Enhanced Mechanical Properties in Esthetic Tantalum Gradient Coated Yttria-Stabilized Zirconia for Dental Applications

MSE Undergraduates: Jasmine Brizuela, Nam de Porceri, Steve Ho, Megan Huynh, Scott Kiehn
Advisors: Drs. Chris Hoo, Shen Dillon, David Kisailus, Jae-Won Kim

Goal

Establish a cheaper, frictionless, and more effective dental restoration paradigm in a world where 1/20 experience a traumatic dental injury each year

Figure 1: Tradeoffs Between Popular Commercial Restorations

Customers won't need to navigate the tradeoffs between fracture toughness (K_{1C}), translucency (CR), and cost between restorations (Figure 1), as this project is pioneering a selection maximizing all 3 attributes

How to Achieve this Goal:

Applying a Tantalum (Ta) Functional Gradient Coating (FGC) to monolithic 6mol% Yttria-Stabilized Zirconia (YSZ)

Process of Experiment

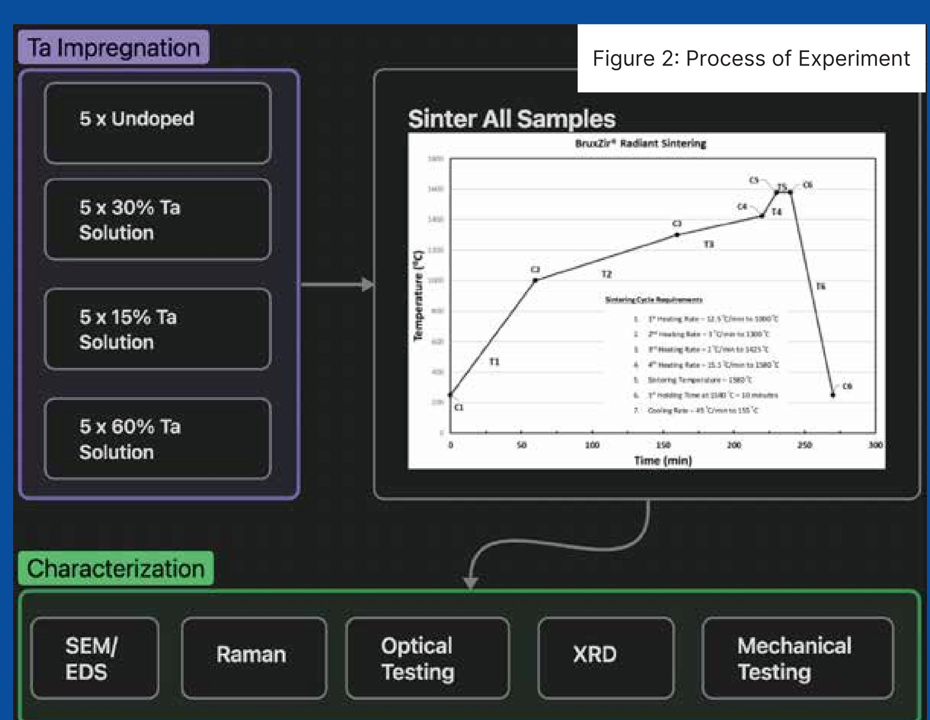


Figure 2: Process of Experiment

Figure 2 Outlines Investigation of [Ta] Influence on Mechanical, Optical, Phase, and Morphological Properties. Ta-YSZ synthesis is Irrelevant to this Experiment

Project Design: Characterization

(Experimental Process Elucidation-the WHY)

Raman + EDS

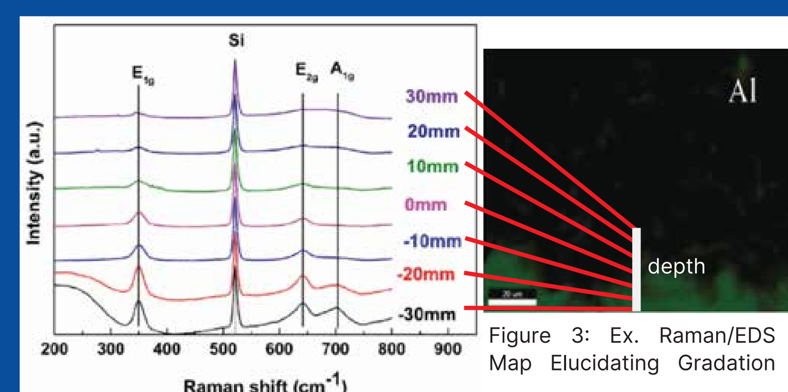


Figure 3: Ex. Raman/EDS Map Elucidating Gradation

Raman and EDS determine Ta's penetration depth and gradation profile in Ta-Doped YSZ cross-section through EDS corroborated Peak Transformation Analysis

