Understanding Crystallization Pathways in MnO_2 Polymorphs

Scientific Achievement

Demonstrated predictive synthesis of MnO_2 polymorphs based on principle of remnant metastability—that synthesizable metastable phases nucleate under thermodynamic conditions where they were once the lowest free-energy phase, and then grow into conditions where they are metastable. Using *in-situ* X-ray diffraction measurements, we verify that this framework can predict which phases are more likely to form as well as the progression order of phases.

Significance and Impact

The successful prediction of phase progression during MnO_2 polymorphs synthesis demonstrates the viability of remnant metastability as a general framework—for predicting synthetically accessible metastable materials and as a practical tool for guiding synthesis.

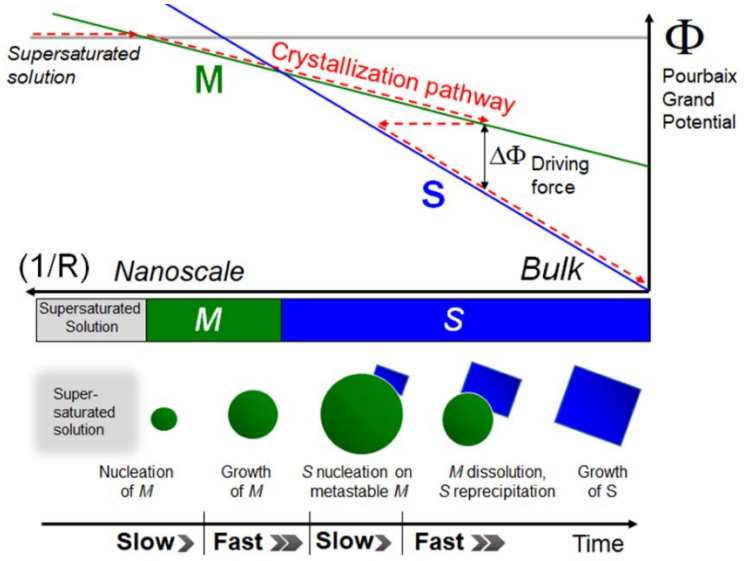
Research Details

Theory: *Ab-initio* predictive framework shows how particle size and solution composition influence polymorph stability during nucleation and growth.

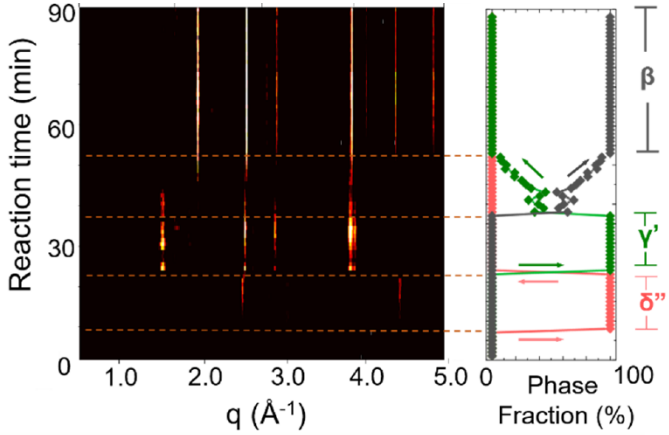
Synthesis: Hydrothermal synthesis with varying solution potassium ion concentrations ([K^+] = 0, 0.2, and 0.33 M).

Characterization: *In-situ* X-ray diffraction observed predicted progression of crystalline polymorphs during synthesis.

Schematic Representation of Remnant Metastability in a Crystallization Pathway



In-situ Observation of Predicted Phase Progression



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