Optimizing Thermal Barrier Coating Performance Through Substrate Texturing

Waste Management at White Mesa Hill

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On my honor as a University student, I have neither given nor received unauthorized aid on this assignment as defined by the Honor Guidelines for Thesis-Related Assignments.

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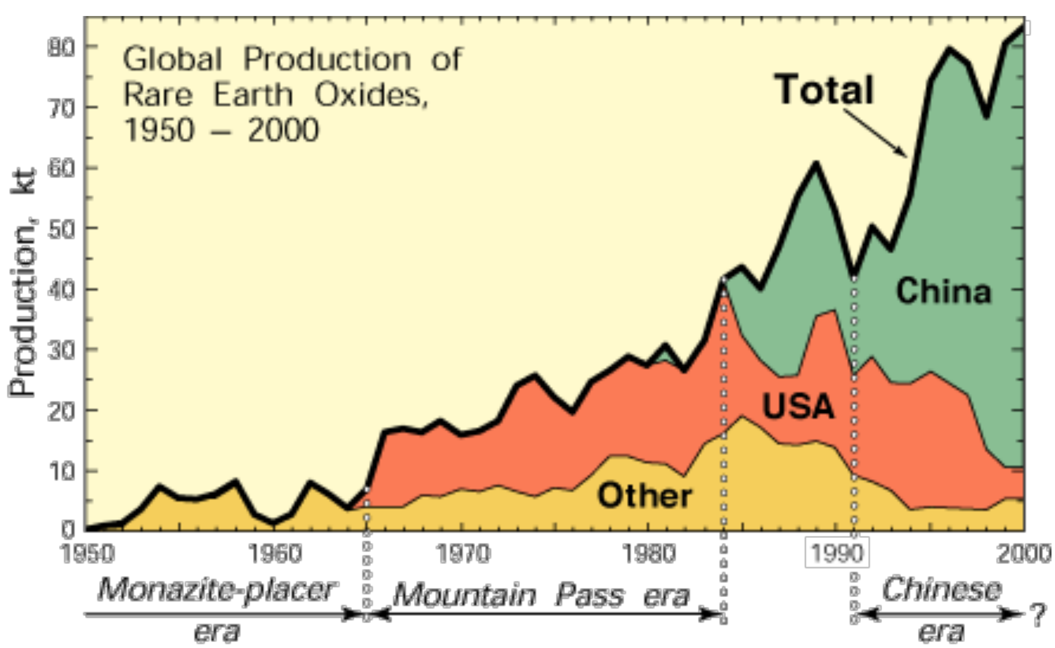
Introduction

In order to keep planes in the air the turbines have to be able to produce massive amounts of energy, as a result the hottest chambers reach temperatures north of 1800 °C. It is important to note that the metals these chambers are made of have melting points in the range of 1400 °C. So, how is it that these turbines haven't melted? That would be thanks to the thermal barrier coatings (TBC's) that are acting as a buffer between the blistering hot air and the metal substrate. Thanks to their thermally insulating properties they are able to deflect the heat. Along with active cooling channels, this prevents the degradation of the structural metal components and allow planes to fly at faster speeds with higher efficiencies.

As the coatings heat up there is a certain amount of thermal expansion that occurs. Since these TBC's are generally made up of various layers of materials, vertical cracks must be engineered into the coating in order to accommodate the varying rates of thermal expansion. These cracks can be introduced to the desired density and locations by processing the metal substrate and creating a surface texture. These peaks and valleys will then be reflected in the coating. After the coating the material can be processed again via heat treatments which will result in the vertical cracking occurring due to stress concentrations at these peaks/valleys. For the technical project, I will be investigating and designing a substrate topography that allows for the optimization of the TBC's adhesion and thermal properties.

The industry standard TBC is Yttria-Stabilized Zirconia (YSZ). This coating is made by having a system that combines the two components zirconia (ZrO2) and yttria (Y2O3). The material is mostly made up of zirconia thanks to its highly desired thermal properties. However, the presence of yttria is crucial to the performance of this material due to the fact that zirconia is not stable at room temperature (Kulyk et al., 2022). Left to its own devices it would undergo a phase change at lower temperatures which would result in a failed coating. The presence of yttrium dioxide prevents this phase change from occurring at lower temperatures, allowing for the coatings to function throughout the temperature cycles that a plane turbine would expect in its lifetime.

