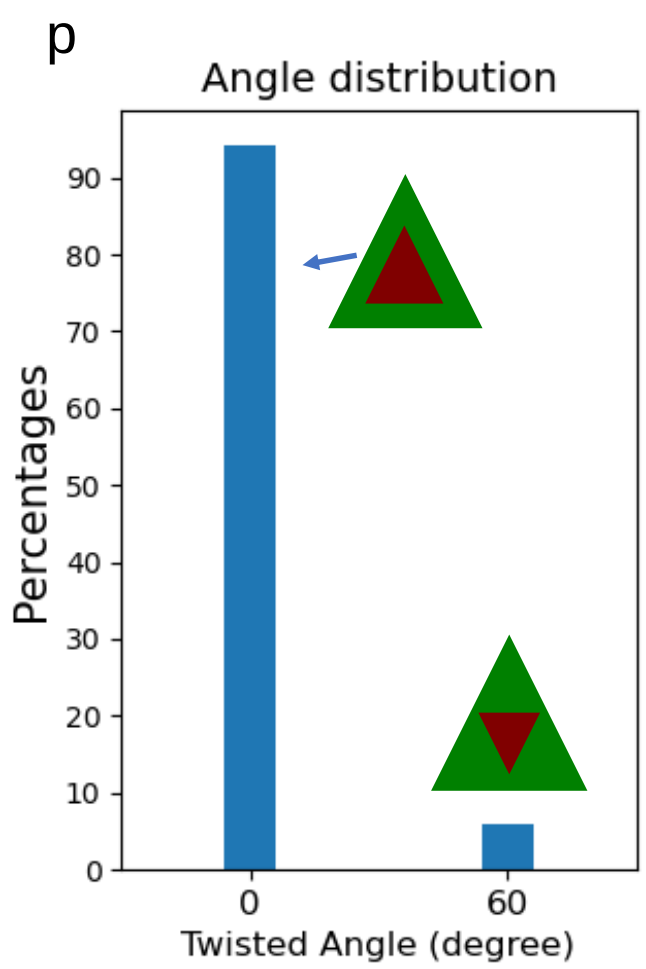
Simplified workflow diagram

Detailed workflow diagram



OpenCV to Predict the Twisted Angles of TMDs





Half intelligence（半智能）

能不能设计一个深度学习的神经网络

去识别双层材料的转角？

能不能设计一个深度学习的神经网络

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难点在于数据集的制作困难！

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MIT and Toyota release innovative dataset to accelerate autonomous driving research

DriveSeg contains precise, pixel-level representations of many common road objects, but through the lens of a continuous video driving scene.

MIT AgeLab
June 18, 2020

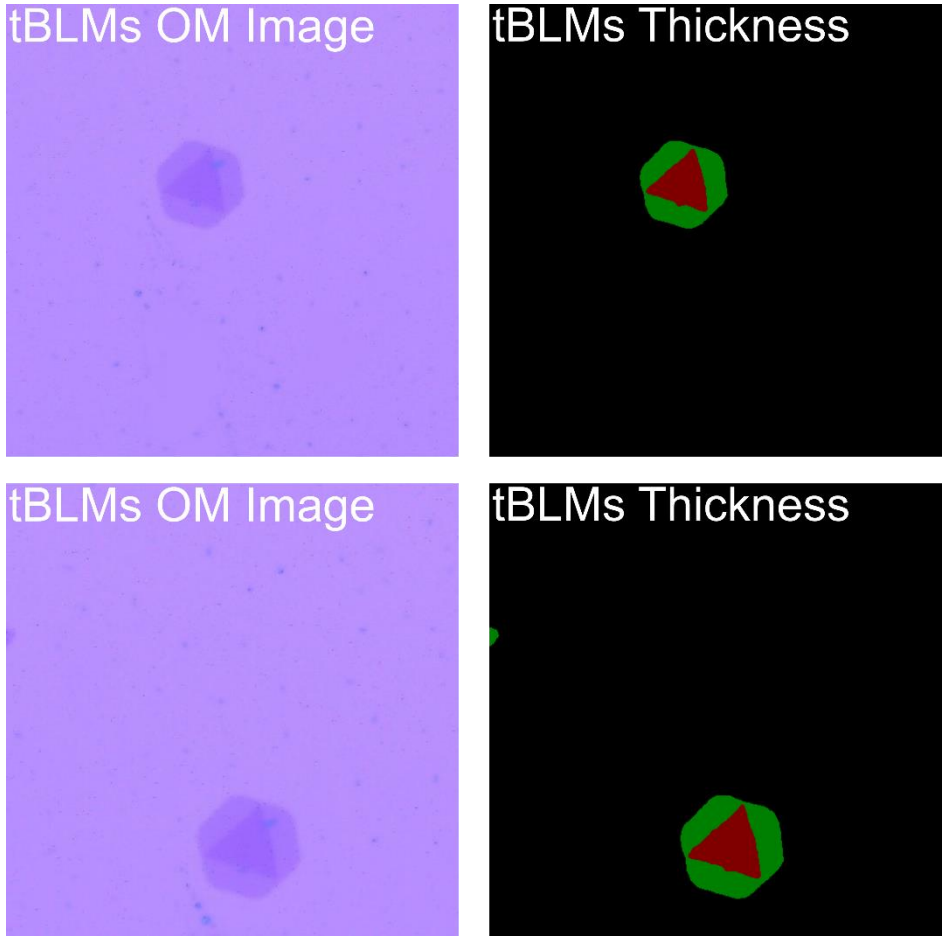
特斯拉CEO马斯克说至少要96亿公里以上，兰德智库认为需要至少跑177亿公里，**相当于在地球和太阳间往返50多趟**。这么大的数据量，要是全靠道路测试是不是会把工程师逼疯？

