Quantitative processing of scanning probe microscopy image with deep learning techniques

Aleksey G. Okunev, Mikhail F. Liz, Anna V. Nartova, Andrey V. Matveev

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In heterogeneous catalysis, one of the main characteristics of the activity of the catalyst is the turnover frequency of the reaction (TOF), which is calculated by the formula:

$$TOF(s^{-1}) = \frac{W}{D} * 100,$$

where W - reaction rate, D - dispersion (0-1)

Introduction

Goals

- Developing a custom method for our dataset
- Analysis of results

Problem statement

Formulation

Problem formulation

- Training data: 8 images
- Test data: 3 images
- Metrics: mean Average Precision (mAP) for segmentation

Problem statement

Data examples

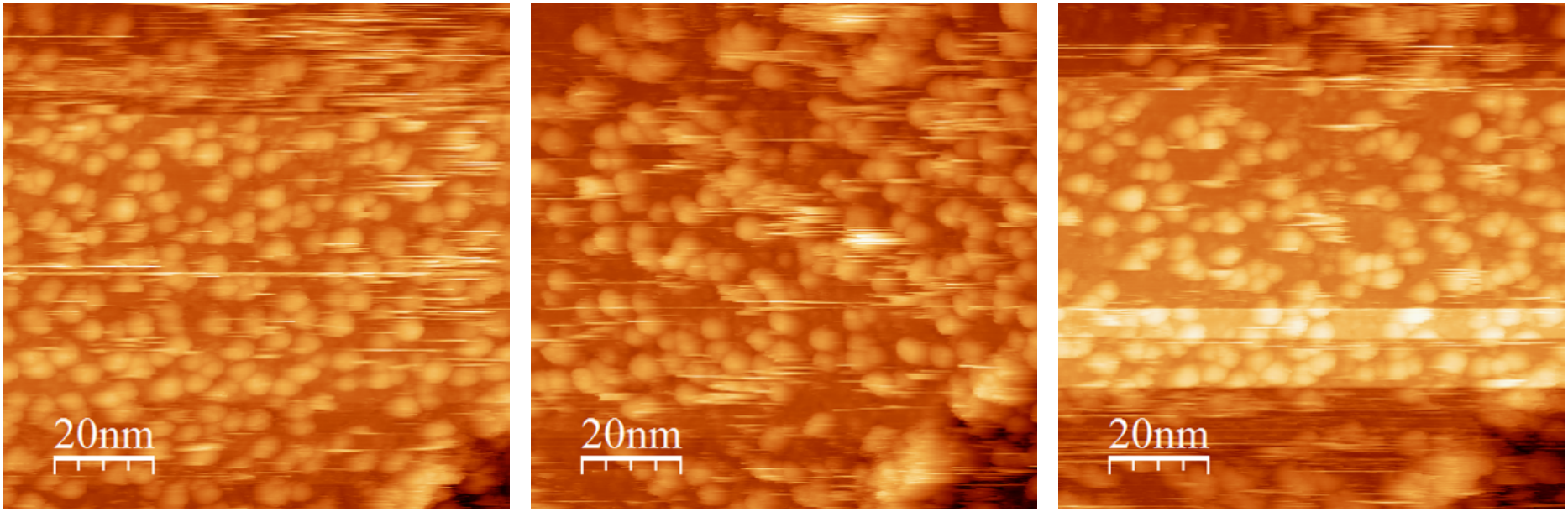
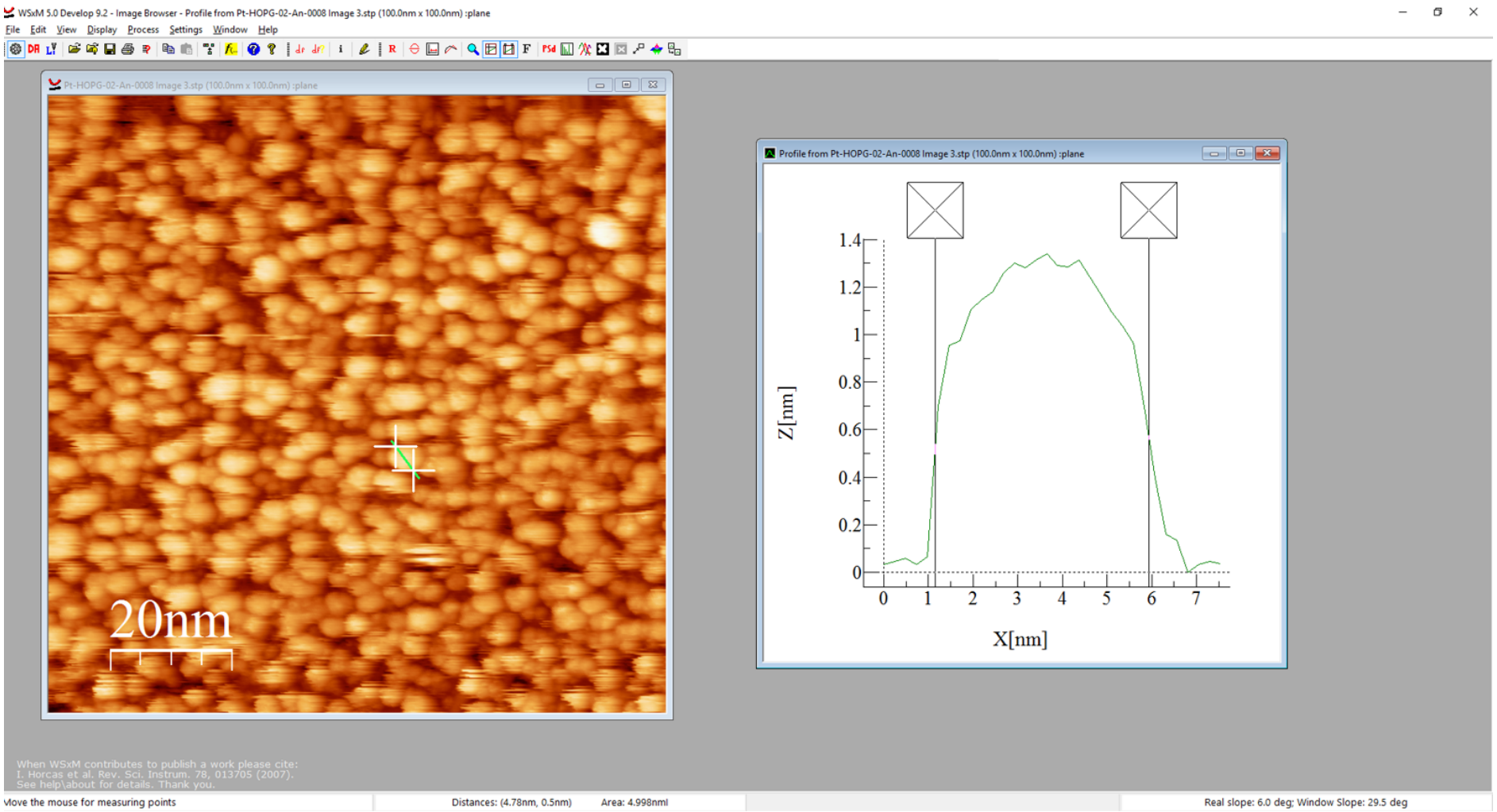