Note: EDS Map and Raman Spectra collage aren't sensibly congruent and only serve to epitomize intention

SEM + EDS

SEM and EDS will help ascertain grain size, structure, and composition between Ta rich and poor domains and reveal causal mechanical and optical property differences

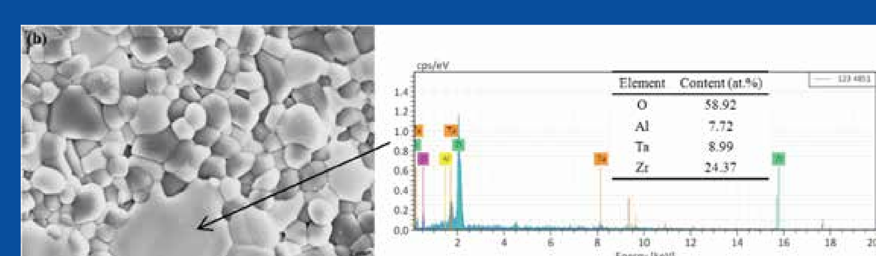


Figure 4: Quantitative EDS Spectra Suggesting Spatially Distinct Ta-Zr-O Phase Precipitation Among Ta_2O_5 Doping

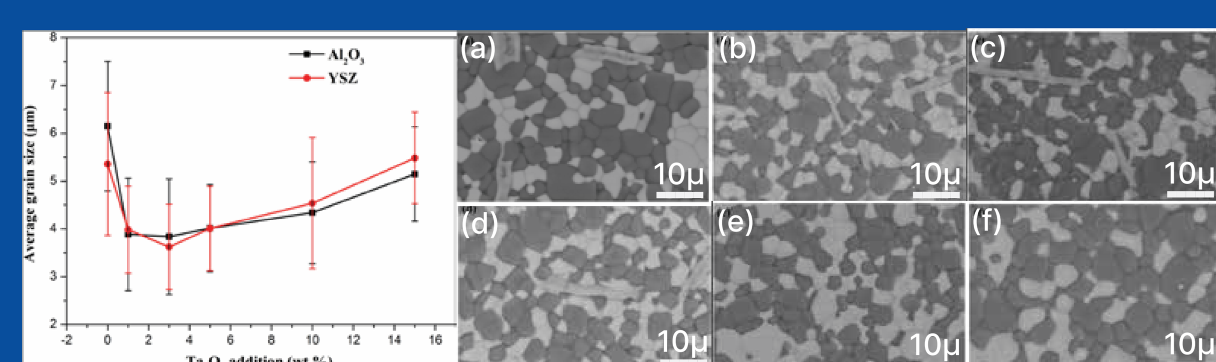


Figure 5: Resultant Ta_2O_5 Addition Effect on YSZ and Al_2O_3 Average Grain Size (left) and Corresponding YSZ Micrographs from Low (a) to High (f) Ta_2O_5 Addition (right) Among 0, 1, 3, 5, 10, and 15wt% Ta_2O_5 Dopant Concentrations