采用**人工产生的数据集**，来模拟无人驾驶的环境，训练模型

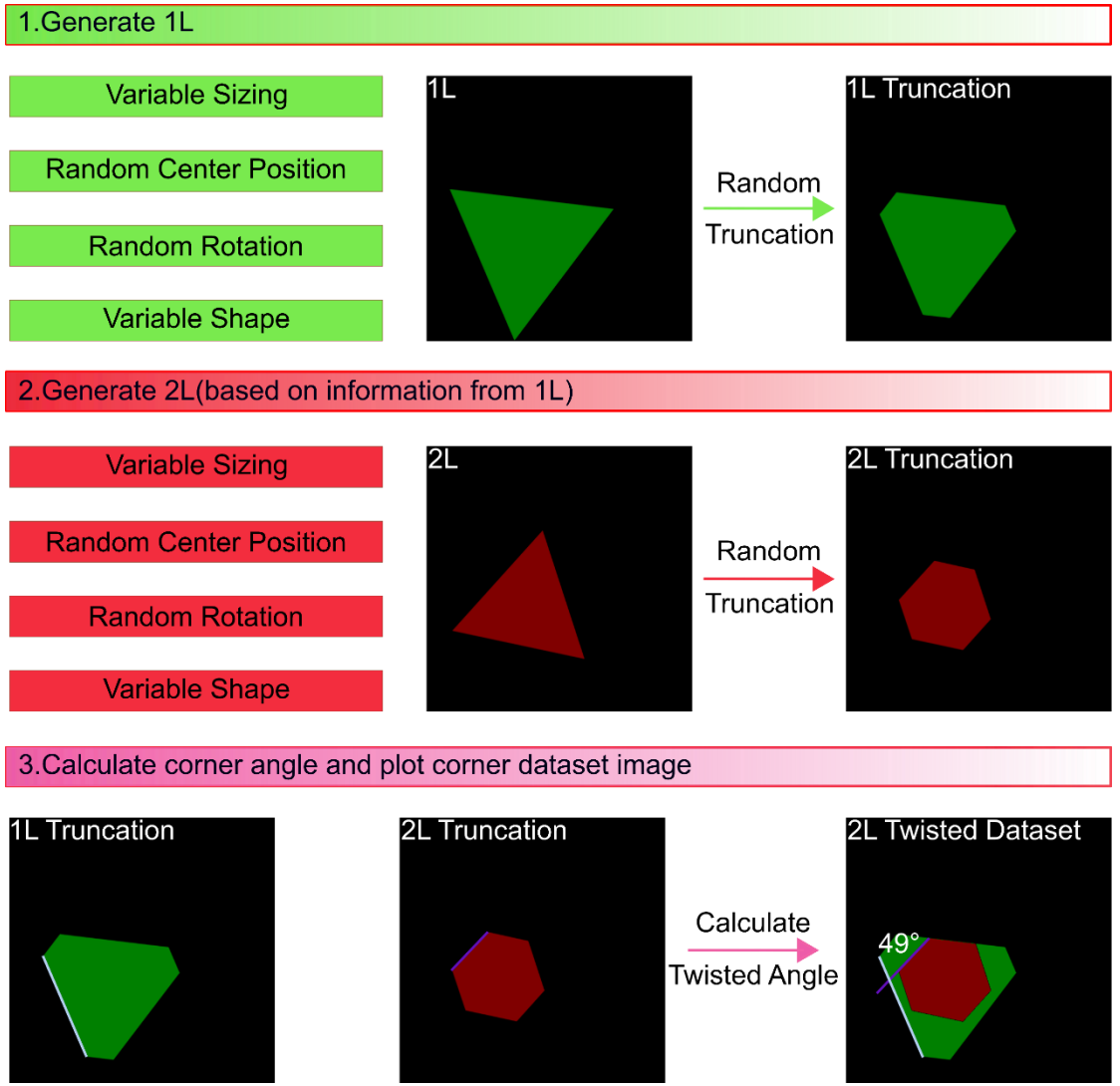
https://news.mit.edu/2020/mit-toyota-release-visual-open-data-accelerate-autonomous-driving-research-0618

Training Dataset Preparation

True Datasets

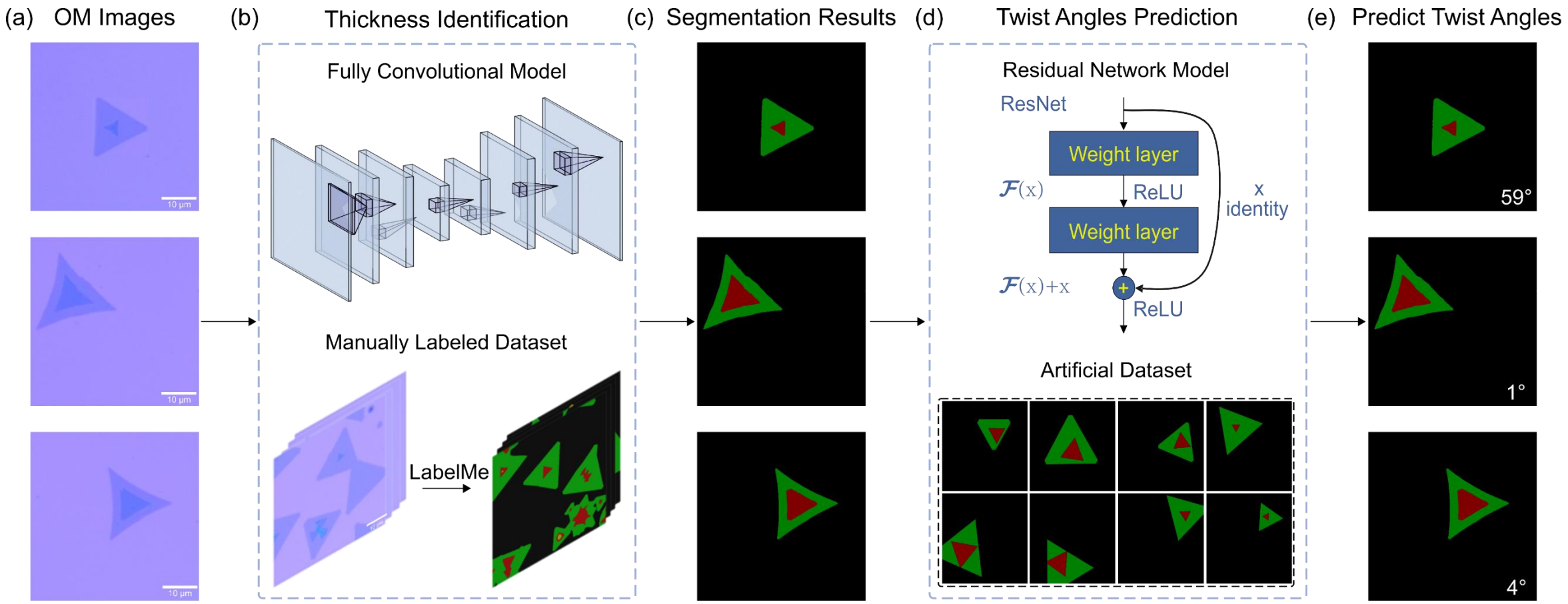


Artificial Datasets



Ping-Heng Tan*, Eduardo R Hernández*, Yong Xie* , **Nano Letters**, 2024, 24, 9, 2789–2797

