Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.27199

High-throughput mineralogical characterization of carbonate (bio)mineralization systems

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Carbonates are a major Eukaryotic and Prokaryotic biomineral type, an important sedimentary sink in the biogeochemical carbon cycle, and the basis for many paleoenvironmental proxies. They are increasingly being considered as long-term carbon stores in different Carbon Capture, Use and Storage (CCUS) strategies, as well as promising materials for replacing carbon-intensive industries (e.g., biocements and bioconcretes in construction). Carbonate crystallisation is under the influence of many physicochemical variables (e.g., temperature, pH, supersaturation, salinity) as well as of inorganic and organic additives that can act as inhibitors or promoters of nucleation and growth, exerting a strong control on the abundance, morphology, and crystal structure of the particulate mineral products. In addition, carbonate formation can be mediated or influenced by the presence of microbial cells, via local chemical changes resulting from their metabolic activity, or via the action of organic molecules produced in the cells' environment. While the impacts of these factors on carbonate mineralization and properties have been extensively studied individually, their combined effects have not been systematically explored. In fact, our current understanding is largely based on empirical studies that investigate the effects of these factors in isolation, providing findings that cannot be easily extrapolated to different conditions, and failing to capture the complexity of natural and engineered systems where multiple chemical and biological variables interact.

We have developed a new high-throughput methodology allowing us to rapidly perform and characterize high numbers of carbonate mineralization experiments, covering a wide multi-dimensional space of chemical variables, and testing the effect of large numbers of organic additives on mineral formation. Carbonate particles precipitating in miniaturized experiments performed in multi-well microplates are systematically imaged at high resolution and classified based on their morphometric parameters using a supervised Machine Learning algorithm. Particle types are then matched with corresponding crystal structures determined by correlative automated Raman spectromicroscopy. *In*-situ imaging and automated Raman analyses directly in the microplate wells also allow for the rapid high-throughput characterization of the morphological and mineralogical properties of carbonate biominerals forming in large numbers of microbial cultures. We will discuss potential future applications of this methodology, notably in microbial biomineralization research.