Yttrium is one of the 17 rare earth elements. Thanks to their atomic configuration the rare earth elements are prized for their ability to produce strong magnetic materials. These magnetic materials are crucial to many marketplaces around the world – most notably defense, renewable energy, and electronics. (American Geosciences Institute. n.d.). Rare earth elements naturally occur in oxidized states and almost without fail in the company of the other rare earth elements. In order to refine these materials strong acids are used and several toxic waste products are left behind; including lead, uranium and thorium (Reed, 2023). Due to the environmental and toxicological hazards much of the refinement and production has been outsourced and the final products imported. Below is a chart depicting the evolution of REE production from 1950-2000 (Sierra Club, 2024).



As seen in figure above there was an era where rare earth elements were mined and refined domestically at a mine called “Mountain Pass Rare Earth Mine.” The sharp decline seen after the 1990’s is a result of a leak from a wastewater pipeline (Cone, 1997). In paying for the spills clean up, fees for failing to report the spill, and financial pressures to find a new waste management process the company running the mine ended up filing for bankruptcy. With this they left behind 17,750 tons of lead sludge that had yet to be treated. In this paper the life story of the lead sludge will be analyzed using the actor network theory framework. It starts at the Mountain Pass mine, travels to White Mesa Hill where it is refined, and finally to its resting place in a containment pond where residual affects are being noticed by the nearby inhabitants.

This paper will analyze the optimization of thermal barrier coatings that utilize rare earth elements to enhance performance in high-temperature applications. Additionally, utilizing actor-network theory it will examine the socio-technical relationship of domestically mining REEs. An emphasis will be placed on the impact it’s had on the communities within the vicinity of processing sites and transport routes.

Optimizing Thermal Barrier Coating Performance Through Substrate Texturing

High temperature material systems often require TBCs with low thermal conductivity to protect components from heat damage via insulation. These TBCs are generally composed of a ceramic, such as yttria-stabilized-zirconia, and deposited onto a substrate with an intermediate ‘bond coat’ to ensure proper adhesion. Since the TBC and the substrate have different coefficients of thermal expansions (CTE), high temperatures and thermal cycling experienced in service creates strain and stress concentrations that can lead to loss of adhesion, oxidation, cracking and failure of the TBC. Once this occurs the bare substrate is exposed to environments in which it is unsuited for, and in the case of turbine engines this can lead to catastrophic failures.

During service the TBC protects the substrate by acting as an insulating mechanism. As such, the highest temperatures are experienced at the surface and decrease the further into the material you go. This temperature gradient is reflected with the thermal expansion since it is directly proportional to the change in temperature. This thermal expansion creates a varied amount of thermal strain within the material. In similar materials the strain is a continuous gradient as a function of temperature. However, at the interfaces of dissimilar materials with different CTEs the amount of strain is no longer continuous but rather a discontinuous gradient, this acts to concentrate the stresses since both materials are bonded and attempting to strain a different amount.

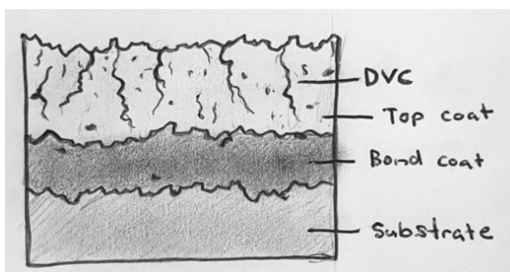


***Figure 1**: Dense Vertical Cracks (DVCs) as seen in a Thermal Barrier Coating System*

Introducing dense vertical cracking (DVC) is one method to improve strain tolerance from CTE mismatch. In this method, vertical cracks form in the TBC during the spray process, or through use due to stress concentrating mechanisms. This will allow the TBC to better expand and contract along with the substrate without losing its adhesion despite their difference in thermal expansion (Chen, Dambra, & Dorfman, 2020). As the substrate expands more than the TBC, the vertical cracks in the TBC will decrease the stress in the TBC by allowing for the upper portion of the TBC to horizontally expand more easily. This form of cracking makes it easier for the coating to tolerate the mismatch of CTE's without sacrificing coating density. This will also help to prevent delamination and buckling of the TBC from the substrate. By controlling the parameters of the spraying procedure, air plasma spraying at close distances can produce stress concentrators that can then induce DVC. However, this method is not conducive to spraying onto engine components with complex geometries. As such, our team has been tasked to induce vertical cracking within the TBC by adjusting the system outside of spray parameters.