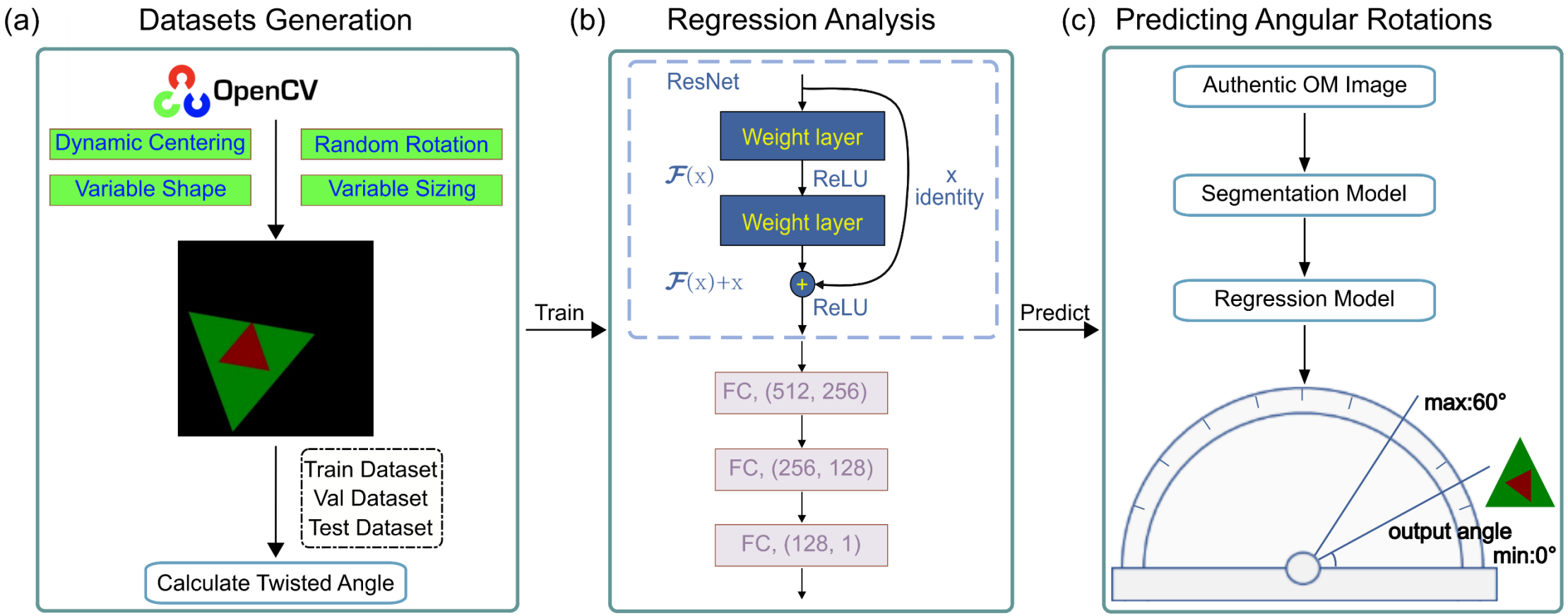
Deep Learning to Predict Twist Angles



第一次实现了转角双层的深度学习识别，完全Full intelligence（全智能）

Ping-Heng Tan*, Eduardo R Hernández*, Yong Xie* ， Nano Letters，2024, 24, 9, 2789–2797

Deep Learning Predict Twist Angles



Deep learning approach for recognizing twist angles in MoS_2 flakes.

(a) Synthetic dataset illustrating varying twist angles in uniformly colored MoS_2 flakes post-segmentation.

(b) ResNet CNN model training using the linear regression approach on the dataset from (a).

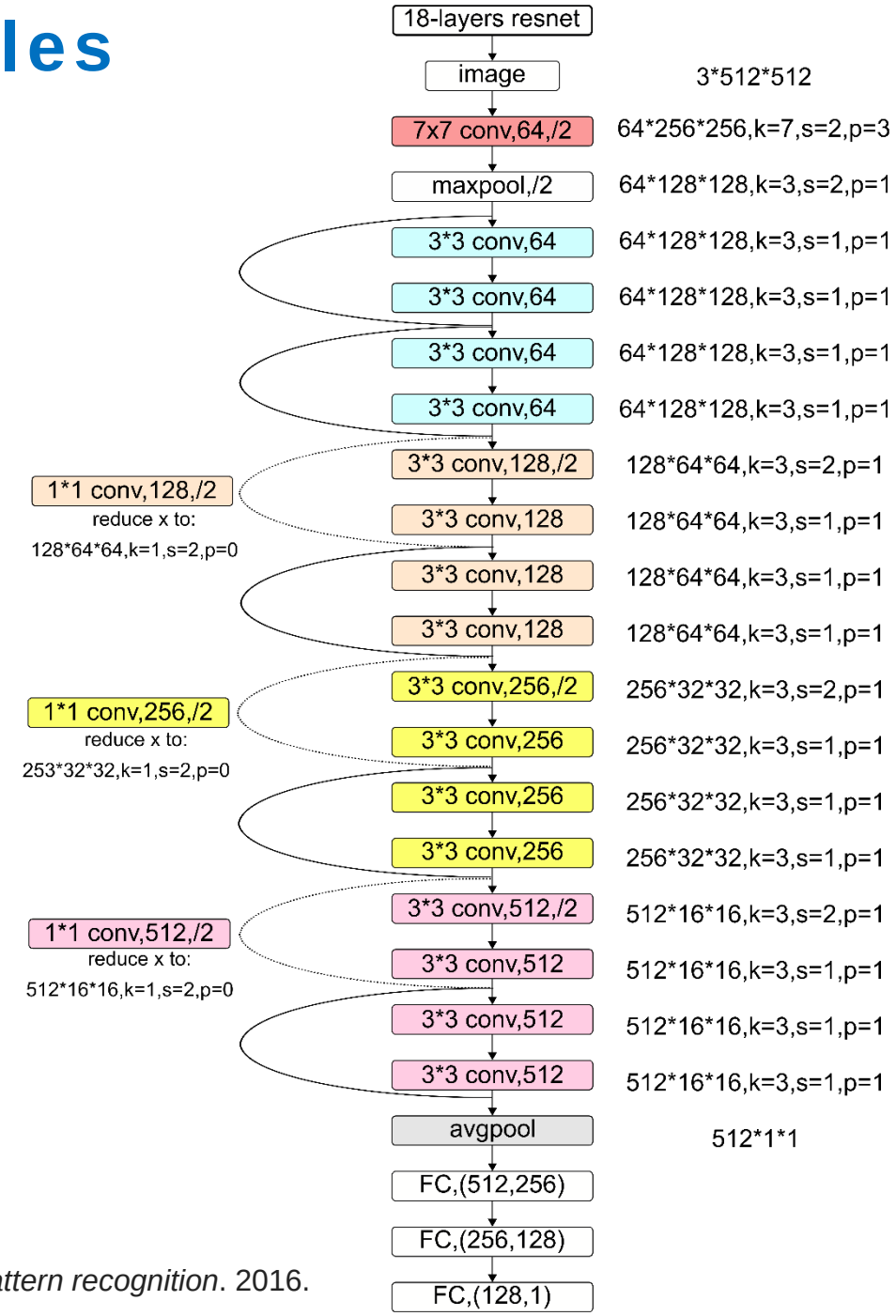
(c) Prediction of twist angles for actual as-grown MoS_2 bilayer samples post-segmentation

