Vertical Growth Models for Analysing Vanadium Dioxide Phase Transition in Thin Films

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Vanadium dioxide (VO_2) possesses a metal-insulator phase transition at ~68 °C that is widely explored for nanophotonic and nanoelectronic applications, such as neuromorphic computing and metasurface-based beam steering. In many of these applications, a key challenge is to accurately model the permittivity of VO_2 during the phase transition. In this work, we propose vertical growth models for this purpose, and show that they outperform the traditional effective medium models in analysing thin film.

The traditional effective medium models treat the intermediate states of VO_2 as an effective medium, where the metallic and the insulating phases are mixed at the microscopic scale. These models assume that, at the macroscopic scale, this mixture is effectively homogeneous in all the three dimensions. However, we argue that this assumption is not valid in thin film analysis. Due to the existence of surface potential energy and the relatively large surface-volume ratio, we believe that the surfaces should be treated differently from the interior, in modelling phase transition in VO_2 thin films. For this purpose, we propose microscopic vertical growth models, where the phase transition is treated as a 2D, layered growth of one phase into another.

As an experimental benchmark, we deposited a VO_2 thin film on a multi-layered substrate and measured its optical reflection as the film temperature was cycled between 25 °C and 110 °C. We then used the Looyange model and the Bruggeman model (two popular effective medium models), as well as our own vertical growth models, to compute the permittivity of intermediate VO_2 states. The permittivity led to the temperature dependent reflection, which provided direct comparison to experimental data. The result shows that, in a wavelength range of ~500 nm around $\lambda = 1550$ nm, the vertical growth models provide closer prediction to experiment as compared the effective medium models.