Physics-based synthetic data model for automated segmentation in catalysis microscopy

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Background:
In catalysis research, the amount of microscopy data acquired when imaging dynamic processes is typically too vast for non-automated analysis. Consistent image segmentation is a common first step to obtain data that can be correlated with time-dependent chemical observable. Developing machine learned segmentation models is challenged by the requirement of more high-quality annotated training data than is available in most cases. In our approach, we thus substitute expert-annotated data with a physics-based sequential synthetic data model.

We study environmental SEM (ESEM) data collected from the process of propanol oxidation to acetone over cobalt oxide. After raising the temperature to 350 °C during the reaction a phase transition occurs, reducing the selectivity of the catalyst towards acetone. This phase transition manifests in the µm-scale ESEM data as the formation of cracks between the pores of the catalyst surface. The aim is to generate synthetic data to train a neural network capable of performing semantic segmentation (pixel-wise labelling) of this ESEM data. Statistical analysis of this data will lead to greater insights into this phase transition.

Method:
To generate synthetic image data that approximates the observed transition, our algorithm composes ESEM images of the pristine room-temperature catalyst with dynamically evolving synthetic cracks satisfying two physical construction principles, gathered from empirical knowledge about the phase transition. First, crack growth propagates along surface paths which avoid close vicinity to nearby pores in the surface. Second, each growing path successively widens and is rendered with increasing contrast over short sequences of frames, allowing the algorithm to mimic the growth of the crack features on the surface. The synthetic dataset generated using this algorithm is then used to train a U-NET-LSTM recurrent convolutional neural network. This network architecture consists of a U-NET component with a convolutional Long Short-Term Memory cell appended.

Results:
To evaluate the quality of the neural network, and by extension the synthetic data generation algorithm, two neural networks were trained. The physics-based network was trained on a synthetic dataset generated as described above, and the random network was trained on a similar synthetic dataset, with the restriction that the crack growth paths avoid close vicinity to pores removed. These models were then benchmarked against each other using a synthetic test set to evaluate the importance of this physics-based component of the synthetic dataset. The results show that the physics-based network has a much lower rate of false positives than the random network, at a cost of a slightly lower rate of true positives. This is reflected in the resulting Dice-coefficients of 0.76 (physics-based) and 0.64 (random).

The physics-based network was then applied to the original ESEM movie, giving a fully semantically segmented dataset as the result. From this, statistics about the evolution of crack features could be extracted. Their analysis revealed that the crack feature is first visible to the ESEM about 100 minutes after the acetone selectivity loss event.

Conclusions:
By integrating physical characteristics of the features on the catalyst surface into a synthetic training data generation algorithm, we obtained a network with superior accuracy and a greatly decreased false positive rate. By taking advantage of the temporal nature of the data through the use of a recurrent Long Short-Term Memory layer, we improved the confidence and accuracy of the model further.

Keywords:

computer vision synthetic data ESEM

Reference:

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