Deep Learning Predict Twist Angles

$$w \sim N(0, \sqrt{\frac{2}{n}})$$

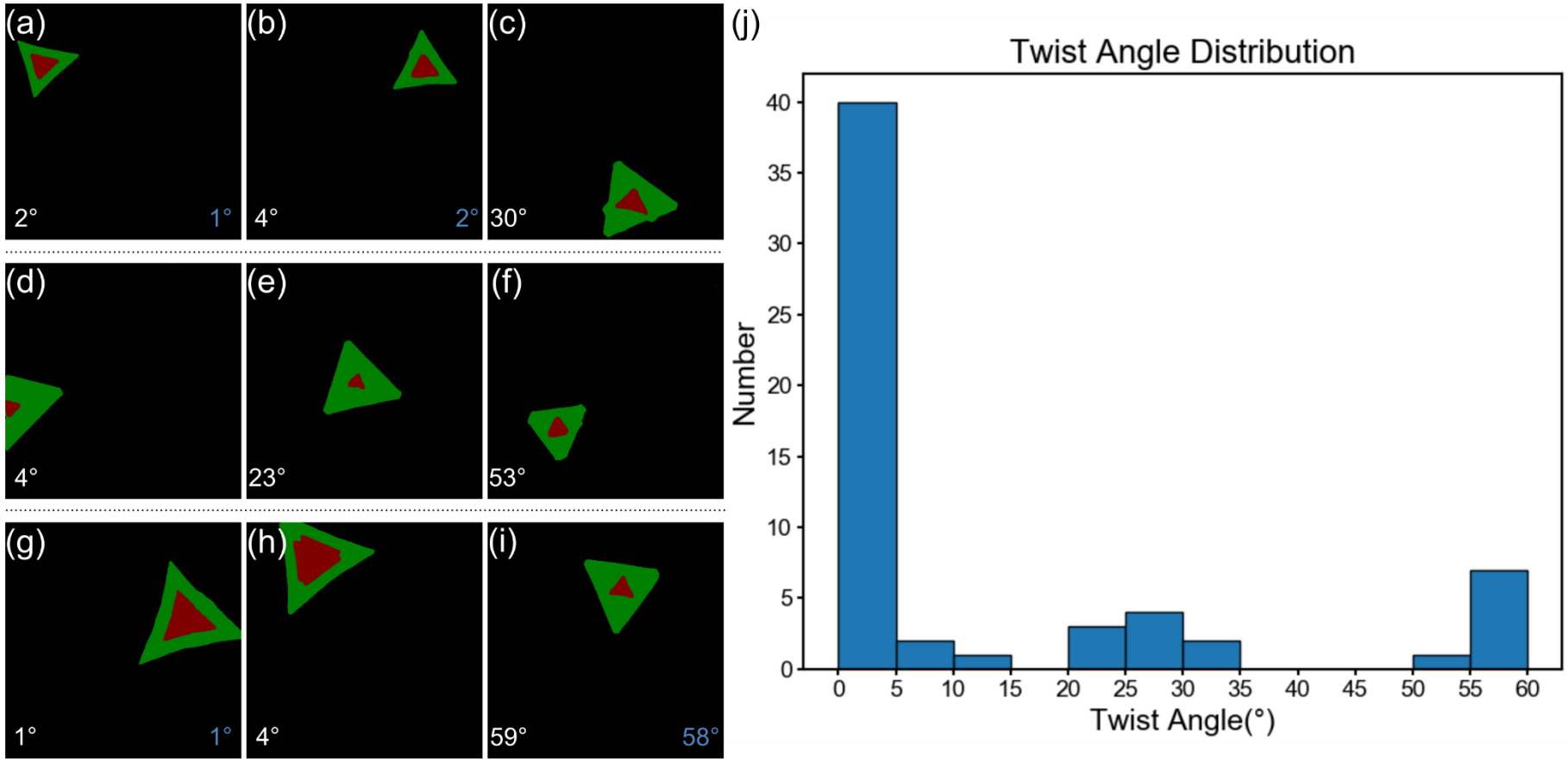
w The weight to be initialized

n The number of input units in the previous layer



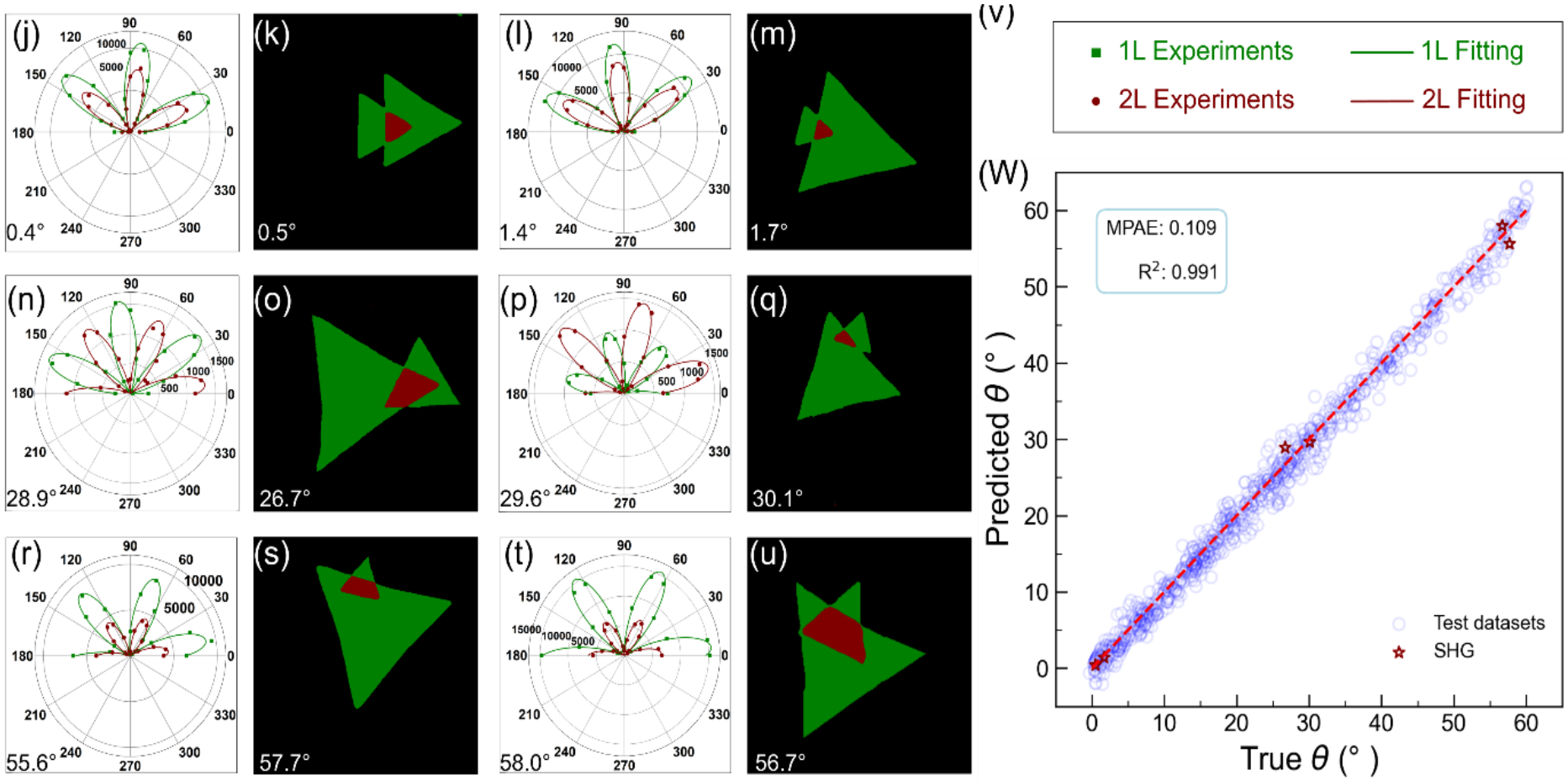
He, Kaiming, et al. *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

