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SESSION 1: MODELS AND METHODS, SALON A

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DFT calculations and experimental study of the lattice distortion on phase transition properties of the polycrystalline VO₂ thin film

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ABSTRACT

Polycrystalline VO₂ thin films with different lattice distortions were fabricated on quartz glass substrates using high power impulse magnetron sputtering. The influences of the lattice distortion of the as-deposited film on phase transition temperature, resistance change, and transmittance were obtained. In addition, using a calculation based on Density functional theory (DFT) methods, the mechanisms of the lattice distortion on phase transition properties are discussed.

KEYWORDS: polycrystalline VO₂ thin film, lattice distortion, phase transition, DFT calculations