In-situ X-ray Diffraction of Inorganic Salt Hydrates for Thermal Energy Storage

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Inorganic salt hydrates are promising phase change materials (PCMs) for low-to-medium temperature thermal energy storage (TES) due to their high volumetric latent heat, cost-effectiveness, and availability [1]. Applications include solar thermal storage, building heating, and industrial waste heat recovery (40–150°C). However, their practical implementation is hindered by performance degradation over repeated melting-solidification i.e., dehydration-rehydration cycles, exhibited as supercooling, phase separation, and loss of storage capacity [2]. Although the bulk thermophysical properties of many salt hydrates have been characterized but the atomic-scale structural dynamics governing reversibility and degradation during thermal cycling remain poorly understood [3].

This study investigates the reversibility and degradation pathways of selected inorganic salt hydrates under cyclic thermal conditions relevant to TES applications. The work is in progress. Using a multi-technique in-situ approach, we aim to correlate macroscopic performance with structural evolution. In-situ variable temperature X-ray diffraction (XRD) will track crystallographic phase transitions [4], lattice parameter changes, and intermediate phase formation during multiple dehydration-rehydration cycles. In-situ Infrared and Raman spectroscopy will directly monitor O–H stretching vibrations of intermediate amorphous and crystalline phases to follow water molecule dynamics during water loss and re-incorporation in real time. We will also use simultaneous TGA-DSC that will provide correlated mass and enthalpy changes.

By comparing structural evolution across cycles under different heating rates and vapor pressures, we aim to identify critical points where irreversibility begins whether through incomplete rehydration, formation of non-reactive phases, or loss of crystallinity. These insights will inform strategies to stabilize salt hydrate PCMs for long-term TES applications, addressing the need for improved cycling stability as identified in recent screening studies [5].

References

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