Amorphous Precursors: A Route to Polymorph Synthesis

Scientific Achievement

Using theory-guided synthesis, we have synthesized TiO_2 thin films with greater than 80% brookite fraction without substrate templating or the presence of helper ions via solid-phase crystallization of amorphous precursors.

Significance and Impact

Polymorph formation pathways are important in many materials systems. Our work demonstrates the viability of using amorphous materials as a high-energy starting point for targeted synthesis of polymorphs higher in energy than the ground-state structure.

Research Details

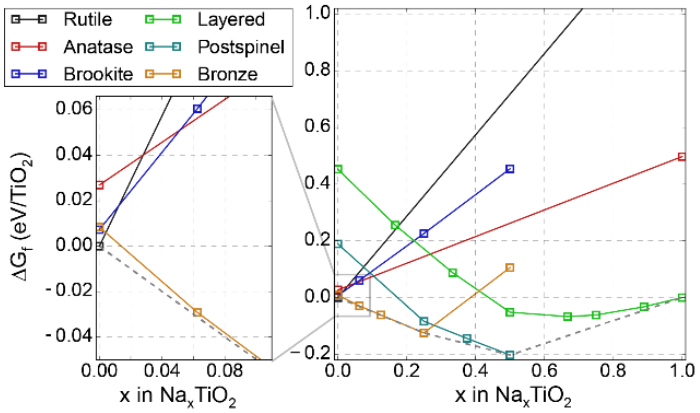
Theory: Density functional theory (DFT) calculations show that Na incorporation does not favor the brookite structure.

Synthesis: Pulsed laser deposition of amorphous films from a TiO_2 target with O_2 background gas on amorphous substrates including Na-free fused silica, low-Na glass, and high-Na glass.

Characterization: *In-situ* and *ex-situ* XRD, HRTEM, and EDS. 2-D micro-Raman mapping quickly identifies polymorphs during formation and helps identify relevant parameters such as precursor properties, film thickness, and anneal temperature.

Haggerty *et al., Sci. Rep.* **7**, 15232(2017).

DFT Calculations



Optical and Raman Measurements