Deep Learning Predict Twist Angles



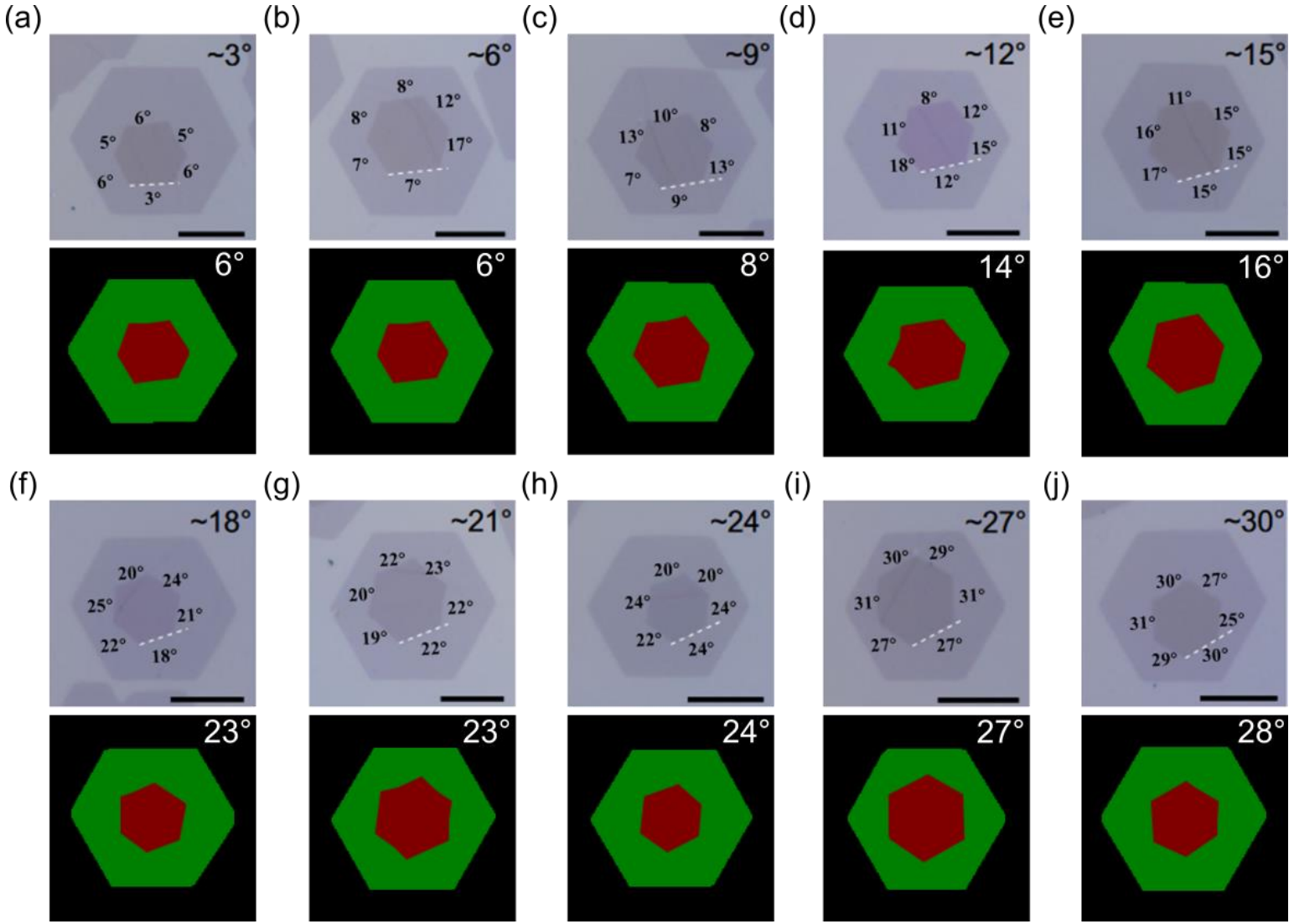
Performance evaluation of the twist angle Identification Model.

Deep Learning to Predict Twist Angles



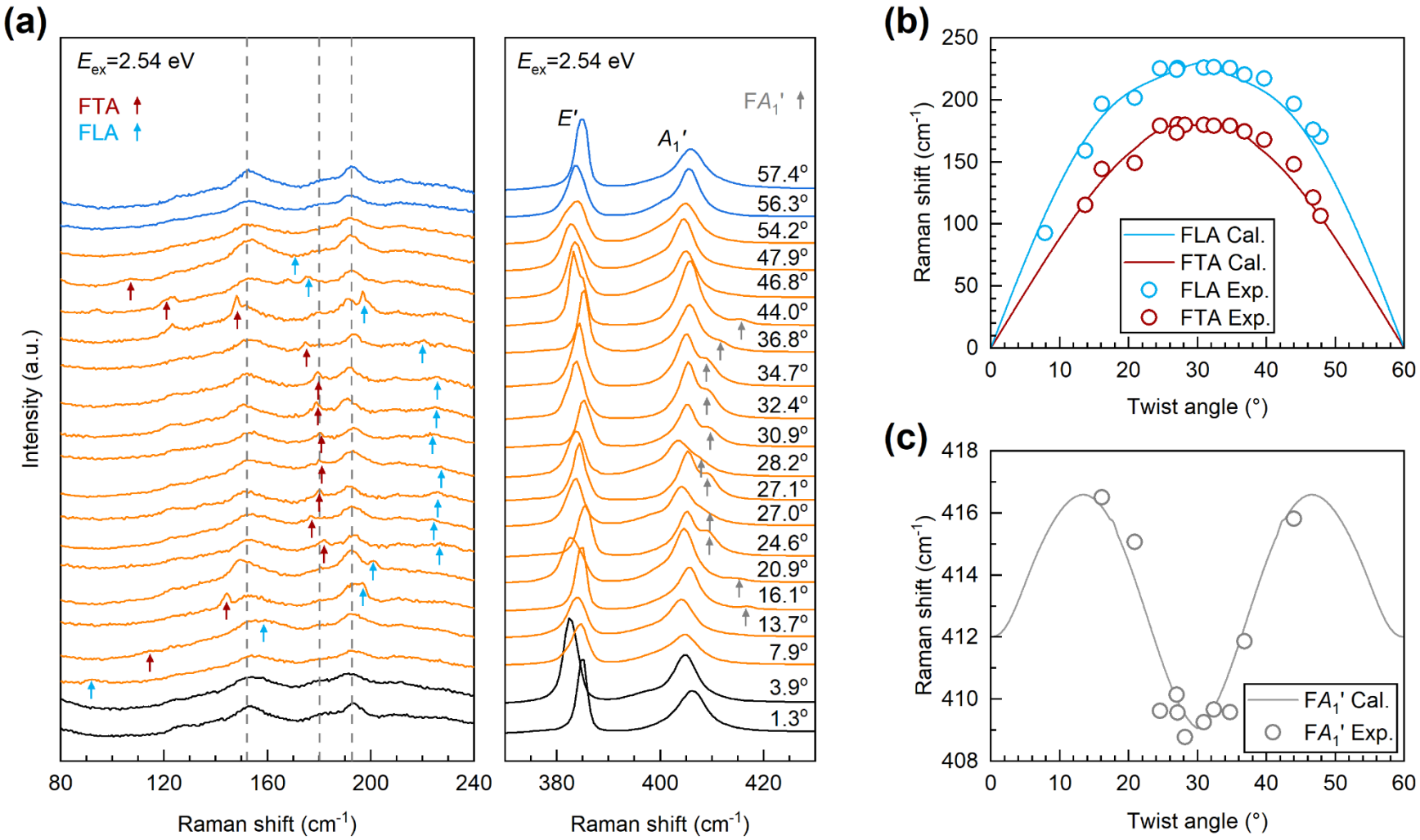
Ping-Heng Tan*, Eduardo R Hernández*, Yong Xie* , **Nano Letters**, 2024, 24, 9, 2789–2797

Deep Learning to Predict Twist Angles



Nat. Commun. 12, 2391 (2021)

Moiré phonons in twisted CVD grown bilayer MoS_2



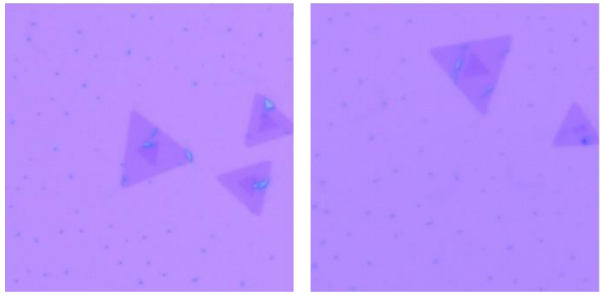
Ping-Heng Tan*, Eduardo R Hernández*, Yong Xie* , **Nano Letters**, 2024, 24, 9, 2789–2797

