MS003

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

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Problem

- ❖ YSZ thin films are being used in countless promising applications
- ❖ Manufacturing YSZ of a desired surface morphology for a new application needs to determine the reagent concentrations required for the task
- ❖ Extensive trial-and-error studies needed to determine reagents and conditions required

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

Solution

- ★ Developed an interactive dashboard to help researchers narrow down set of reagent concentrations to generate YSZ of desired surface morphology using Python and StreamLit.
- ★ Minimizing the need for trial-and-error studies helps:
  - ➔ Speed up research timelines
  - ➔ Minimize wastage of resources
  - ➔ Reduce environmental impacts of synthesis

Introduction

- Yttrium-stabilized Zirconia (YSZ)
  - Ceramic
  - ZrO_2 stabilized by doping with Y_2O_3

- Hydrothermally synthesized YSZ:
  - Low thermal conductivity
  - Solid electrolyte
  - Countless <u>novel and promising applications</u>

Cell-cultured meat Medical implants

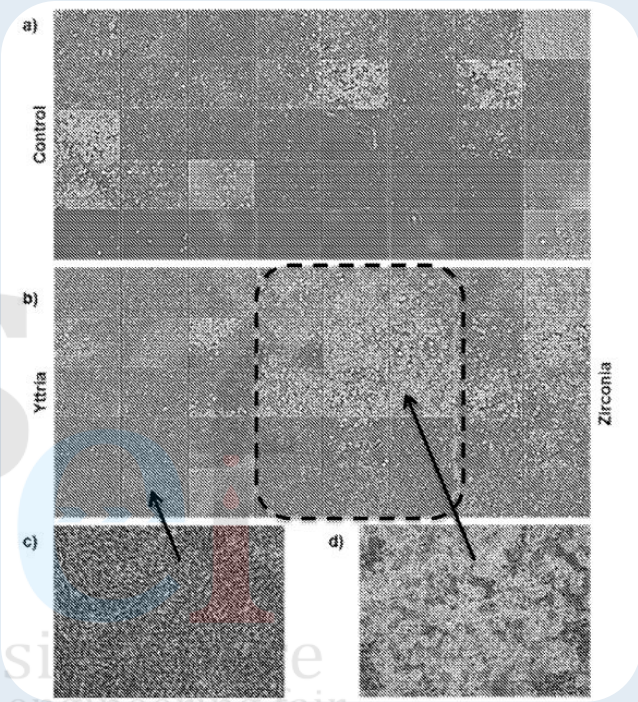

Figure 1:
An increase in differentiated adipocytes with lipid formation was observed on the (b) Y_2O_3 - ZrO_2 coated substrate as opposed to (a) the control substrate
Source: Dykas et al, 2019

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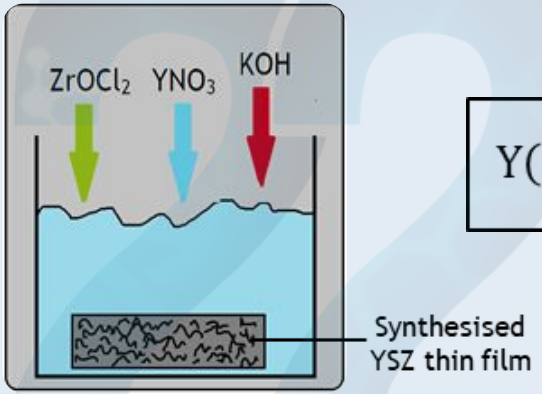
Introduction

Figure 2: Illustration of the hydrothermal synthesis of YSZ in an autoclave.