Figure: Nanoparticles deposited on highly oriented pyrolytic graphite (HOPG)

Problem statement

Program WSxM



U-Net

Training

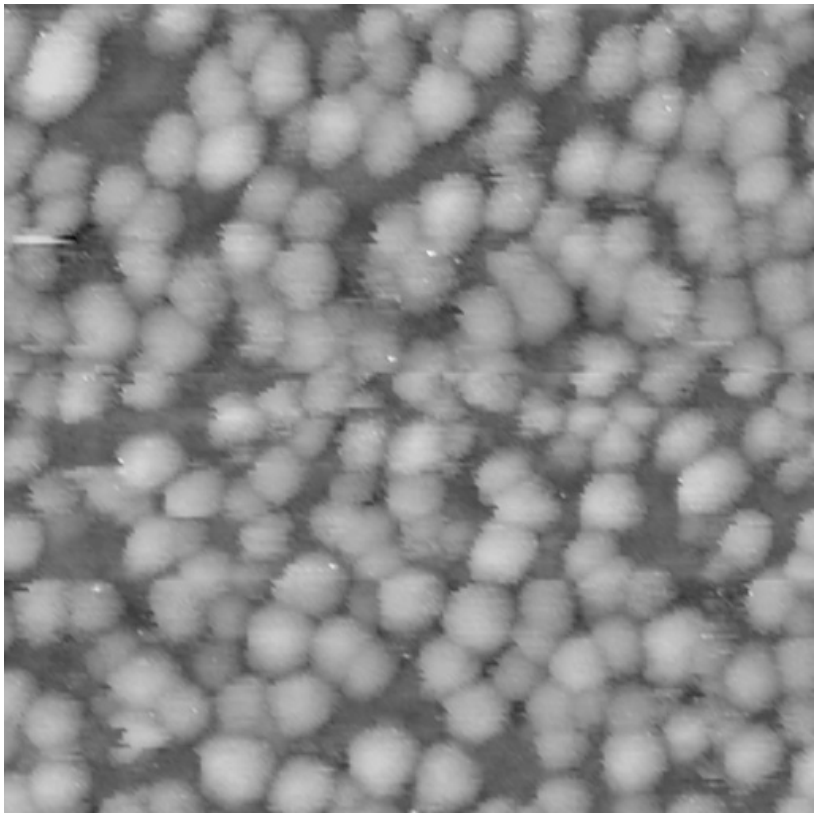


Figure: Original image

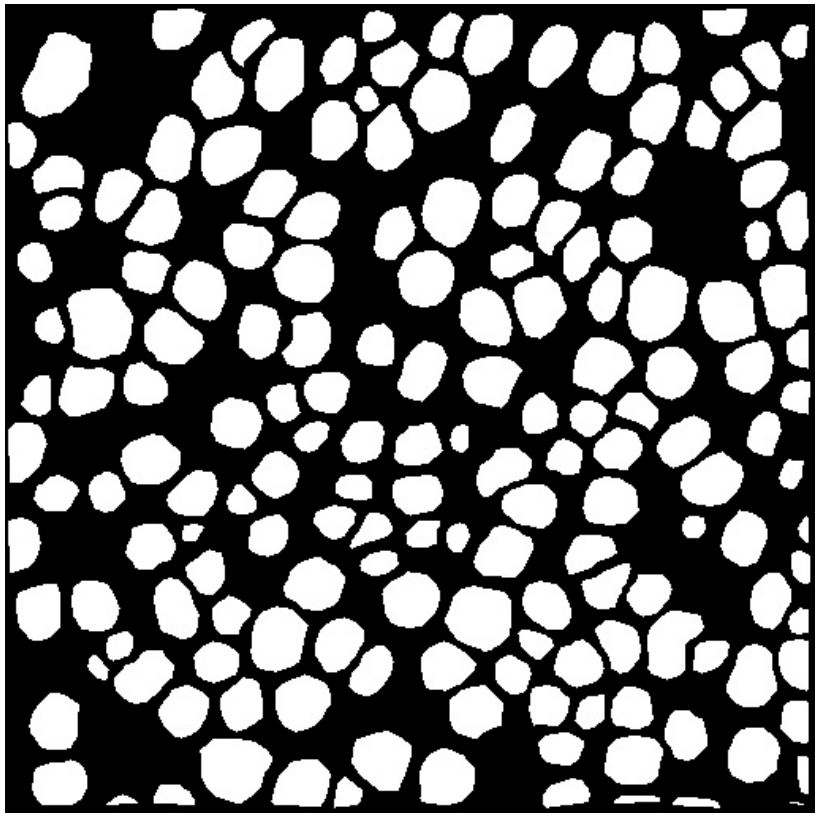


Figure: Main mask

U-Net

Training

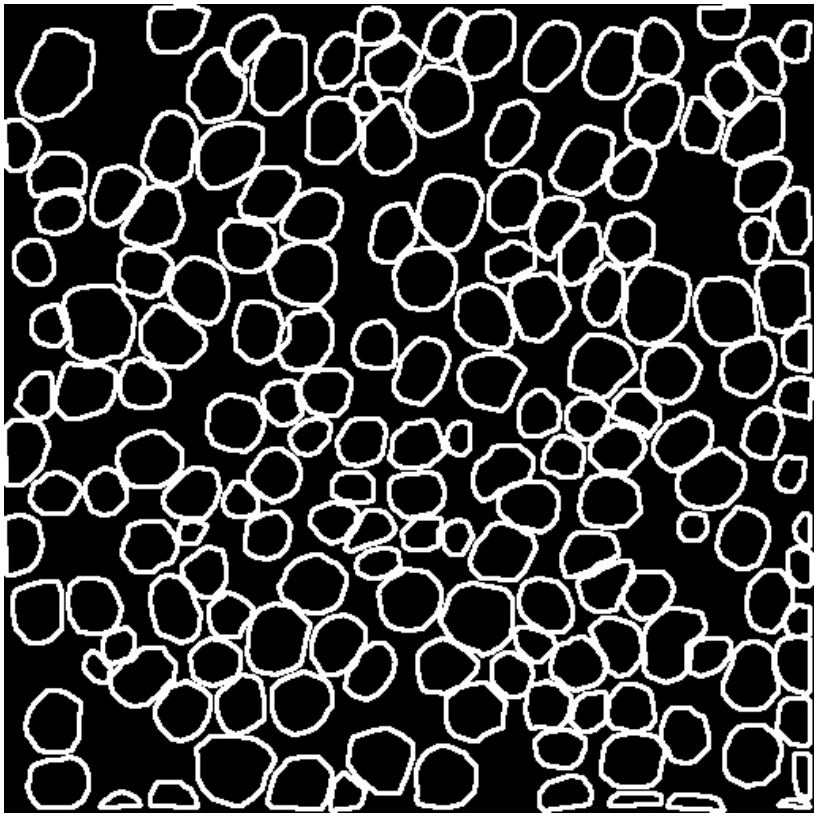


Figure: Border mask

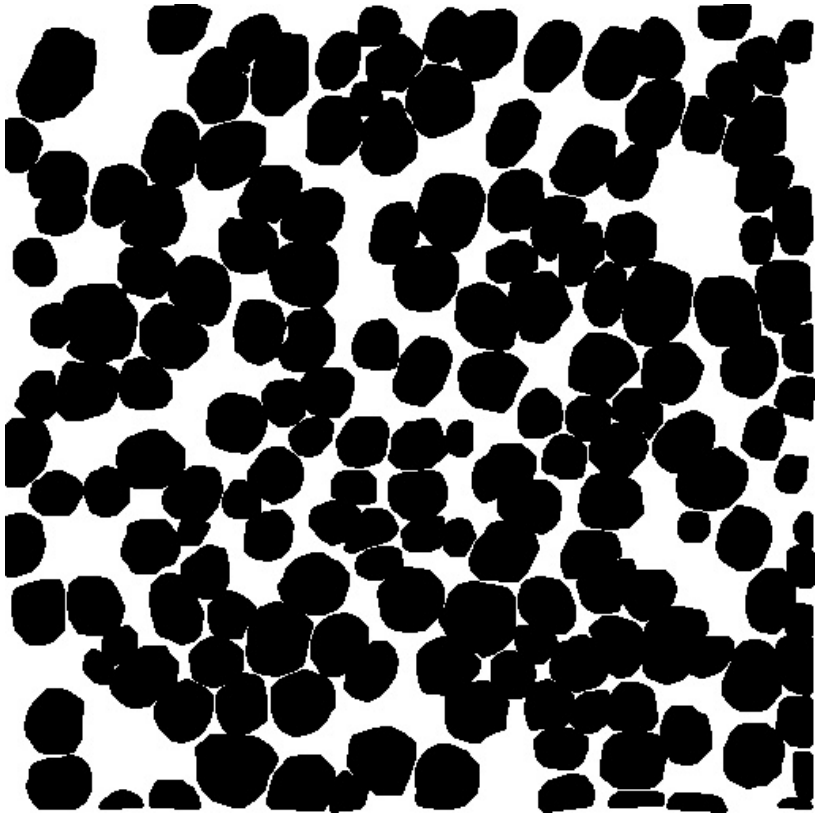


Figure: Background mask

U-Net

Training

First stage

- Masks: mask - border, border, 1 - mask - border
- Encoder: EfficientNet-b3
- Optimizer: Adam
- Loss: Focal + Dice
- Scheduler: ReduceLROnPlateau

Second stage

- Masks: from first stage
- Model: from first stage
- Optimizer: Adam
- Loss: Weighted Focal + Dice Loss, weights: border - 0.8, other - 0.2
- Scheduler: ReduceLROnPlateau

We also conducted an additional experiment: we used an open dataset with labeled cells in order to pre-train the U-Net network on these data.

