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Coherent X-ray Diffraction Imaging to Investigate morphology of Calcium Carbonate Microparticles

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Coherent X-ray diffraction imaging (CXDI) is a phase retrieval technique that reconstructs a real-space image from the corresponding Fraunhofer (far-field) diffraction patterns that must be oversampled in the reciprocal space. The measured diffraction patterns of an object are directly related to the Fourier transform of the electron density of the sample. CXDI is a lensless imaging technique that retrieves the sample's structural information using the observed Fourier space amplitude and iteratively recovered phase. The phase recovery algorithm alternates a guess of the phase between real and Fourier spaces using known constraints –positivity of the electron density and a support constraint that defines the region within which the electron density is non-zero. The method, therefore, requires the particles to be isolated and have a size that falls within the size of the beam to ensure the oversampling condition is met. CXDI requires advanced coherent X-ray sources like synchrotrons combined with state-of-the-art detectors and iterative phase retrieval algorithms.

As part of our ongoing research on understanding nucleation and growth, we utilised CXDI to investigate the morphological development of calcium carbonate ($CaCO_3$), an important constituent in shells and other exoskeletal structures. We can control the developing morphology of $CaCO_3$ through additives, concentrations, and the confinement of precursors.

In this presentation, we will present an in-depth review of the CXDI methodology and demonstrate its use within the study of the 3D internal and external morphologies of a range of $CaCO_3$ particles with voxel sizes as high as 11 nm.

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