Source: Self-made



$$Y(NO_3)_3 + ZrOCl_2 + KOH \xrightarrow[\text{autoclave}]{aq.medium} \text{YSZ thin film}$$

Concentrations of reagents → pH of solution → Solubility → Rate of deposition → **Surface Morphology**

Objective

- 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
- Interactive Dashboard:
  - Grid of $[Y(NO_3)_3]$,$[ZrOCl_2]$ tuples
  - Slider input for [KOH]
  - Displays SEM/TEM images of YSZ films obtained from empirical literature
  - pH and solubility contour lines in the grid to identify required pH and solubility bands

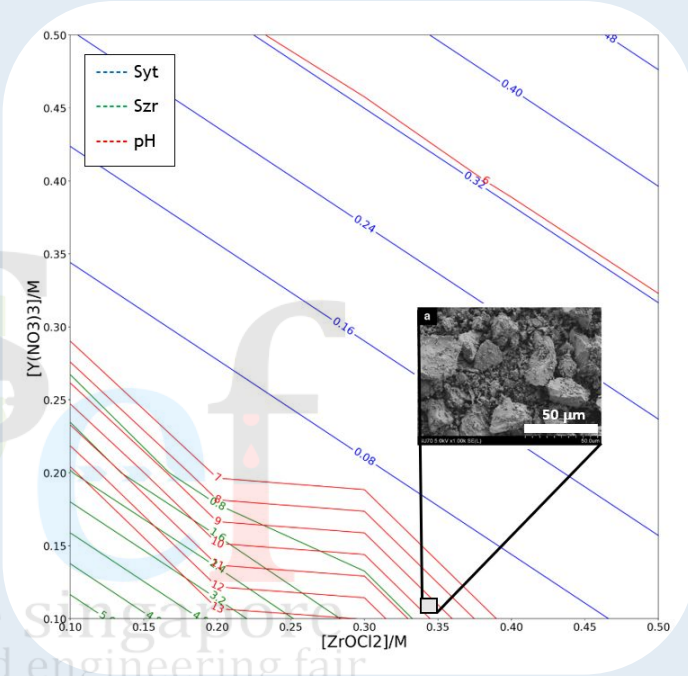


Figure 3:
Solubility surface plot for YSZ with SEM Micrograph of 8mol% YSZ powder synthesised by coprecipitation at pH 9-10 (Zarkov et al, 2015)

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Methodology: Phase 1

pH of the solution depends on [OH^-] from KOH. Some [OH^-] reacts to form species of Y and Zr in solution.

Chemical equilibrium equations for the formation of the compounds are used to find [OH^-] and pH in solution. These can be represented as:

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

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

Solubilities of Y and Zr are computed from total concentrations of all Y and Zr species formed in solution.

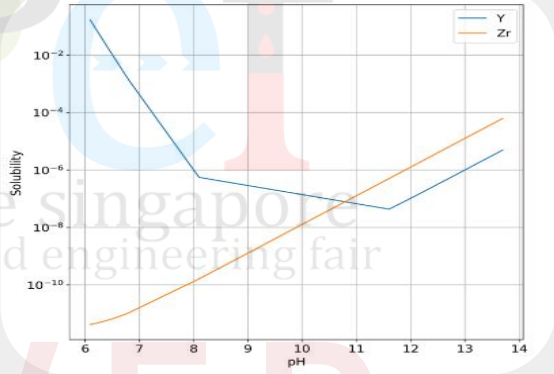

Figure 4: Graph of Solubilities of Yttria (blue) and Zirconia (orange) vs pH

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Methodology: Phase 1

1 Microsoft Excel

Generated preliminary graphs of solubility based on empirical data and equilibrium equations

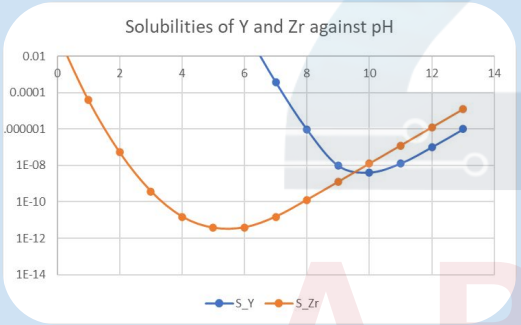


Figure 5: Graph of Solubilities of Yttria (blue) and Zirconia (orange) vs pH

2 Google Colab

Used root-finding "toms748" algorithm to find point where solution mixture net charge = 0. Iterated through various [KOH] to plot solubility/pH.

