Semantic segmentation of Atomic Force Microscopy images of calcite topography

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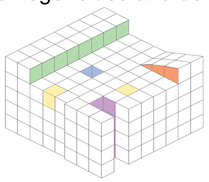
PROBLEM STATEMENT

- Mineral dissolution/precipitation reactions are critical in many natural and industrial contexts.
- High resolution imaging techniques allowing a direct observation of the surface during the reaction revealed that they involve different dissolution mechanisms caused by an uneven local distribution of surface energy due to inhomogeneities and defects in the mineral lattice.



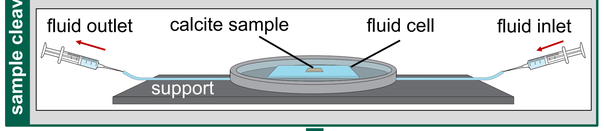
Typical features in the crystal lattice
- step
- line defect
- impurities
- point defect
- screw dislocation

- We rely on a multimodal Gaussian model to capture the spatial heterogeneity of *in-situ* and real time topography measurements of calcite samples subject to dissolution at far from equilibrium conditions acquired via Atomic Force Microscopy (AFM). Each Gaussian mode is associated with a characteristic dissolution pattern.
- We resort to an imaging segmentation technique to cluster topography data into different regions depending on the dissolution mechanism. Stochastic model parameters are then inferred on the data of the regions.

METHODS

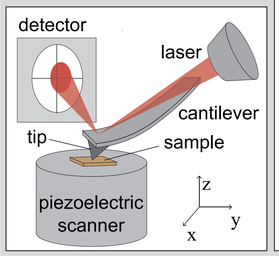
sample cleavage & cell preparation

- Sample: freshly-cleaved calcite
- Solution: Milli-Q water
- Frame time interval: 5 min
- Observed window size: 6 × 6 μm²
- Horizontal resolution: 11.7 nm
- Flow rate: 36 ml h⁻¹



AFM imaging

AFM measurements in contact mode



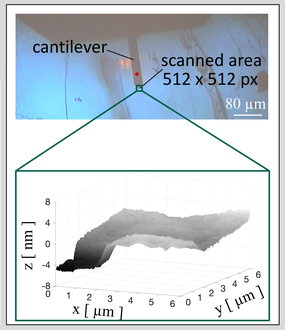
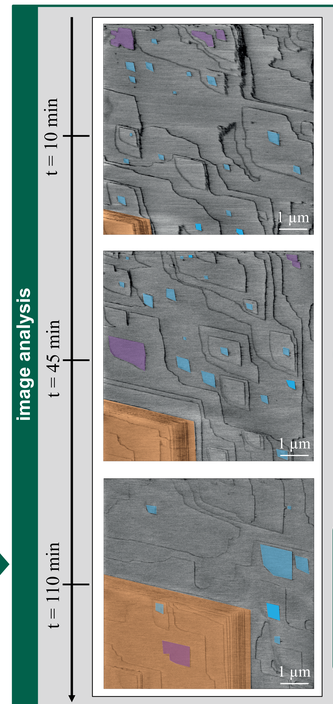


image analysis



Main dissolution mechanisms:
- Monolayer etch-pits nucleation
- Monolayer etch-pits spreading and coalescence
- Deep multilayer etch pit spreading

each one is associated with a sample frequency mode

image semantic segmentation model to identify the different regions

stochastic model

- We compute sample statistics of
  $Z'(x) = Z(x) - \langle Z \rangle$ — Zero-mean fluctuation of Z
  $\Delta Z(s) = Z(x+s) - Z(s)$ — Increment of Z over lag s
- We interpret Z' and ΔZ data with a Gaussian Mixture Model (GMM):

$$Z'(x) = c \cdot N(\mu_A, \sigma_A) + (1-c) \cdot N(\mu_B, \sigma)$$

The model depends on seven parameters

μ_A μ_B	mean	
σ_A σ_B	standard deviation	
ρ_A ρ_B	spatial correlation	
c	contribution coefficient	

