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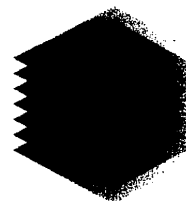
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# Simulations Mapping Stress Evolution in High Temperature Ceramic Coatings under Thermal-Mechanical Conditions

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Finite element simulations representing thermal barrier coatings on turbine blades enabled mapping of the stress evolution within the multi-layer configuration under thermal-mechanical conditions. The study aims to accurately model the transient strain behavior throughout a load cycle due to plasticity, creep, and oxide growth. The results were compared with *in-situ* experimental quantitative measurements performed previously using synchrotron X-ray diffraction. The studies verify the stress within the thermally grown oxide for critical combinations of temperature and load. These numerical models can be used to predict in-cycle stresses that lead to eventual failure of the coatings.

## I. Introduction

THERMAL barrier coatings (TBC) have been of interest to the aerospace industry for application on turbines since the 1950s, and became widely used in the 1980s after the development of the now industry standard Yttria Stabilized Zirconia (YSZ). The low thermal conductivity of these coatings allows them to adequately protect the blade substrate from high operating temperatures, which can be in excess of 1000°C. However, at high temperatures the multilayer nature of the applied coating can lead to crack propagation and delamination due to the mismatch of thermal expansion coefficients and the induced thermal gradients. Through various studies, failure in TBCs is observed to originate from the stress experienced at the interface between the inter-metallic bond coat and thermally grown oxide (TGO) layer. The TGO layer developed is the intermediate layer in the system that grows between the substrate and the topcoat with thermal cycling and the resulting oxidation. TGO stress is associated with eventual failure of the system, and as such these stresses are to be examined in the model. Under loading, the TBC fails due to a number of factors. These include TGO growth, interfacial roughness<sup>1</sup>, creep in the system, complex loading<sup>2</sup>, and thermal expansion mismatch of each layer of the TBC system<sup>3,1</sup>.

Modeling of the material behavior under thermal-mechanical cycling is essential to investigating both the stress propagation and damage effects. Numerous studies have been done on modeling crack propagation and delamination of the TBC coatings under various thermal and mechanical fatigue conditions<sup>4,5,6,7</sup>. It has been found that the failure of the coating system often occurs, resulting from the high stresses developed in and around the TGO-Bond Coat interface. These conditions cause rumpling of the rigid TGO layer creating significant localized stresses, which cause crack initiation and propagation<sup>8</sup>. Work has been done by researchers to obtain closed-form solutions of thermal residual stress field under the effects of non-linear coupled temperature gradient effects, TGO growth, and elastoplasticity deformation during thermal cycling<sup>9</sup>.

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<sup>2</sup> Physicist, Argonne National Laboratory.

<sup>3</sup> Senior Scientist, sendilr@i-a-i.com.

While there has been significant experimental research done in the after cycling fatigue effects, validated predictions of the stress evolution throughout the thermal-mechanical cycle are limited. To meet the challenges of studying turbine blades under operating conditions, thermal and mechanical loads have been applied to samples to simulate the in-cycle conditions, while allowing *in-situ* measurements using X-ray diffraction in our recent work<sup>10</sup>. These high-resolution strain measurements are then used to validate nonlinear material behavior, which causes stress relaxation throughout a cycle.

Finite element models, which include creep and TGO growth, were developed to show the transient strain evolution of the TBC layers while being raised to and held at high temperature. Different creep models are tested for the bond coat and TGO layers to compare the stress relaxation realized from the experimental results. A validated model of the in-cycle strain behavior allows for the creation of models predicting TGO failure under cyclic loads. For models simulating cyclic loading conditions, swelling behavior is included in the element material models to represent growth of the TGO layer. This study will show the stress progression throughout a high-cycle life span of a coated turbine blade.

## II. Experimental

Parameters for the numerical simulation were based on experimental studies of Electron Beam Physical Vapor Deposition (EB-PVD) coated nickel-based super-alloy substrate samples which have been subjected to thermal-mechanical load cycles and monitored in-cycle *via* synchrotron x-ray diffraction strain measurements. Simulating the fatigue analysis of the coatings, the samples were pre-cycled to various stages of a TBC life cycle. Three samples were manufactured for as-coated, 50 cycles, and 200 cycles. These samples, with dimensions shown in Figure 1, were subjected to a load cycle representative of that experienced by a turbine blade.

Three tensile mechanical stresses of 16, 32, and 64 MPa, were applied throughout separate thermal cycles to simulate the centrifugal loads on turbine blades. For each test, the samples were subject to uniform heating to a temperature of 1120 °C. The samples were then held at high temperature for duration of one hour. Strain measurements were collected for each layer at the data collection points shown in Figure 2.

The tensile specimens, shown in Figure 1, were used to allow for *in-situ* strain measurements in the layered profile. The applied thermal loading cycle is shown in Figure 3. The high energy beam of 86 keV was oriented as shown in Figure 2 while moving the sample laterally for the depth-resolved layer measurements as shown in Figure 4. The X-ray images were taken with a 2D CCD and analyzed for strain development across each layer while paying particular attention the strain evolution in the TGO region. Further detail on the experimental setup is described by Diaz *et al*<sup>11</sup>.