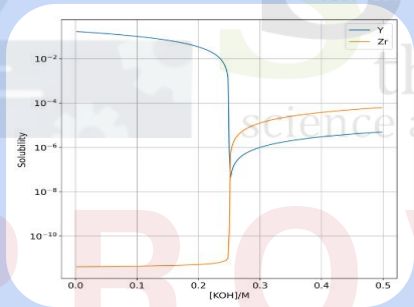


Figure 6: Graph of Solubilities of Yttria (blue) and Zirconia (orange) vs [KOH]

3 Streamlit
Anaconda
PyCharm

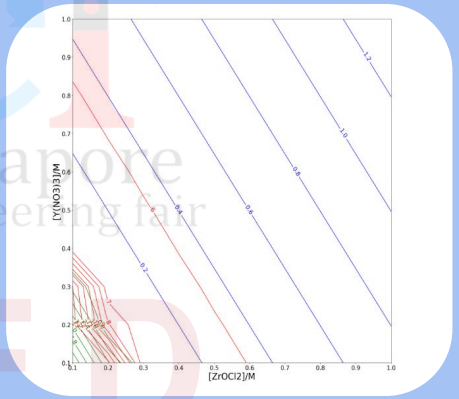


Figure 7: Final Solubility Surface Contour Plot

Methodology: Phase 2

To complete the model, we leverage existing empirical literature to append a selection of SEM/TEM images of YSZ surfaces to the grid, each at the concentration tuple it was synthesized under.