Mechanical Testing

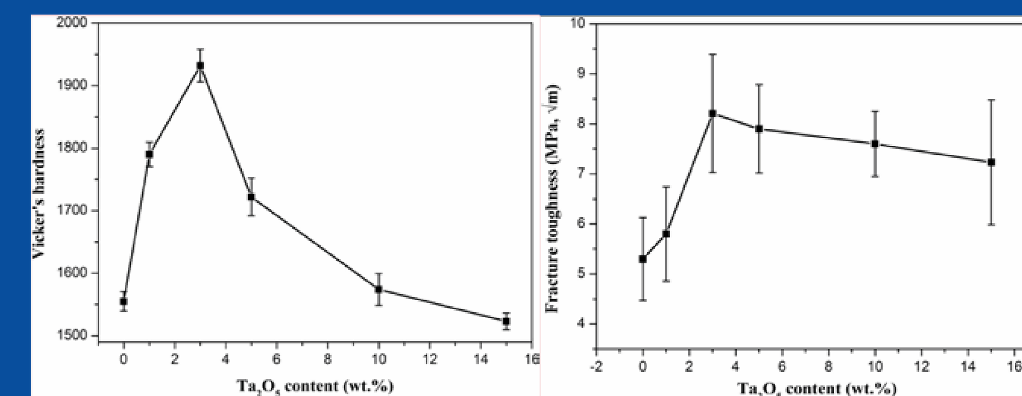


Figure 6: Effect on Vicker's Hardness (left) and Fracture Toughness (right) Among 0, 1, 3, 5, 10, and 15 wt% Ta_2O_5 Dopant Concentrations.

Mechanical Testing quantifies increase in hardness /toughness (microindentation), and (TBD) flexural strength (3-point bending) upon low variable Ta concentration

XRD

XRD illustrates the degree to which YSZ's monoclinic (m), tetragonal (t), and cubic (c) phases transform upon varying Ta dopant concentration, and the resultant phase(s) Ta manifests itself as within YSZ

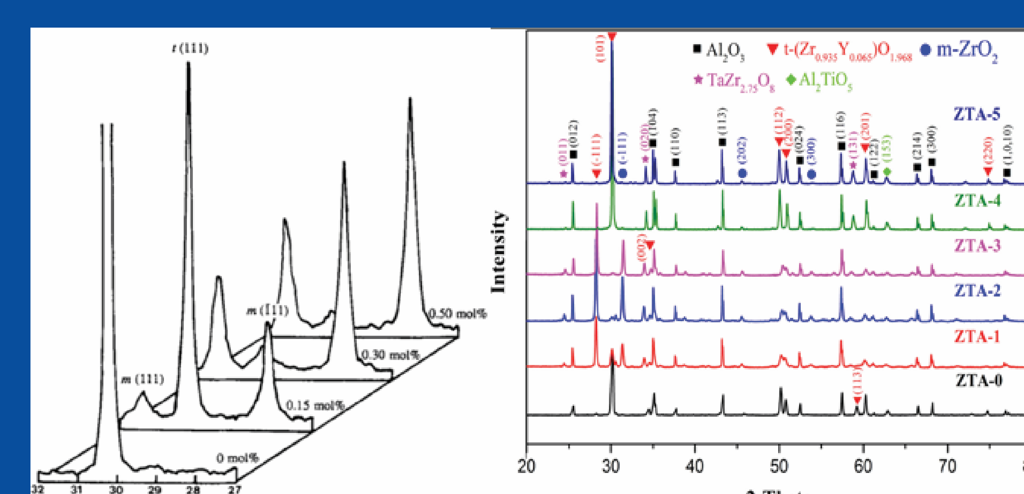


Figure 7: Increasing Ta_2O_5 concentration's inverse effect on tetragonal YSZ phase stability (left), and significant $TaZr_{2.75}O_8$ phase precipitation (right) for YSZ toughened alumina (ZTA) of increasing (ZTA-0 to 5) Ta concentration

Optical Testing

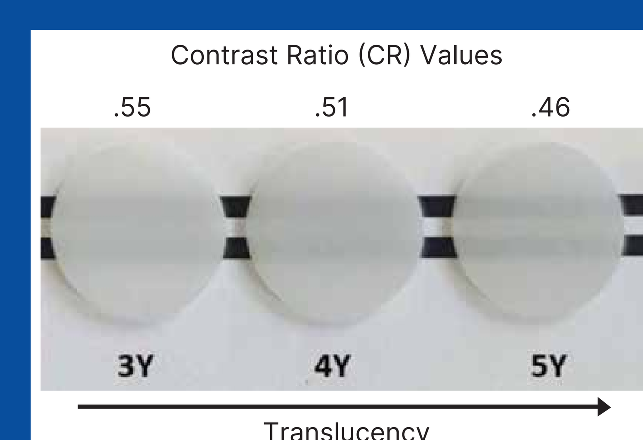


Figure 8: In-line Visual translucency increase (quantified via CR decrease) among augmented yttria concentration (3, 4, 5 mol%) in YSZ