The approach our team will be taking is rather than using the spraying parameters to induce the DVC, we will create textures on the bond coat using ultra-short pulse lasers. Ultra-short pulse (USP) lasers are at the cutting edge of laser machining. The laser is pulsed using an electronic shutter with a period that is on the order of femtoseconds (Žemaitis, 2020). Due to this very short emission period, thermal effects of this processing method surrounding the laser focal point are minimal, yielding an effectively "heat-free" process. Compared to other lasering methods, such as Long Pulse Lasering (~100ns pulse duration), USP lasering minimizes microcracks, recast layers, and splash (Tang, 2022).

There are many variables to adjust for texture production; scan speed, laser power, pattern, spacing, height, width, etc. Therefore, the experimental process will be split into two phases. The first phase will focus on optimizing the patterning of the substrate, informed by finite element analysis models. We plan on testing roughly four textures and testing them in conjunction with an untextured control sample. Once we determine which texture performs the best, we will then begin a second round of more detailed testing. This will involve varying specific parameters of our chosen geometry, such as spacing, thickness, or depth, to further optimize TBC performance. This performance will be characterized by the effect of thermal tests on oxidation, crack propagation, and the adhesion of the coating.

Waste Management at White Mesa Hill

In order to process a single ton of rare earth elements it is estimated that almost 2000 tons of waste are produced (13kg of dust, 9,600-12,000 cubic meters of waste gas, 75 cubic meters of wastewater, and one ton of radioactive residue) (Nayar, 2021). Using the Mountain Pass Rare Earth Mine as a case study, the aim is to discover how the waste is managed and how it affects surrounding communities. Throughout this waste management process there are a lot of actors that need to be factored in. The most impactful actors are the regulating committees, the refining processors, the waste treatment facilities, and the neighboring communities. These neighboring communities are at constant risk due to their proximity to the transportation, processing and storage of the hazardous waste.

When it became apparent that the mine at Mountain Pass was going to be shutting down, an urgency was placed on determining how to process the 17,750 tons of lead sludge that had accumulated in their holding pools. The lead sludge was known as a "characteristic hazardous waste" under the regulations of the Resource Conservation and Recovery Act (RCRA). However, thanks to the high concentration of uranium in the lead sludge White Mesa Mill was able to justify reclassifying it as "source material," placing it under the Nuclear Regulations Comissions supervision and allowing them to transport and process it (The Grand Canyon Trust, 2000).

The practice of accepting alternative feed sources arose from the diminishing price of uranium making the ore processing less economically viable. It is cheaper for polluters, such as the mine, to send their radioactive waste to the mill rather than the proper waste processing facilities. In this model the mill is able to produce the uranium while also collecting fees in exchange for processing/discarding the alternative feeds. Once processed by the mill, the discarded waste is placed into holding pools, from this arises the concern of mixing various alternative feeds together. The chemical reactions that take place within these holding pools can result in toxic fumes, degradation to the pool liners, and the formation of even more hazardous compounds. The ground pools pose great threats to the environment via leakage into ground water systems and the dispersion of fumes.

In order to analyze this problem, the network of relationships between the hazardous waste, environment, regulation committees, waste handlers and surrounding communities will be considered. Hazardous waste is a byproduct of the nuclear economy and desires for advanced technologies. The regulation committees are tasked with weighing the value of surrounding communities, the safety of the country, and worldwide economic factors in order to form their policies. The environment is afflicted by waste processing residues and potential leakage failures, which in turn threaten to harm the neighboring communities. This network has many complicated implications and relationships that will be weighed through further investigation.