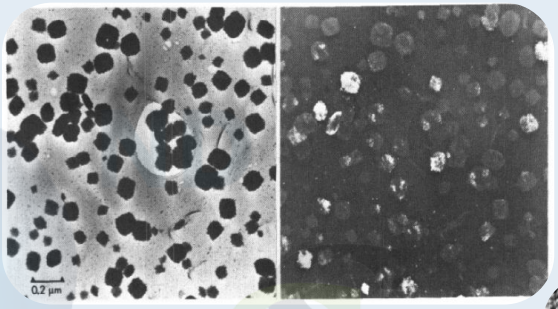


Figure 8:
Bleier's synthesis
Source: Bleier et al., 2011

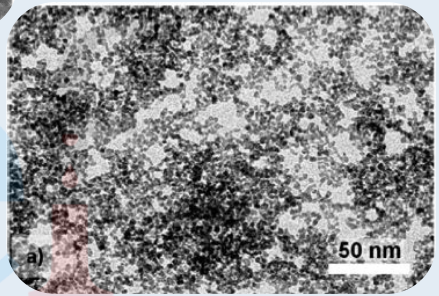


Figure 9:
Kubrin's synthesis
Source: Kubrin et al., 2013

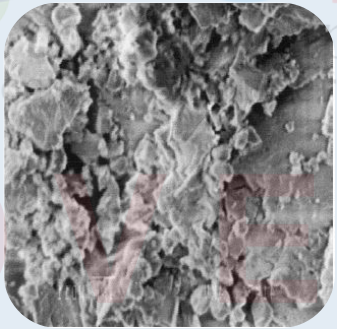
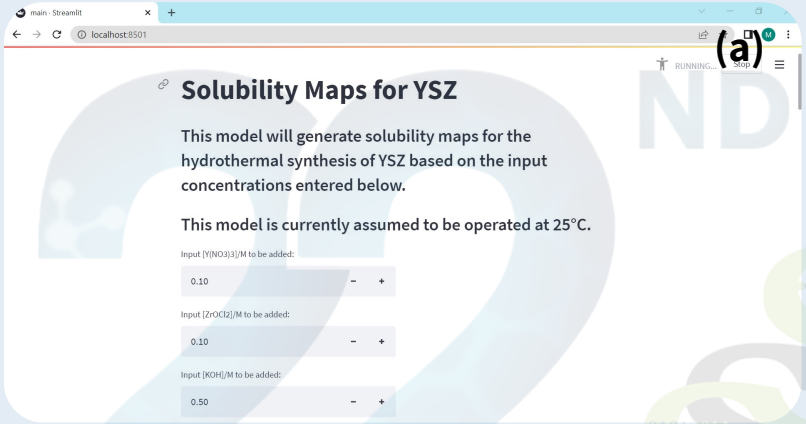
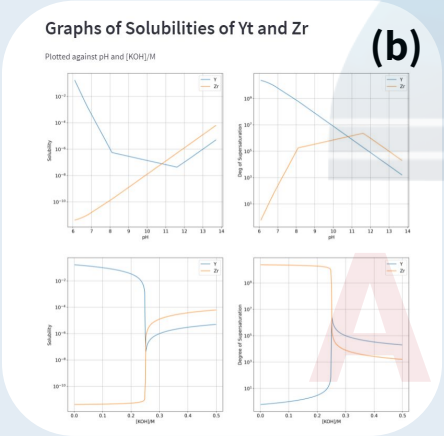
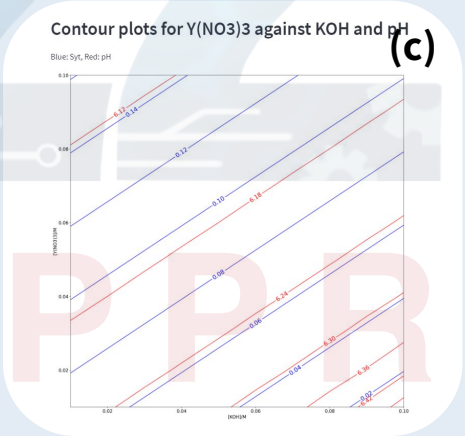


Figure 10:
Piticescu's synthesis
Source: Piticescu et al., 2000

Results: Interactive StreamLit Dashboard







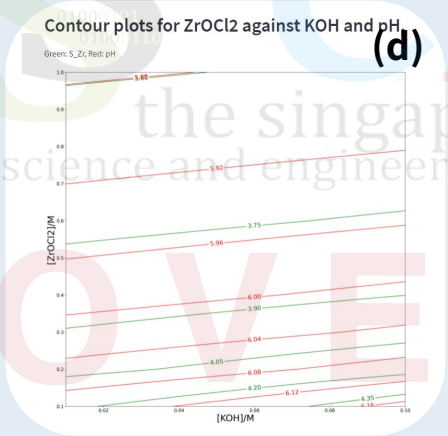


Figure 11:

