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AI assisted quantification of the metastability of ACC in the presence of metallic ions

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The understanding of calcium carbonate minerals formation through amorphous calcium carbonate (ACC) precursors is relevant for various system e.g., biomineralization of marine calcifiers which represents one of the long-term sinks of carbon on Earth [1] and as scavengers of metals and radionuclides [2]. To this end we conducted droplet microfluidic experiments [3] to investigate the time of life of ACC and their transformation into more stable minerals in presence of metal ions (M) such as Mg, Sr and Ba. In such experiment hundreds of droplets are generated and the mineralogical transformation are monitored by time lapse microscopy. To maximize the throughput of these experiments, we developed an automatic approach that combines classical machine learning algorithms and computer-vision techniques to analyze large datasets of experimental data and to understand the behavior of ACC under various conditions. The use of computer-vision techniques plays a critical role in automating the analysis of complex datasets.

The proposed computer-vision procedure was established by combining traditional image processing techniques with an original convolutional neural network (CNN). The CNN was based on the U-net architecture [4] and was developed in Python. To develop the U-Net CNN model, the first step involves manually annotating a set of ACC images to identify regions of interest. Next, the model is trained using the annotated images, where the goal is to minimize the difference between the predicted output and the ground truth labels. Finally, the trained model is used to segment new ACC images into regions of interest. The U-Net CNN model achieved a high accuracy in segmenting ACC images, demonstrating its potential for use in the analysis and characterization of complex mineral structures. In addition, classical machine learning algorithms were used to assess the results and to identify and analyze different patterns of behavior between different sets of experiments quantifying the time of life of ACC in presence of metallic ions.

References

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