Evaluating Crystal Facets for Photoelectrochemical Water Splitting

Semantic segmentation of Cu_2O nanocrystals

Rouven Spiess
rouvens@stanford.edu

CS230
Winter 2020

Motivation

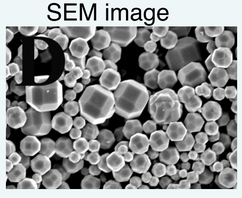
Photelectrochemical Water Splitting could be a promising way for **producing Hydrogen from Solar Energy** Cuprous oxyde Cu_2O Microcrystals are interesting candidates, as of their aboundance on earth and non-toxicity. The electrocatalitic activity depends largely on the facet type, thus, **a method for determining the exposed facets is paramount to increase devices performance**

Cu_2O nanocrystal facets

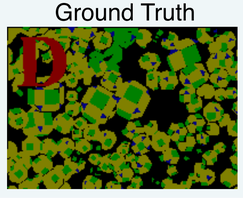
Dataset

26 Scanning Electronic Microscopy (SEM) images representing cubic, octahedral and 26-facet polyhedra crystals. The **total amount of data is 1MB** The images are labelled manually to deliver the ground truth images.

SEM image



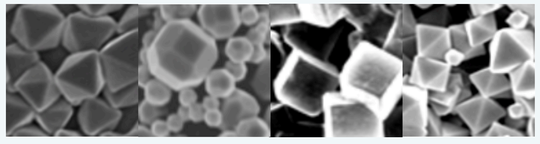
Ground Truth



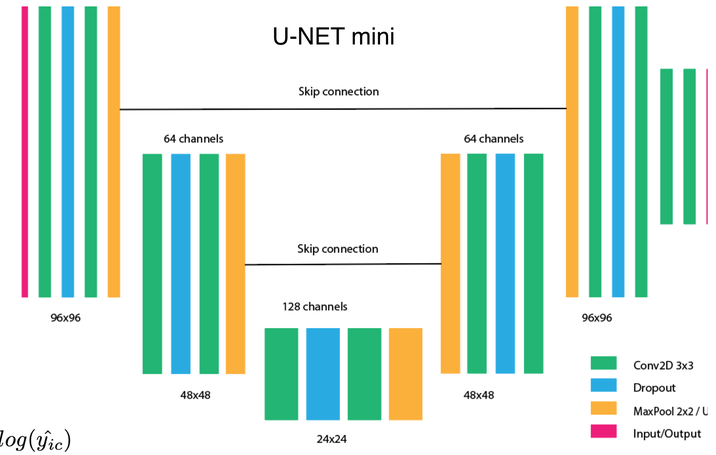
Data Augmentation

As the dataset is small, a proper data augmentation strategy is key We can take advantage that SEM images are rotation invariant by applying random rotations and augmenting the data massively. Other transformations include shear, grid distortion and zoom.

Augmented images



Network and Training

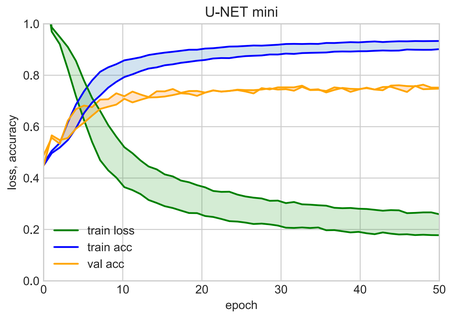


Loss function

$$\mathcal{L}(y, \hat{y}) = \sum_{i=1}^{P} \sum_{j=1}^{C} y \cdot log(\hat{y_{ic}})$$

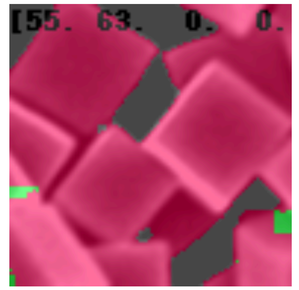
Architecture	# Parameters
U-NET mini	473,203
U-NET Vanilla CNN encoder	4,504,192
U-NET VGG-16 trained on ImageNet	12,351,219

Architecture	train acc	dev acc	dev IoU
U-NET mini	0.93	0.76	**0.60**
U-NET Vanilla CNN	0.92	0.71	0.51
U-NET VGG-16	0.96	0.76	0.58



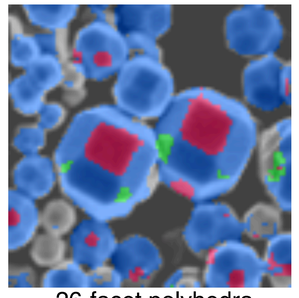
U-NET architecture is suitable for semantic segmentation and small datasets
The following U-NET variants are tested:
•UNET Mini
•Vanilla CNN U-NET
•VGG-16 U-NET pret-rained on ImageNet
Overall, the models present a **high variance problem,** which can only moderately be mitigated by regularization techniques.

Results



Cubes

Octahedra



26-facet polyhedra

Performance

Class	IoU	PA
(100)	0.48	0.54
(111)	0.44	0.52
(110)	0.54	0.81
background	0.62	0.79
mean	**0.52**	**0.66**

Discussion and Future Work

Semantic segmentation problems can be solved with low amount of data, **SEM images provide enough spatial information** to be augmented. U-NET architectures, with either **low number of parameters or pretrained weights** are powerful methods to train on limited datasets.
As project continuation, **Synthetic data generation**, where the crystal geometries are build from scratch, could be an **interesting alternative to manual labelling**, which is time consuming. This should be coupled with a **domain transfer technique**, e.g. by training a GAN to match the original distribution.

Sun Shaodong, Song Xiaoping, Sun Yuexia, Deng Dongchu, Yang Zhimao. (2012). The crystal-facet-dependent effect of polyhedral Cu2O nanocrystals on photocatalytic activity. Catal. Sci. Technol.. 2. 925-930. 10.1039

Shang, Y. Guo, L. (2015). Facet–Controlled Synthetic Strategy of Cu2O–Based Crystals for Catalysis and Sensing. Adv. Sci., 2: 1500140.

Zixi Liu, Wanling Liu, Jiyao Yuan, Bismuth Vanadate (111) Facet Detection, CS229 Final Report, December, 13, 2018.

Ferrer, Mateus & Fabris, Guilherme & Faria, Bruno & Martins, João & Moreira, Mário & Sambrano, J.. (2019). Quantitative evaluation of the surface stability and morphological changes of Cu2O particles. Heliyon. 5(10):e02500 · October 2019.

Ronneberger, O., Fischer, P., Brox, T., U-Net: Convolutional Networks for Biomedical Image Segmentation}. (2015).

Ulku I., Akagunduz E., A Survey on Deep Learning-based Architectures for Semantic Segmentation on 2D Images.(2020).