inferred on regions A and B

inferred on geometric proportion

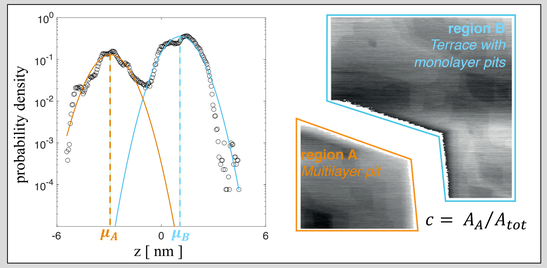
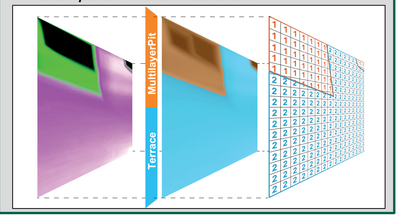


IMAGE SEMANTIC SEGMENTATION & RESULTS

pre-processing & labelling of training and test images

Image semantic segmentation = process of assigning a class label to each pixel of an image

- Images are processed to remove measurement artifacts and they are displayed with a high-contrast colormap (green – magenta).
- We define two labels:
  1 Region A **Multilayer Pit**
  2 Region B **Terrace**
- We assign pixel labels to 280 images (240 training images + 40 test images) using Matlab *Image processing and computer vision* toolbox.

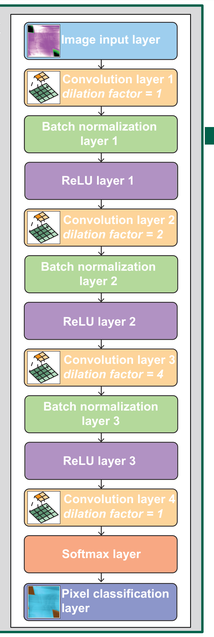


definition of Convolutional Neural Network architecture & training

- In the context of image analysis, Convolutional Neural Network (CNN) are deep machine learning architectures able to assign categories/recognise objects in input images.
- We define a CNN with 13 layers using Matlab *Deep learning* toolbox :

input layer:	*reads image and normalises data.*
convolution layer:	*applies a kernel that calculates a local weighted sum as it slides through the input. A dilation factor may be selected to increase the receptive field.*
batch normalization layer:	*standardises inputs to each mini-batch.*
ReLU layer:	*applies a threshold to each element and sets any value less than 0 to 0.*
softmax layer:	*converts the input into probabilities applying softmax function.*
pixel classification Layer:	*takes the values from the softmax function and assigns each input to one of the classes.*

- Network is trained with 240 images with 900 iterations requiring a computational time of 60 min.



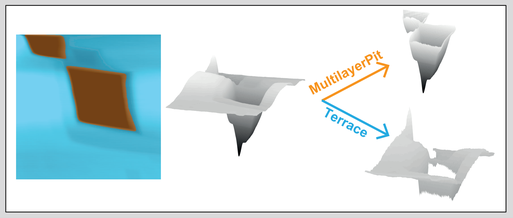
network metrics

- We test the trained network against 40 images comparing predictions with known labels:

Mean accuracy = **0.99**

results

- We use the trained network to segment several unknown topography maps. Segmentation results are used as masks to extract topography regions.



REMARKS

- Image semantic segmentation resulted to be very accurate in subdividing the mineral regions associated with different dissolution patterns.
- GMM parameters inferred on segmented regions provide an accurate representation of the sample frequency distribution.
- After training, the network is able to segment input images instantaneously.
- Future developments include the introduction of a third pixel class to subdivide nucleated monolayer etch pits from terraces.

REFERENCES

- Tahmasebi, P., Kamrava, S., Bai, T., Sahimi, M. Machine learning in geo- and environmental sciences: from small to large scale. Advances in Water Resources 142 (2020). doi.org/10.1016/j.advwatres.2020.103619