Spectrophotometry of 6mol% YSZ indicates enhanced transparency value of ~ .41 upon linear regression. Ta concentration may increase this value slightly, yet still remain competitive

Project Design: Theory

(Mechanisms and Feasibility-the HOW)

Phases

High concentrations of Yttria (6mol%) stabilize the cubic phase of ZrO_2 at room temperature, enhancing translucency but compromising mechanical properties. Yet, Ta impregnation restores these properties, while maintaining elevated transparency values

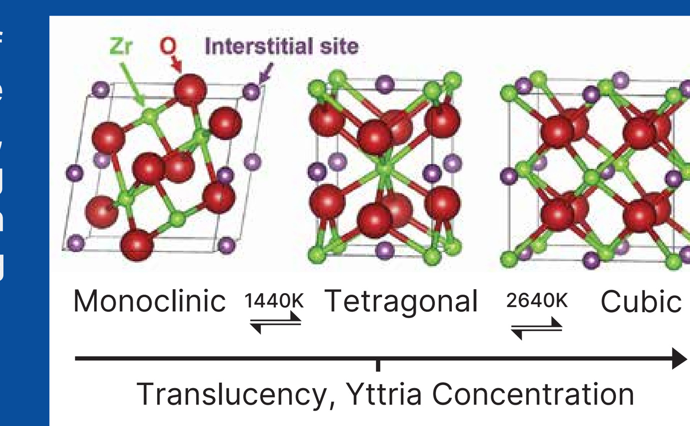


Figure 9: Equilibrium [Y] and Temp. dependent Crystal Structures of Zirconia

Tantalum Impregnation

Ta easily substitutes Zirconium: Similar ionic radius, electronegativity, and valence manifests as the defect behavior shown below in Figure 10

$$2Ta_2O_5 \rightarrow 4Ta_{Zr}^{\bullet} + V_{Zr}^{''''} + 10O_O^X$$

$$Y_2O_3 + Ta_2O_5 \rightarrow [2Y_{Zr}' + 2Ta_{Zr}^{\bullet}] + 8O_O^X$$

Figure 10: Ta Defect Behavior Within YSZ

To balance out the excess charge upon substitution, oxygen vacancies annihilate; oxygen promptly accumulates within the YSZ lattice, decreasing t/c phase stability

Optical Properties

Translucency values increase due to non-birefringent properties special to high yttria concentration induced cubic YSZ grains (Figure 11)

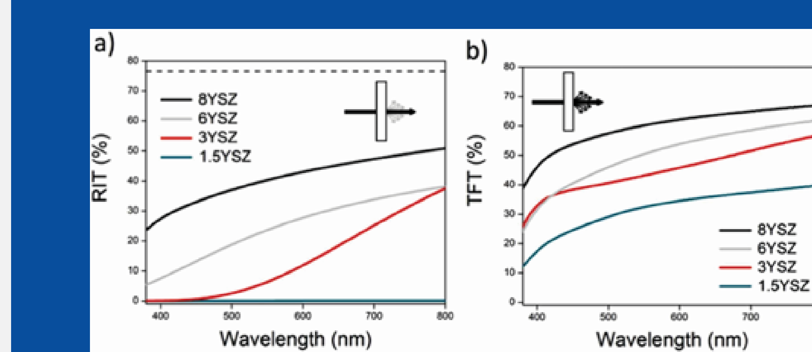


Figure 11: Real In Line (RIT) and Total Forward Transmission (TFT) of 1.5mol% - 8mol% Yttria Concentrations in YSZ, Revealing Translucency Increase

Mech. Properties

Enhanced Ta-YSZ mechanical properties emerge from increased m phase transformation toughening due to decrease in t/c phase stability observed in XRD, and from smaller densified grain structure due to the Hall-Petch effect, and observed via SEM. (Figure 12)

