Grain Boundary Diffusion of Magnesium into Yttria-Stabilized Zirconia

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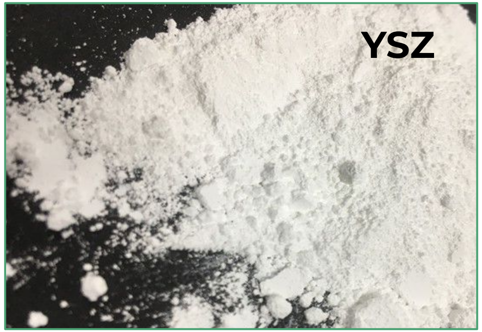
Purpose:

The purpose of this experiment was to see how accurate our calculations were in predicting how much time was needed to completely dissolve MgO into YSZ in a mixed powder solution at constant temperatures.



Approach for Time Calculations:

YSZ: 347.7 g/mol

MgO: 40.304 g/mol , 10 mol %

$$\text{YSZ} = \frac{90(347.7\ \text{g/mol})}{90(347.7\ \text{g/mol})+10(40.304\ \text{g/mol})} \times 100\% = \mathbf{98.7\ w.t.\ \%}$$

YSZ = 98.7 w.t. %
MgO = 1.30 w.t. %

Using Case Four: Transient Infinite Diffusion of a Thin Layer

$$C_i = \frac{N_i}{\sqrt{4\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right)$$

$\frac{N_i}{\sqrt{4\pi Dt}}$ is an approximation, so $C_i = \exp\left(\frac{-x^2}{4Dt}\right)$

$$t = \frac{-x^2}{4D\left(\ln\left|C_i\right|\right)}$$

x = 1µm = 1.0 x 10^{-6} m
$D_{\text{Mg in YSZ at 1500°C}}$ = 1.26 x 10^{-15} m^2/s
$D_{\text{Mg in YSZ at 1600°C.}}$ = 9.00 x 10^{-15} m^2/s
C_i of MgO = 0.013

At 1500°C :

$$t = \frac{(-1.0 \times 10^{-6}\ m)^2}{4(1.26 \times 10^{-15}\ m^2/s)\left(\ln\left|0.13\right|\right)} = \mathbf{45.7\ seconds}$$

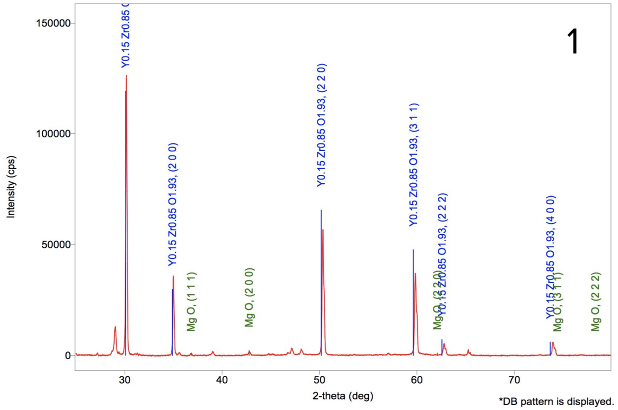
At 1600°C :

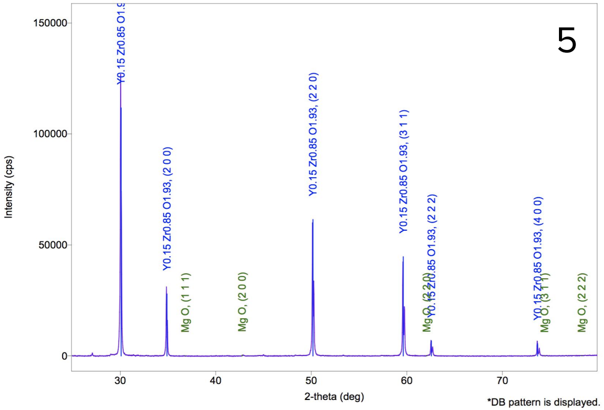
$$t = \frac{(-1.0 \times 10^{-6}\ m)^2}{4(9.00 \times 10^{-15}\ m^2/s)\left(\ln\left|0.13\right|\right)} = \mathbf{6.40\ seconds}$$