Deep Learning to Predict Twist Angles

		Thickness Classification Model				Twist Angle Regression Model
Model Name		DeepLabV3	FCN	LR-ASPP	U-Net	ResNet
Training Epoch		300	300	300	300	600
NN Training Time		29m24s	25m18s	17m18s	34m18s	14h25m33s
Frames Per Second (FPS)	CPU	1.16	1.32	9.80	3.56	14.3
	GPU	45.66	50.35	201.25	125.63	479.6

Conclusion

1.拍摄光学显微镜图片



3.厚度识别模型

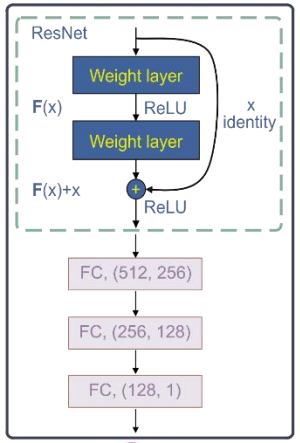
DeepLabV3

FCN

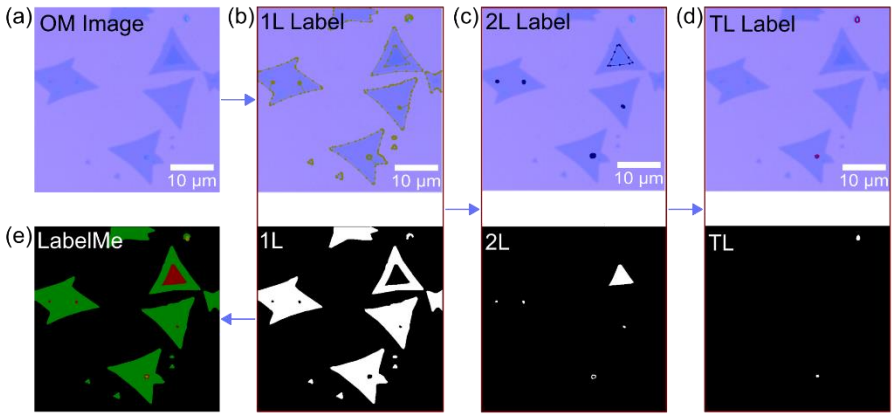
LR-ASPP

U-net

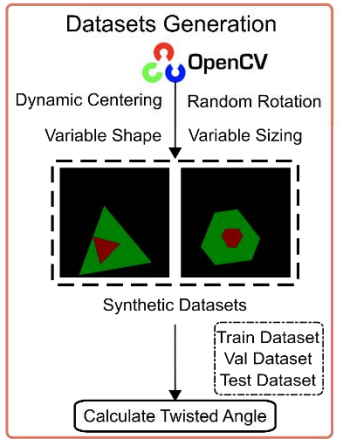
5.转角识别模型

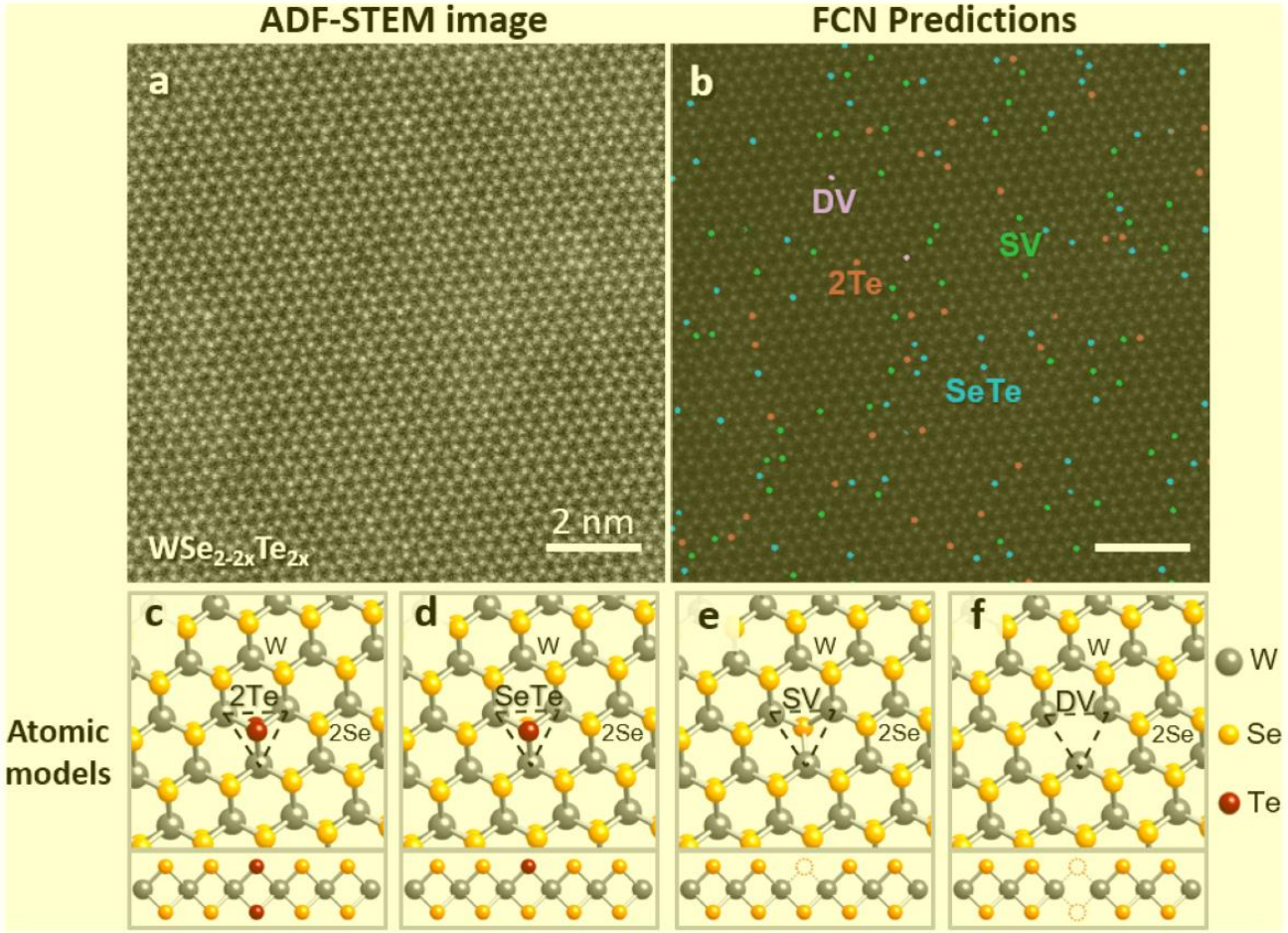


2.制作厚度识别数据集



4.人工转角数据集





NANO LETTERS

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Deep Learning Enabled Strain Mapping of Single-Atom Defects in Two-Dimensional Transition Metal Dichalcogenides with Sub-Picometer Precision

Chia-Hao Lee, Abid Khan,[#] Di Luo,[#] Tatiane P. Santos, Chuqiao Shi, Blanka E. Janicek, Sangmin Kang, Wenjuan Zhu, Nahil A. Sobh, André Schleife, Bryan K. Clark, and Pinshane Y. Huang*

