#### **UC** Irvine

**SSOE** Research Symposium Dean's Awards

#### Title

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

#### Permalink

https://escholarship.org/uc/item/5jv122z0

#### Authors

Kiehn, Scott Duy Huynh, Megan Hong Ho, Steve Jiaxiang <u>et al.</u>

#### **Publication Date**

2024-03-15

#### **Copyright Information**

This work is made available under the terms of a Creative Commons Attribution License, available at <a href="https://creativecommons.org/licenses/by/4.0/">https://creativecommons.org/licenses/by/4.0/</a>

Peer reviewed

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

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



Customers won't need to navigate the tradeoffs between fracture toughness  $(K_{10})$ , 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 5mol% Yttria-Stabilized Zirconia (YSZ)

# **Process of Experiment**



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

# **Project Design:** Characterization

#### Raman + EDS



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

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 5: Resultant Ta<sub>2</sub>O<sub>5</sub> Addition Effect on YSZ and Al<sub>2</sub>O<sub>3</sub> Average Grain Size (left) and Corresponding YSZ Micrographs from Low (a) to High (f) Ta<sub>2</sub>O<sub>5</sub> Addition (right) Among 0, 1, 3, 5, 10, and 15wt%  $Ta_2O_5$  Dopant Concentrations



(Experimental Process Elucidation—the WHY)

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

#### SEM + EDS

Figure 4: Quantitative Spectra EDS Suggesting Spatially Ta-Zr-O Distinct Phase Precipitation Among Ta<sub>2</sub>O<sub>5</sub> Doping

## **Roles & Contact**

ame	Role	Émail
egan Huynh /ISE)	Team Lead, Mechanical and Optical Testing Lead	mhhuynh1@uci.edu
teve Ho /ISE)	XRD Lead, SEM/EDS Technician	sjho1@uci.edu
cott Kiehn /ISE)	SEM/EDS Lead, Raman Spectroscopy Technician, Mechanical Testing Technician	skiehn@uci.edu
am de Porceri /ISE)	XRD Technician, Mechanical Testing Technician	ndeporce@uci.edu
asmine rizuela (MSE)	SEM/EDS Technician	jsbrizue@uci.edu
r. Jae-Won im	Corporate Advisor	JaeWon.Kim@glidewell dental.com

#### **Mechanical Testing**



Figure 6: Effect on Vicker's Hardness (left) and Fracture Toughness (right) Among 0, 1, 3, 5, 10, and 15 wt% Ta<sub>2</sub>O<sub>5</sub> 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<sub>2</sub>O<sub>5</sub> concentration's inverse effect on tetragonal YSZ phase stability (left), and significant TaZr<sub>2.75</sub>O<sub>8</sub> 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 5mol% YSZ indicates enhanced contrast ratio value of 0.46. Ta concentration may increase this value slightly, yet still remain competitive in industry



# UCI Samueli School of Engineering Gidewell

# **Project Design: Theory**

Phases High concentrations of Yttria (5mol%) stabilize the cubic phase of ZrO<sub>2</sub> at room temperature, enhancing translucency but compromising mechanical properties. Yet, Ta impregnation restores these properties, while maintaining elevated transparency values

## **Tantalum Impregnation**

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

$2Ta_2O_5 \to 4Ta_{Zr} \bullet$	$+ V_{Zr}^{~~} + 100_{0}^{~~X}$	(
$Y_2O_3 + Ta_2O_5 \rightarrow  $	$[2Y_{Zr} + 2Ta_{Zr}]$	$+ 80_0^{X}$

Figure 10: Ta Defect Behavior Within YSZ

# **Optical Properties** — Mech. Properties —

Translucency values increase due to Enhanced Ta-YSZ mechanical non-birefringent properties special to high properties emerge from increased m ytrria concentration induced cubic YSZ phase transformation toughening due



Concentrations in YSZ, Revealing Translucency Increase

Monoclinic 1440K 2640K Translucency, Yttria Concentration Figure 9: Eguilibrium [Y] and Temp. dependent

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

grains (Figure 11) 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

## References

Richards, D. One billion people have experienced a traumatic dental injury (2018). Nature Portfolio.

Mao, F., et al. Combinatorial magnetron sputtering of AgFeO2 thin films with the delafossite structure (2016). Materials & Design

Sathish, M. et al. A critical review on functionally graded coatings: Methods, properties, and challenges (2021). B: Engineering Part

Yudong S., et al. Effect of Ta2O5 addition on the microstructure and mechanical properties of TiO2-added yttria-stabilized zirconia-toughened alumina (ZTA) composites (2018). Ceramics International

Kim, DJ., Tien, TY. Phase Stability and Physical Properties of Cubic and Tetragonal Zr02 in the System Zr02-Y203-Ta205 (1991). Journal of the American Ceramic Society

Roitero Et al. Ultra-fine Yttria-Stabilized Zirconia for dental applications: A step forward in the quest towards strong, translucent and aging resistant dental restorations (2023). Journal of the European Ceramic Society

Zmak, I., et al. Hardness and Indentation Fracture Toughness of Slip Cast Alumina and Alumina-Zirconia Ceramics (2019). Materials

Dong, Y., et al. A computational study of yttria-stabilized zirconia: II. Cation Diffusion. (2016) Acta Materialia.

Akhlaghi, O., et al. Transparent high-strength nanosized yttria stabilized zirconia obtained by pressure-less sintering (2022). Journal of the European Ceramic Society Glidewell Dental