

Structural analysis by stochastic differential scanning calorimetry

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Integration of second harmonic generation (SHG) imaging with differential scanning calorimetry (DSC) enables a thermal and physical analysis of single-particle stochastic phase transformations in organic crystals, which collectively contribute to the ensemble-averaged thermal transients interrogated by DSC. The SHG-activity of a crystal is highly sensitive to the specific molecular packing arrangement within a noncentrosymmetric lattice, providing access to structural information otherwise unavailable by conventional imaging approaches.^{1,2} Consequently, lattice transformations associated with dehydration/desolvation events were observed by SHG imaging and correlated to phase transformations observed in the DSC measurements.

Following the studies of a model system, stochastic differential scanning calorimetry (SDSC) was performed to interrogate samples of crystalline trehalose dihydrate which exhibit complex phase-transition behaviors.³ In general, the structural analysis of trehalose dihydrate during heating is complicated by the existence of varying polymorphs that form under different conditions, leading to an ongoing debate on how the polymorphs of trehalose are connected to each other during various thermal/phase transformations.⁴ Since significant structural differences can arise due to polymorphic transition, trehalose dihydrate was analyzed by SDSC using an integrated DSC-SHG microscope to probe crystal form throughout its phase transitions.

References

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