Bridging real and reciprocal-space nanoimaging of biogenic calcite: Bragg coherent diffraction, ptychography, and cryo X-ray fluorescence

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Presentation type: Oral **Presentation time:** 09:00-09:15

Synthetic approaches to strain engineering struggle to control internal lattice distortions reproducibly: morphologically identical nanocrystals exhibit heterogeneous strain. Coccolithophores (unicellular algae) biomineralize calcite with long-recognized morphological consistency and, we now find, equally consistent internal strain. Holococcoliths, the calcite scales produced by cells in haploid phase, show spherically symmetric strain fields across biological replicates; heterococcoliths, produced in the diploid phase, exhibit strain complexity that scales with chiral morphology. The cell controls both crystallographic orientation and impurity distribution beyond what morphological templating alone explains. Resolving the mechanism requires reading both the lattice distortions and the chemical perturbations that drive them.

We approach the question by combining real- and reciprocal-space X-ray nanoimaging on the same single coccolith crystals. Bragg coherent diffractive imaging (BCDI) at ID01 of the ESRF-EBS resolves three-dimensional lattice strain at sub-10 nm resolution and 10 strain sensitivity. Ptychographic X-ray computed tomography (PXCT) at ID16A maps quantitative electron density at similar resolution, exposing intracrystalline density variations. Cryogenic X-ray fluorescence computed tomography (cryo-XRF-CT) on intact, plunge-frozen coccolithophore cells localizes the chemical origin of the measured strain at 35 nm voxel resolution with single-element sensitivity down to tens of atoms per voxel. The workflow builds on our recent implementations of cryo-correlative X-ray microscopy and self-supervised denoising for multi-element XRF detectors.

Applied to both life-cycle phases, the approach exposes two regimes of impurity-strain coupling. In holococcoliths the Sr enrichment toward the crystal rim results in transition from compressive to tensile lattice strain, leading to self-limited growth. In heterococcoliths the strain field becomes strongly anisotropic and follows the broken morphological symmetry, co-localized with asymmetric Sr distributions. At substitutional levels around 0.25 atomic percent (Sr/Ca), strain and impurity co-evolve with a non-linear, anisotropic lattice response that deviates from Vegard's law, corroborated by density functional theory.

By resolving both the lattice signature and the chemical origin of symmetry breaking at the single-nanocrystal level, our tri-modal workflow turns biogenic calcite into a quantitative testbed for impurity-driven strain engineering. The same correlative approach extends to other complex materials in which composition and lattice strain are entangled at the nanoscale. Probing them requires complementary techniques operated at their current limits, where the methods and the understanding of the phenomena they reveal are co-developed.