(a) Interactive StreamLit Dashboard updates as input values are varied

(b) Graphs of solubilities for Y and Zr

(c) Contour plot for Y system

(d) Contour plot for Zr system

Results: Preliminary Solubility Surface Plots

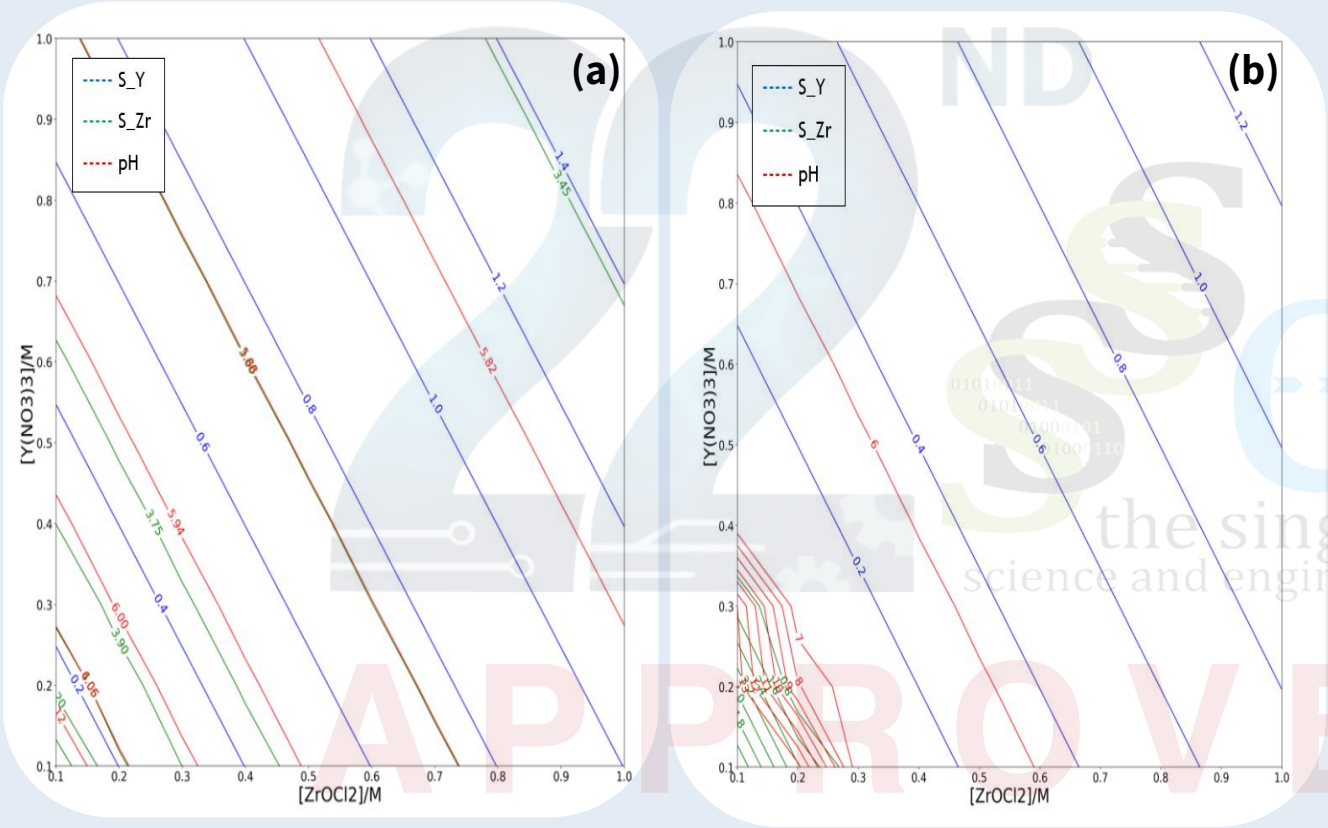


Figure 12: Solubility surface plot for YSZ. Each point is a tuple of ([Zr], [Y]) for (a) [KOH] = 0.1M and (b) [KOH] = 0.5M. [KOH] is adjusted by slider on dashboard, given [KOH]≤0.5M.

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Results: Final Solubility Surface Plots