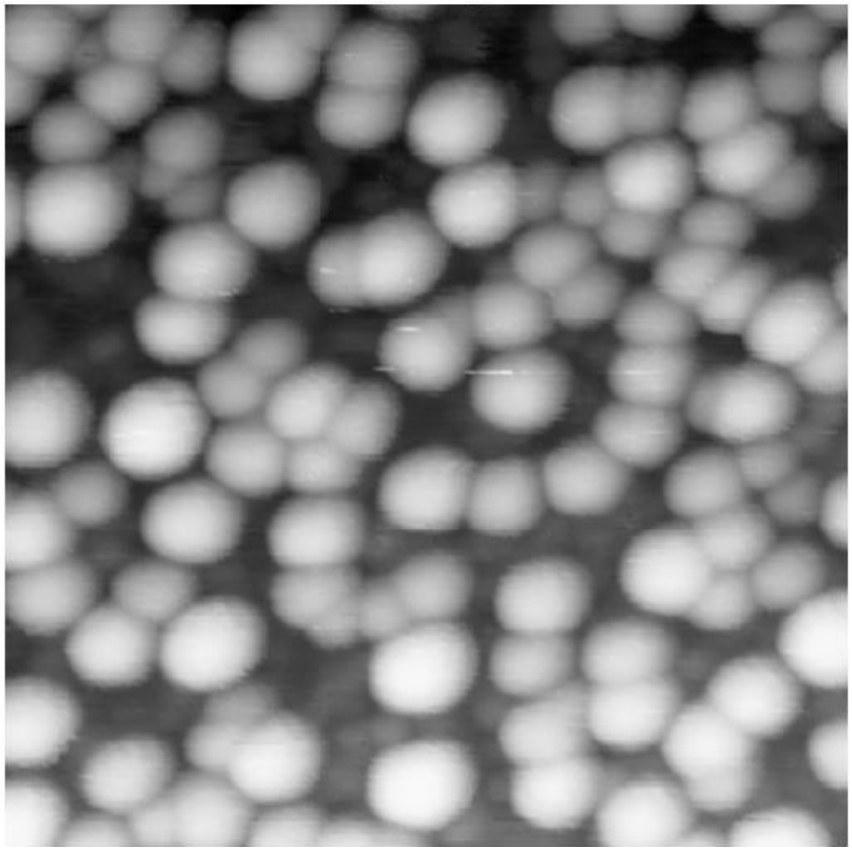
U-Net

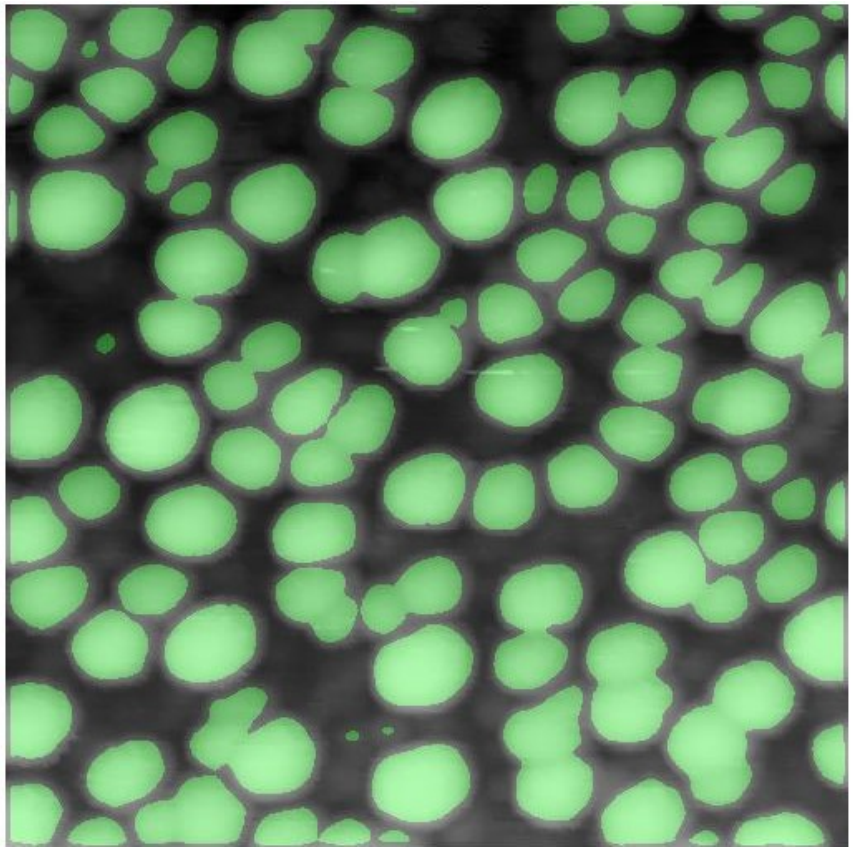
Postprocessing

Model output is three masks: cells insides, cells borders and background. We apply softmax for this masks and get each pixel maximum. After that we apply Watershed algorithm to a channel with a full masks and borders and got the final mask.

Results

Example of the U-Net





Results

Table of results

Results	
Method	mean Average Precision
U-Net	0.01
U-Net + post-processing	0.09
U-Net + post-processing + pre-training	0.12

Thank you for your attention!