Abstract

Yttrium-stabilized Zirconia (YSZ) is a key ceramic material, with its thin films used in countless applications including solid-oxide fuel cells. It is also studied in novel contexts, including cell-culture meat and medical implants.

There are several ways of synthesizing YSZ thin films. One promising method is hydrothermal synthesis due to its speed, energy-efficiency, suitability for large-scale processing and minimal environmental impact.

The surface morphology of YSZ thin films produced via hydrothermal synthesis depends on YSZ solubility. However, currently no model exists to predict YSZ solubility as the chemical equilibrium equations needed are not readily available.

In this work, we collected the equilibrium constants for speciation from various sources and verified them against each other. We derived simultaneous equations from these equilibria and solved them to predict solubility. To develop a modelling tool for the scientific community, we also developed an interactive dashboard where researchers can key in the reagent concentrations added and determine the solubility equilibria of Y and Zr. Researchers can view a Scanning Electron Microscope image to visualise the surface morphology at each reagent set. They can determine the image closest to their desired morphology and narrow experimental efforts to the concentration sets likely to produce YSZ closest to it.

By minimizing the need for trial-and-error studies, this model helps researchers generate useful insights into the growth mechanics of YSZ, honing their growth strategy for their desired output. This speeds up research timelines, minimizes the wastage of resources and reduces the environmental impacts of synthesis, allowing us to develop a more sustainable hydrothermal synthesis process for YSZ.