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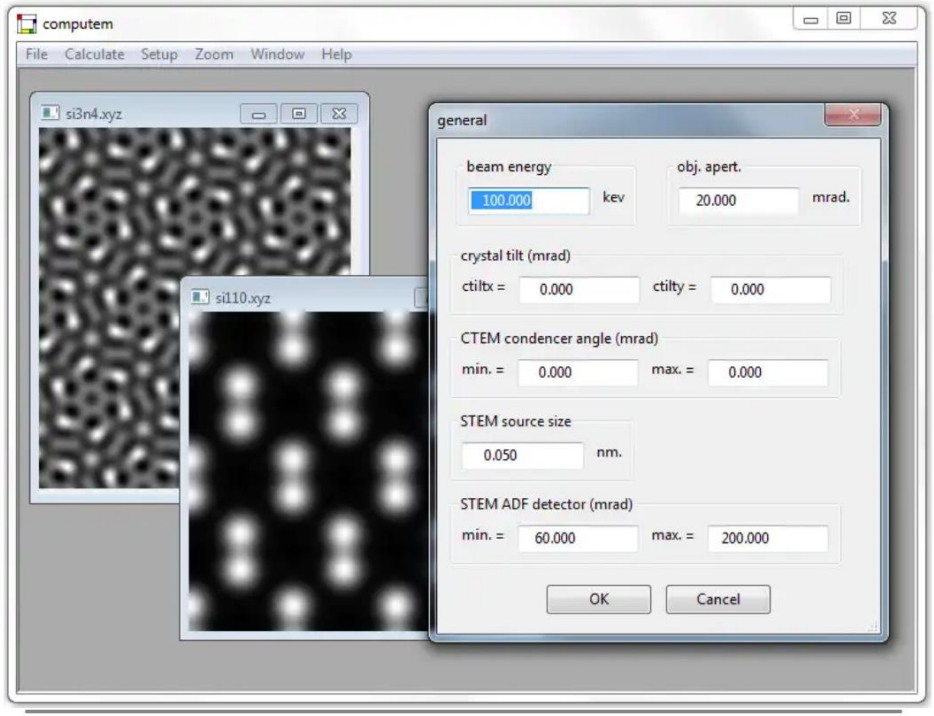
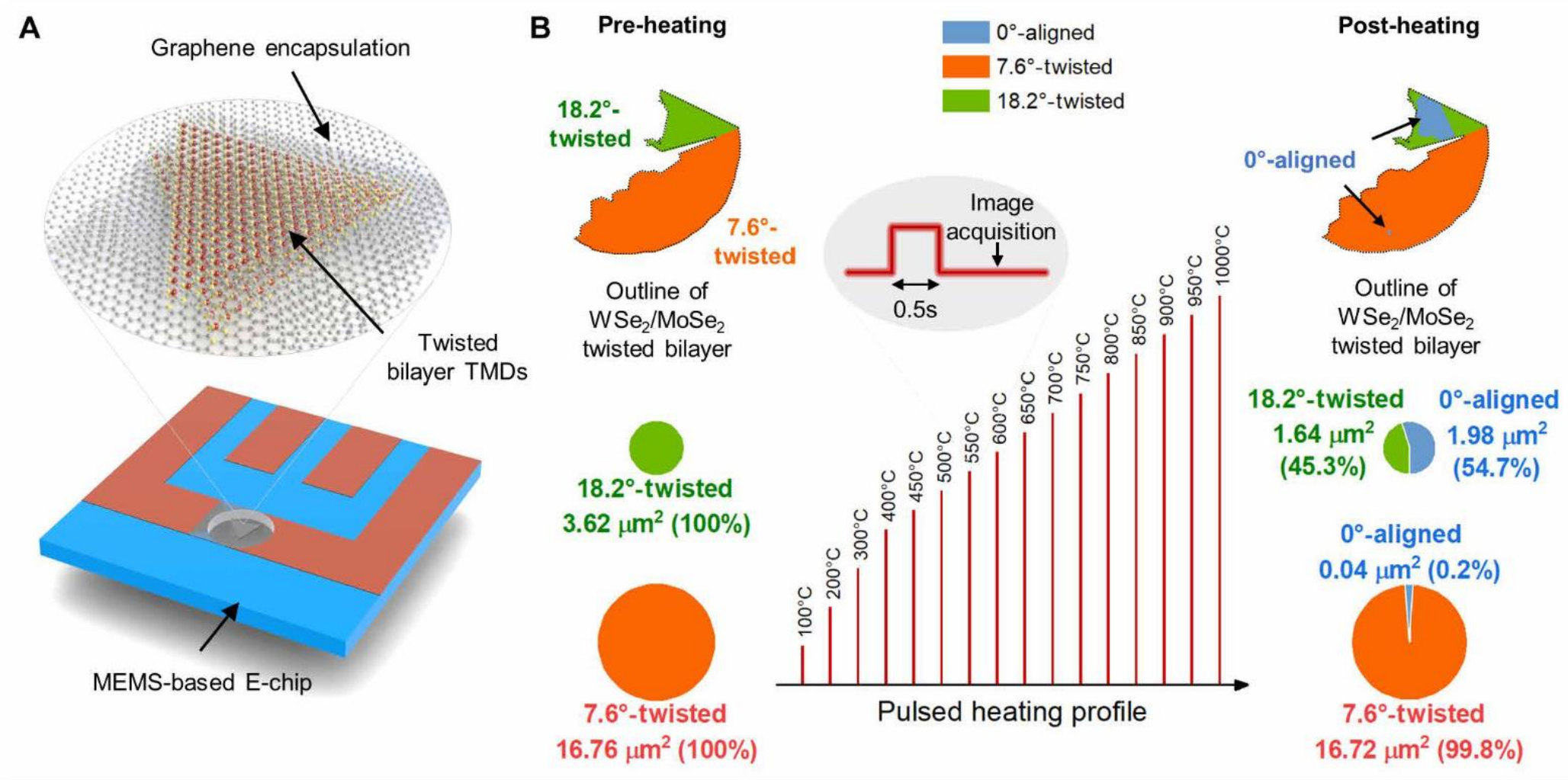
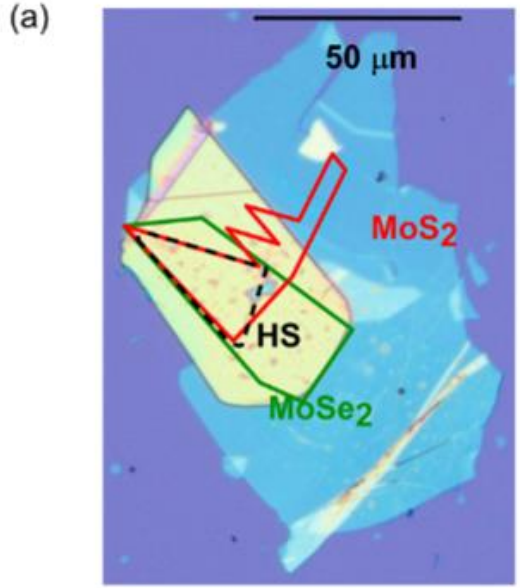
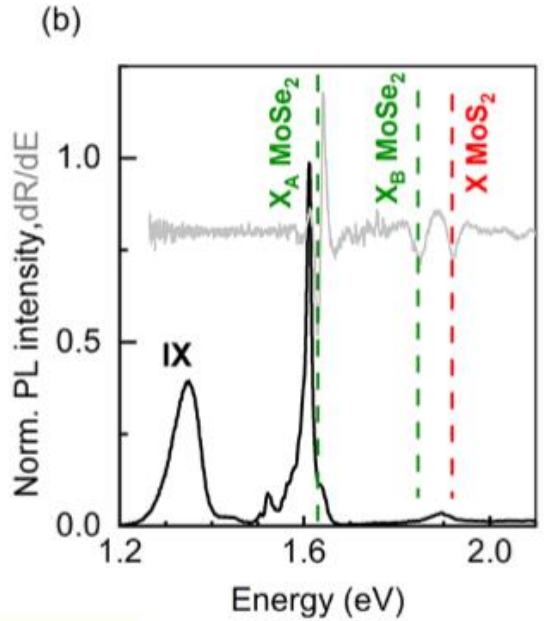