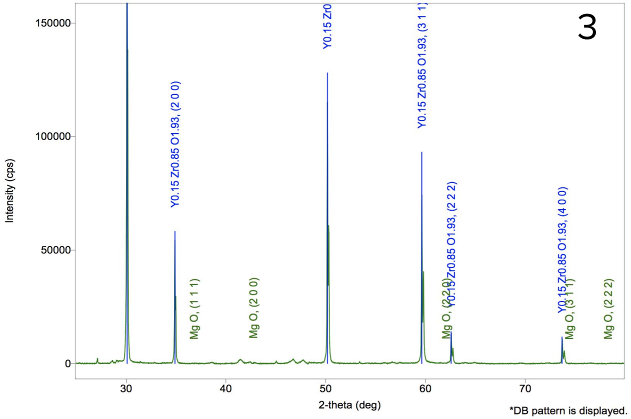
Results for Mixed Powders:

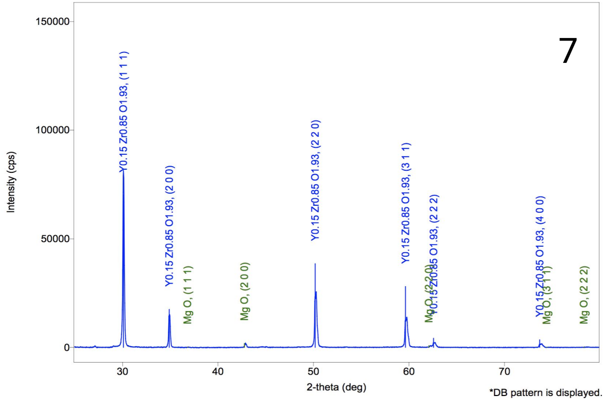
Group:	Temp (°C):	Time (mins):
1	1600	120
3	1600	3
5	1500	120
7	1500	3

Results for Mixed Powders:









Group:	Temp (°C):	Time (mins):
1	1600	120
3	1600	3
5	1500	120
7	1500	3

Reviewing our Calculations:

@ **T = 1500°C**, we predicted that if we held the powders for **45.7 seconds** we would see full dissolution of MgO into YSZ.

@ **T = 1600°C**, we predicted that if we held the powders for **6.40 seconds** we would see full dissolution of MgO into YSZ.

However, the different times that we held the powders **experimentally** were **3 minutes and 120 minutes** rather than the calculated time.

The calculated time frames are **too restrictive on** the capability of **the furnace**. The **smallest amount** of time the allows for **appropriate** heating and cooling was **3 minutes**. And the larger period, 120 minutes, was used to see if a larger window has a drastic effect on the diffusion.

Future Suggestions:

When calculating the time **firsthand**, our group decided to choose **Case 4**, Transient Infinite Diffusion of a Thin Layer.

Yet, **approaching the problem again**, we would instead try to use **Case 6**, Transient Finite (Symmetric) Spherical Diffusion, because there is an assumption of **self-similarity** that refers to **diffusion** proceeding in the **same way** throughout the space:

$$\frac{C}{C_s} = 1 - 2e^{(-Dt\,(\frac{\pi}{R})^2)}$$

$$t = [-\frac{R^2}{\pi^2 D} ln(0.5(1 - \frac{C}{C_s}))]$$

$$D_{1600°C} = 9 * 10^{-11} cm/s^2$$

$$D_{1500°C} = 1.26 * 10^{-11} cm/s^2$$

$$C = 1.3\ wt\%$$

$$C_{s1600°C} = 100\ wt\%$$

$$t_{1500°C} = 56.8\ s$$

$$t_{1600°C} = 7.95\ s$$

Purpose of MgO and YSZ pellet experiments

1. To test theory vs reality
2. To test theory in context

MgO pellet- YSZ pellet diffusion w/ respect to set times and temperatures

Case 4: Time 1&3: 16 hours= 5.76 E4 s/ Time 2&4: 8 hours =2.88E4 s Temp 1&2: 1600 degrees C/ Temp 3&4: 1500 degrees C

D@1600 C= 9.00E-15m^2/s / D@1500 C= 1.26E-15 m^2/s Ni=100 wt% C= 5 at% MgO/ Mg= 0.6 wt%

Position (x)= sqrt(-ln(C*sqrt(4piDt)/Ni)*4Dt)