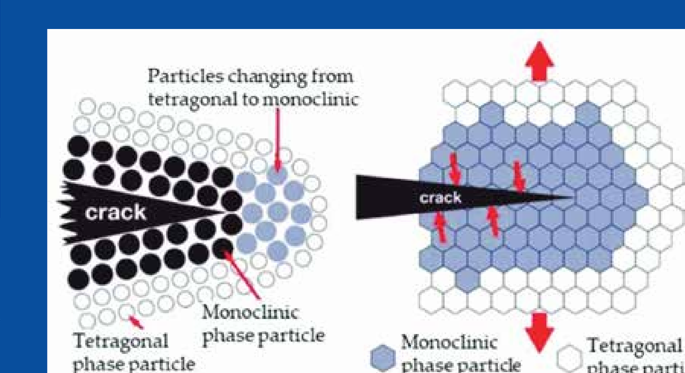
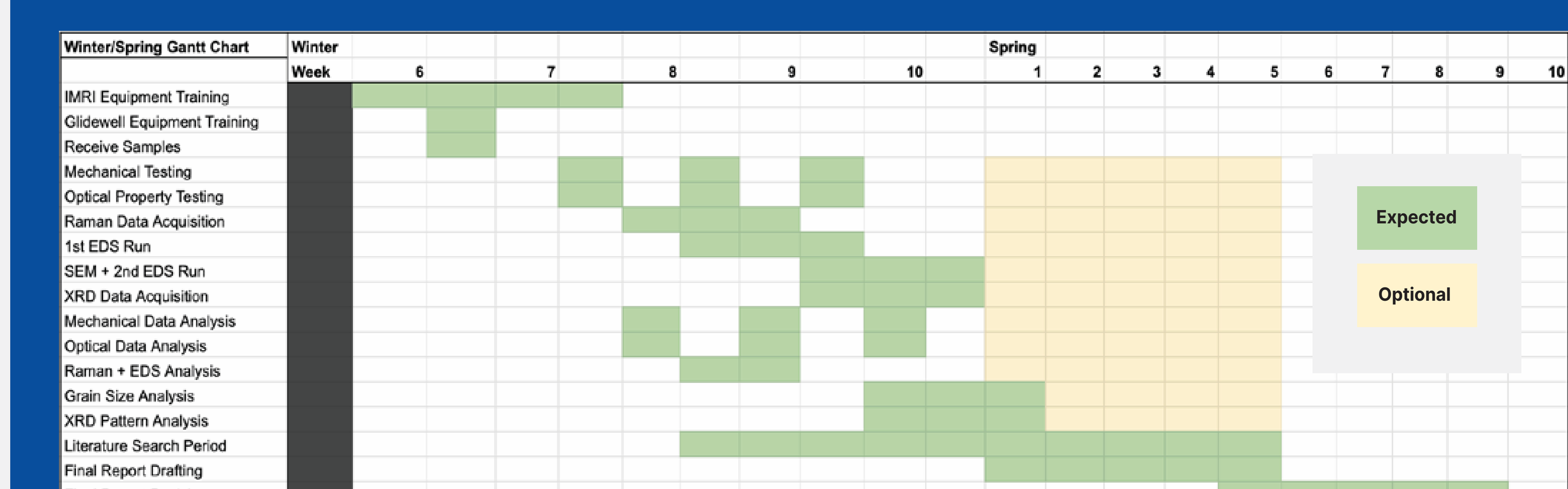


Figure 12: M Phase Transformation Toughening Schematic

Timeline



Roles & Contact

Name	Role	Email
Megan Huynh (MSE)	Team Lead, Mechanical and Optical Testing Lead	mhhuynh1@uci.edu
Steve Ho (MSE)	XRD Lead, SEM/EDS Technician	sjho1@uci.edu
Scott Kiehn (MSE)	SEM/EDS Lead, Raman Spectroscopy Technician, Mechanical Testing Technician	skiehn@uci.edu
Nam de Porceri (MSE)	XRD Technician, Mechanical Testing Technician	ndeporce@uci.edu
Jasmine Brizuela (MSE)	SEM/EDS Technician	jsbrizue@uci.edu
Dr. Jae-Won Kim	Corporate Advisor	JaeWon.Kim@glidewelldental.com

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