Developing a modelling tool for hydrothermal deposition of Yttrium-Stabilized Zirconia (YSZ) thin films

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Engineering Problem and Objectives

To manufacture YSZ of a desired surface morphology for a new application requires the determination of the reagent concentrations required.
The state-of-the-art is to find this by extensive trial-and-error studies to determine reagents and conditions required.
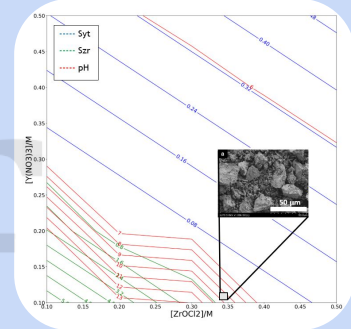
The objective is to develop a modelling tool with an interactive dashboard to help researchers narrow down the set of concentrations which could generate their desired YSZ surface morphology.
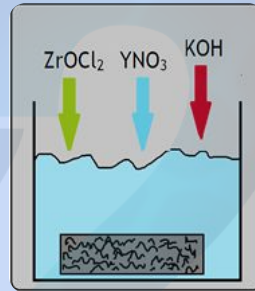

Source: Self-made

Data Analysis and Results

Figure illustrates a resultant solubility surface plot for YSZ. The SEM image of Zarkov's synthesis is an example of a surface morphology which a researcher might desire for their application. If the researcher scrolls over the grid and identifies this SEM image as the surface morphology closest to their desired morphology, they can narrow the set of reagent concentrations they test.
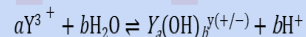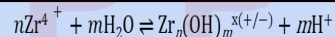

Source: Self-made

Project Design

Concentrations of reagents → pH of solution → Solubility → Rate of deposition → Surface Morphology
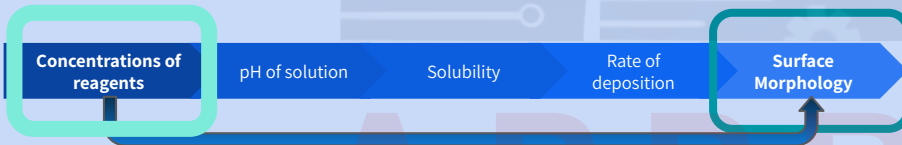
Leveraged chemical equilibrium equations and empirical data to develop model.

$$nZr^{4+} + mH_2O \rightleftharpoons Zr_n(OH)_m^{x(+/-)} + mH^+$$

$$aY^{3+} + bH_2O \rightleftharpoons Y_a(OH)_b^{y(+/-)} + bH^+$$

Interpretations and Conclusions

Model helps to minimize the need for trial-and-error studies, which in turn helps to:

➔ Speed up research timelines
➔ Minimize wastage of resources
➔ Reduce environmental impacts of synthesis

Model addresses the unmet need for a tool to help researchers narrow down range of reagent conditions to test