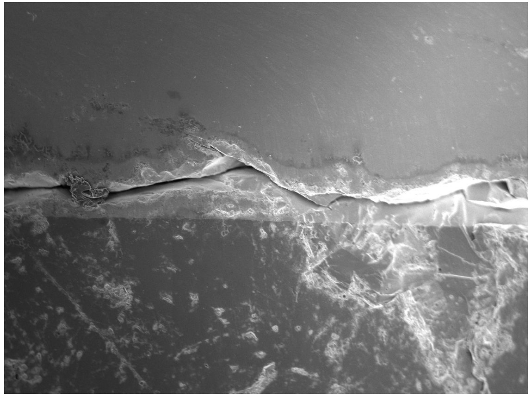
x (case 1)= 1.74E-4 m

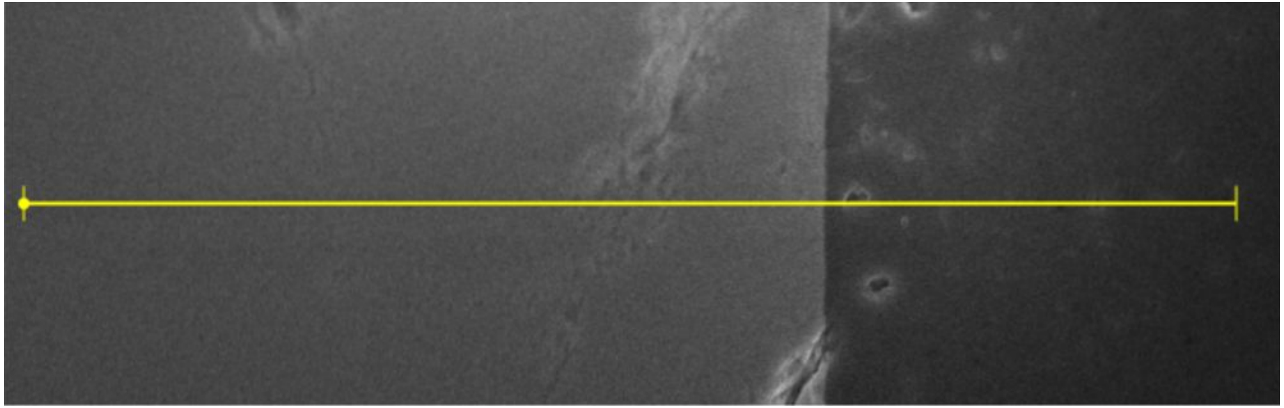
x (case 2)= 1.24E-4 m

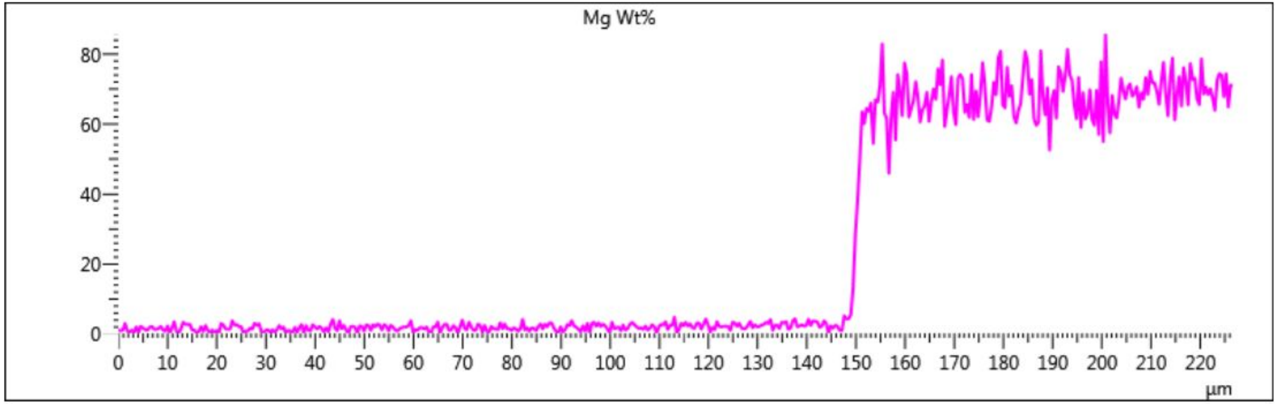
x (case 3)= 6.71E-5 m

x (case 4)= 4.80E-5 m

SEM/EDS Results







Results

~ 15 μm

Results do not match calculations

Future Approaches

Case 2

$C = 0.5C_s + 0.5C_s \text{erf}\,[x/(2(Dt)^{½}]$

$\text{erf}\,[x/(2(Dt)^{½}] = 1 - 2C/C_s = 0.994$

$\text{erf}(z) = 0.994$

$z = 1.95$

$x = 2z(Dt)^{1/2}$

C = 5 at% = 0.604 wt%

C_s = 100 at% = 100 wt%

$D_{1500°C} = 1.26 \times 10^{-11} cm^2/s$

Results

$x_{8h} = 23.5\ \mu m$

$x_{16h} = 33.2\ \mu m$