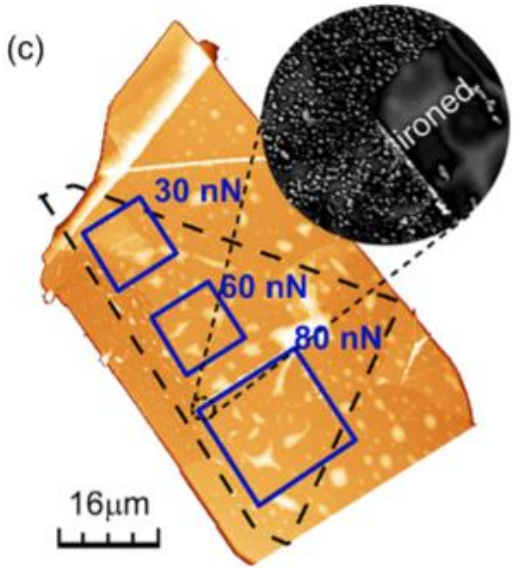
Computem

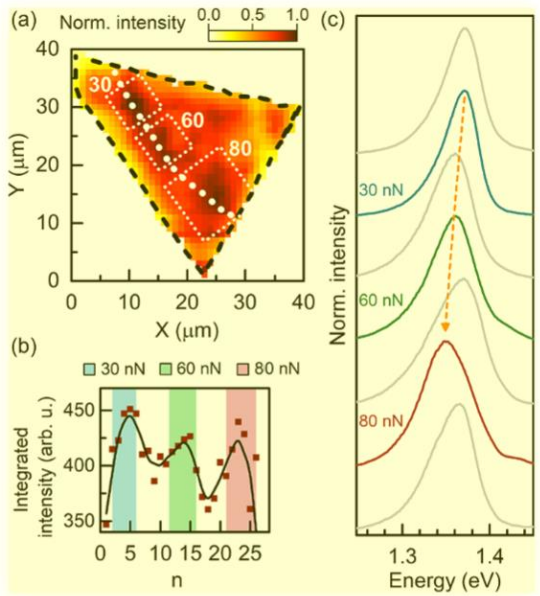


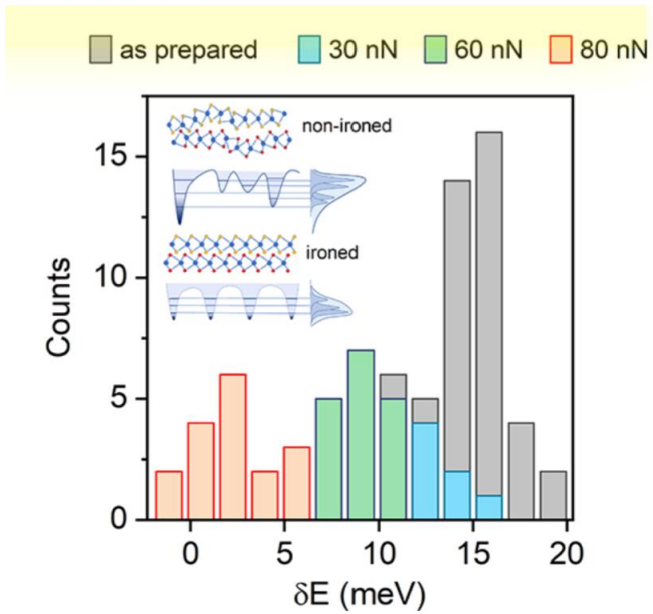
Atom- by- atom imaging of moiré transformations in 2D transition metal dichalcogenides, Science Advance, Huang











NANO LETTERS

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Approaching the Intrinsic Properties of Moiré Structures Using Atomic Force Microscopy Ironing

Swaroop Kumar Palai, Mateusz Dyksik, Nikodem Sokolowski, Mariusz Ciorga, Estrella Sánchez Viso, Yong Xie, Alina Schubert, Takashi Taniguchi, Kenji Watanabe, Duncan K. Maude, Alessandro Surrente, Michal Baranowski, Andres Castellanos-Gomez, Carmen Munuera,* and Paulina Plochocka*

Cite This: *Nano Lett.* 2023, 23, 4749–4755 Read Online

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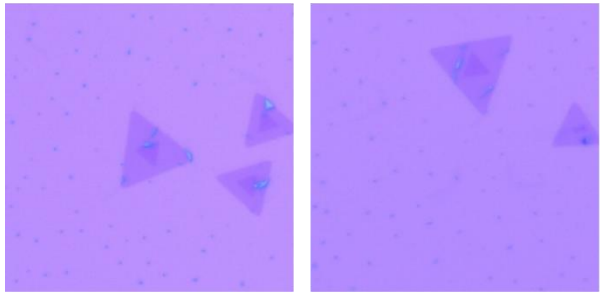
- 西电：马晓华、李培咸、周楠
- 半导体所谭平恒教授、武恒博士、周岩博士、张昕研究员
- 马德里材料科学研究所：E. R. Hernandez教授

Thanks for your attention!

Conclusion

1.拍摄光学显微镜图片



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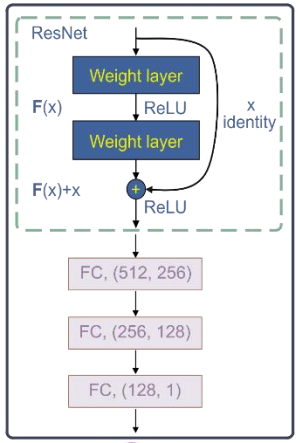

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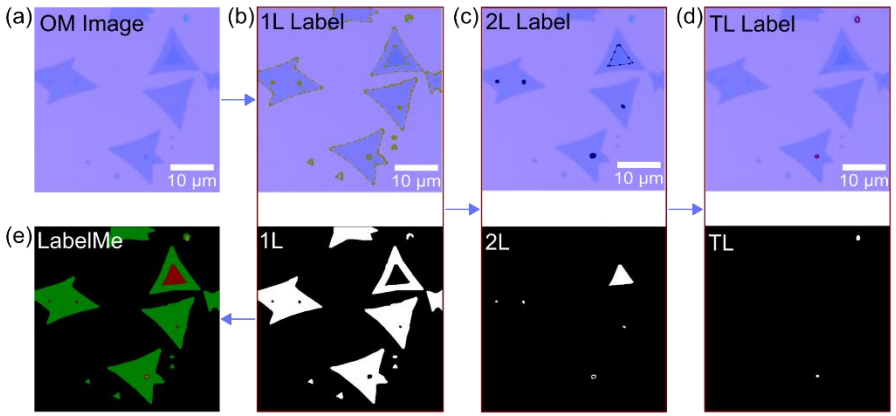

4.人工转角数据集