In the coming semester, research will be conducted to investigate the relationship past and present between the network of actors mentioned above. The data will be compiled from various reports, regulation policies, testimonies, news articles, and financial statements. The evidence will be put out as independent artifacts before being cross analyzed to determine which actors influenced certain outcomes. In doing so, the network interrelating these various artifacts will expose the intricate relationship holding them together.

Conclusion

Through this semester I will research and deliver an optimized laser processed geometry that improves the thermal cycling and adhesion of thermal barrier coatings. In order to test this, we will design various patterns to be produced with assistance from CCAM and PulseTex and their facilities. We will then receive the samples and conduct various tests to determine which design works best. his development will improve the ability to tailor the properties and performance of thermal barriers on complex geometries such as in turbine engines.

For the STS portion I will utilize the actor network theory to research how the various acting parties in this web of waste management interplay and affect each other. I'm especially curious to analyze the relationship between regulators, businesses and market demands. Additionally, I will look into the responses to concerns posed by the nearby Navajo Nation inhabitants. With this I will be able to build a portion of the complex network that revolves around the mining of crucial elements for many technological developments.

References

American Geosciences Institute. (n.d.). What are rare earth elements and why are they important? Retrieved October 10, 2024, from https://www.americangeosciences.org/critical-issues/faq/what-are-rare-earth-elements-and-why-are-they-important

Chen, D., Dambra, C., & Dorfman, M. (2020). Process and properties of dense and porous vertically-cracked yttria stabilized zirconia thermal barrier coatings. *Surface and Coatings Technology, 404,* 126467. https://doi.org/10.1016/j.surfcoat.2020.126467

Cone, M. (1997, April 24).Desert Lands Contaminated by Toxic Spills. Los Angeles Times. https://www.latimes.com/archives/la-xpm-1997-04-24-mn-51903-story.html

Grand Canyon Trust. (2000, December 19*). Mountain Pass Mine - Redefining Characteristic Hazardous Waste to Ship it to White Mesa. ArcGIS Online*. https://storymaps.arcgis.com /stories/e3fc81532d94456dbafbff151f2d3851

Grand Canyon Trust. (n.d.). *White Mesa Uranium Mill*. Retrieved November 8, 2024, from https://www.grandcanyontrust.org/white-mesa-uranium-mill

Kulyk, V., Duriagina, Z., Kostryzhev, A., Vasyliv, B., Vavrukh, V., & Marenych, O. (2022). The Effect of Yttria Content on Microstructure, Strength, and Fracture Behavior of Yttria-Stabilized Zirconia. *Materials (Basel, Switzerland)*, *15*(15), 5212. https://doi.org/10.3390/ma15155212

Nayar, J. (2021, August 12). Not so "green" technology: The complicated legacy of rare earth mining. Harvard International Review. https://hir.harvard.edu/not-so-green-technology-the-complicated-legacy-of-rare-earth-mining/

Reed, J. (2023, September 26). *A once-shuttered California mine is trying to transform the rare earth industry. Grist*. https://grist.org/energy/a-once-shuttered-california-mine-is-trying-to-transform-the-rare-earth-industry/

Rim, K. T., Koo, K. H., & Park, J. S. (2013). Toxicological evaluations of rare earths and their health impacts to workers: a literature review. *Safety and health at work*, *4*(1), 12–26. https://doi.org/10.5491/SHAW.2013.4.1.12

Sierra Club. (2024, March). *Critical Minerals and Rare Earth Elements*. https://www.sierraclub.org/minnesota/blog/2024/03/critical-minerals-rare-earth-elements

Tang, S., Wang, C., Hua, C., Yang, L., Wu, Y., Sun, X., Song, P., & Huang, B. (2022). Surface texture of substrates prepared by femtosecond laser for improving the thermal cycle life of TBCs. *Ceramics International, 48*(4), 5775–5786. https://doi.org/10.1016/j.ceramint.2021.11.125

Žemaitis, A., Gečys, P., Račiukaitis, G., & Gedvilas, M. (2020). Efficient ablation by ultra-short pulse lasers. *Procedia CIRP, 94*, 962–965. https://doi.org/10.1016/j.procir.2020.09.083