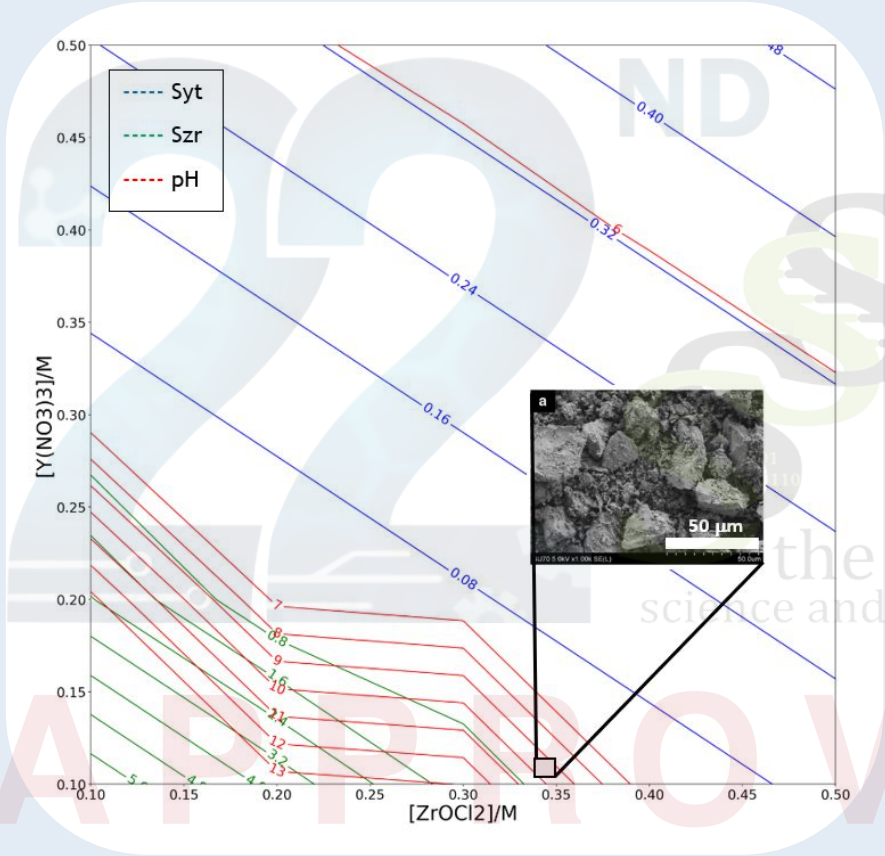


Figure 13: Solubility surface plot for YSZ with SEM Micrograph of 8mol% YSZ powder synthesised by coprecipitation at pH 9-10 (Zarkov et al, 2015) [KOH] =0.5M

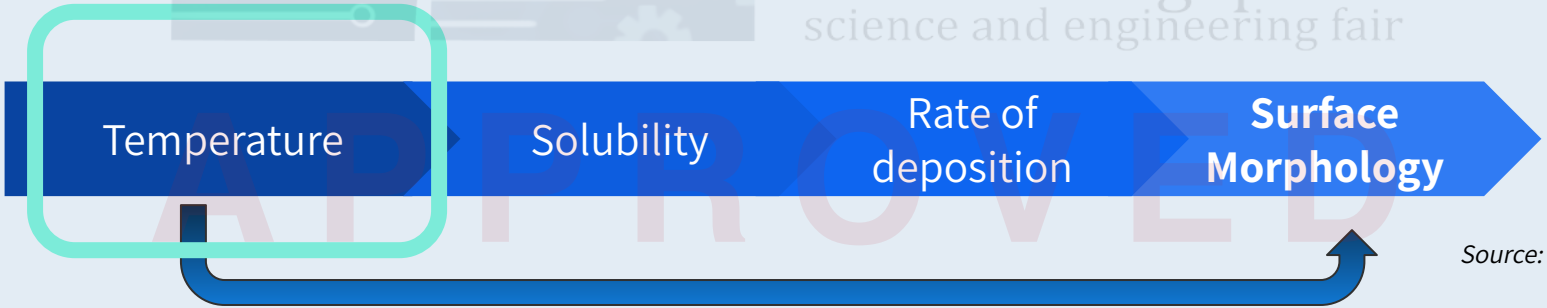
Conclusions & Future Work

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

Future work:

- Validating the model + Making it open-source for other researchers to add their data
- Using YSZ to improve the sensitivity of paper-based diagnostics
- Adding temperature dependence



Source: Self-made

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A. R. Burkin, H. Saricimen, and B. C. H. Steele, “Preparation of Yttria Stabilized Zirconia Powders by High Temperature Hydrolysis,” Trans. J. Br. Ceram. Soc., 79, 105 (1980).

E. P. Stambaugh, J. H. Adair, I. Sekercioglu, and R. R. Wills, “Hydrothermal Method for Producing Stabilized Zirconia,” U.S. Pat. No. 4 619 817, Oct. 28, 1986.

Judge’s Acknowledgement Form

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