

ABSTRACT - POSTER

Tuning the Switch: How to Influence the Kinetics and Thermodynamics of the Structural Phase Transition in W-Doped VO₂ Microparticles

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Abstract:

Vanadium dioxide (VO₂) is a promising material for energy-efficient smart windows due to its thermochromic properties. At a critical switching temperature (T_0) of 68 °C, VO₂ undergoes a reversible structural phase transition (SPT) from the semiconducting monoclinic VO₂(M) to the metallic rutile VO₂(R) phase. This SPT involves changes in solar infrared (IR) transmittance, with VO₂(M) transmitting IR light below its T_0 and VO₂(R) blocking it above its T_0 . To tune the thermochromic properties to application-specific requirements and realize maximum performance, it is important to understand the thermodynamics and kinetics of the STP and how those characteristics can be influenced.^{1,2}

This research investigates the thermodynamics and kinetics of the STP in thermochromic VO₂(M). We focus on understanding how T_0 can be efficiently reduced and which parameters influence the phase transition kinetics. For this purpose, W-doped VO₂ microparticles (17 - 34 μm, 0.5 - 2.5 at.% W) were synthesized through a hydrothermal method, and the effect of W⁶⁺ incorporation on the formation of different VO₂ crystal phases was studied.

Structural and morphological analyses confirm that W⁶⁺ is crucial for promoting the formation of phase-pure monoclinic and rutile VO₂. Furthermore, differential scanning calorimetry (DSC) indicates switching enthalpies ranging from 15 to 35 J/g, along with a decrease in T_0 as the W⁶⁺ content increases. However, deviations from ideal behavior arise from the inhomogeneous distribution of W⁶⁺ in the VO₂ crystals.

A comprehensive isoconversional kinetic analysis reveals that the rate of the phase transition is limited by nucleation kinetics. This results in a temperature-dependent activation barrier that steeply increases as the temperature approaches T_0 . Activation energies were found to range from 10³ to 10⁴ kJ/mol. Hence, significant overheating or undercooling is required to achieve a rapid thermochromic switch when implementing this material in smart windows.

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References

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