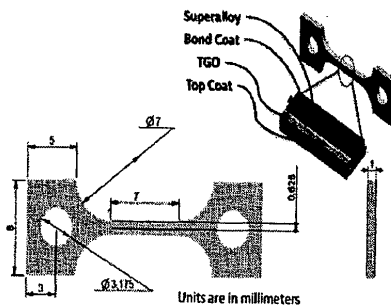


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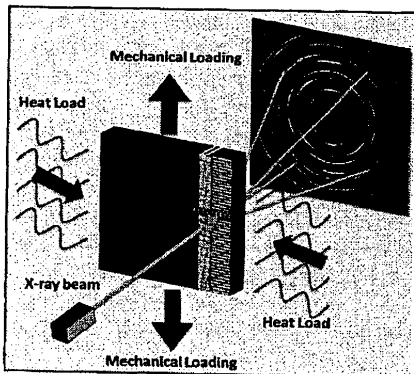
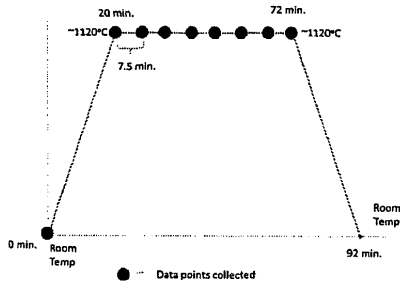


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**Figure 3. In-Situ Load Cycle Data Collection**

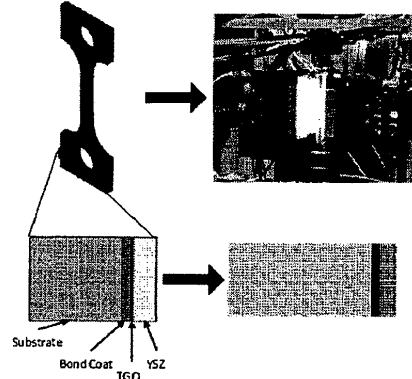
the variation of the stress-free temperatures between layers, the entire model was assumed to have a stress-free temperature of 1000°C.

The substrate, bond coat, TGO, and top coat, were modeled at 1 mm, 50 μm, 0.5 μm, and 125 μm, respectively. It was assumed that the substrate would be large enough relative to the other layers, particularly the TGO, since it was of greatest importance. The TGO layer was set to 0.5 μm in order to represent the as-coated stages of TGO growth in the TBC sample. The material properties were kept consistent with the work of Hernandez *et al*<sup>6</sup> based on the similarity of the properties to the experimental setup. The temperature dependent material properties are shown in Table 1.

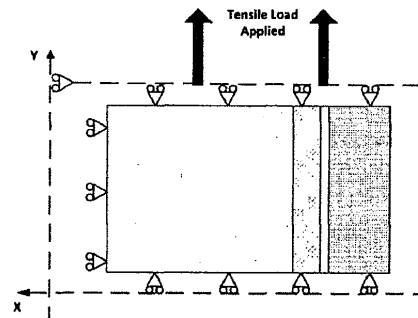
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stress-free temperatures are assigned to each material. While further investigation is being done into



**Figure 4. Specimen Coating Model**



**Figure 5. Boundary Conditions**

**Table 1. Temperature Dependent Material Properties**

	Substrate		Bond Coat		TGO		YSZ	
	RT	HT	RT	HT	RT	HT	RT	HT
Elastic Modulus, E [Gpa]	215	148	140	70	360	340	13	16
Poisson Ratio, ν	0.3	0.3	0.322	0.351	0.24	0.24	0.22	0.28
Coefficient of Thermal Expansion, CTE [ $10^{-6}$ 1/K]	11.5	18.8	8.6	16.6	6.0	8.7	9.0	11.5
Thermal Conductivity, λ [W/mK]	15	30	8.7	27.5	23	5	1.88	1.60
Density, ρ [ $g/cm^3$ ]	7.75	7.29	7.80	7.43	4.00	4.00	5.00	4.84
Heat Capacity, $C_p$ [J/kgK]	400	580	390	700	769	1261	500	630

$$\dot{\epsilon} = C1\sigma^{C2}\exp\left(-\frac{C3}{T}\right) \quad (1)$$

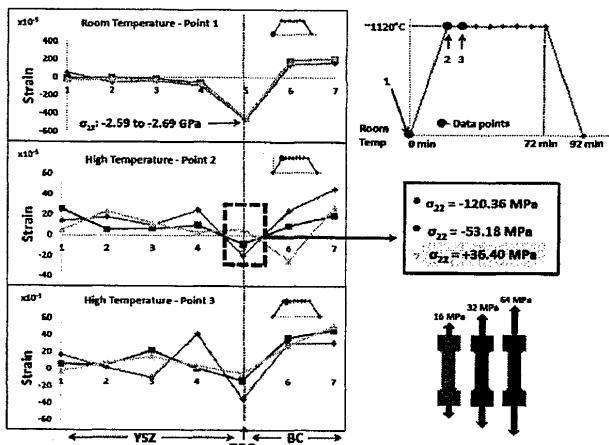
**Table 2. Creep Constants**

	C1	C2	C3
TGO	1.08e-10	2.3	51,000
Bond Coat	8.96e-15	3.0	35,840

#### IV. Results

With the model assumptions that each layer is perfectly planar with minimal roughness, only the in-plane stresses and strains are comparable between the model and experimental results. Shown below in Figure 6 from Diaz *et al.*<sup>14</sup> are the in-plane strains resulting from the XRD analysis. The strain profile across the depth of the layers is shown for each mechanical load at the first three data collection points of the cycle. This confirms from

previous studies the highly compressive nature of the TGO layer at room temperature<sup>7</sup>. The first high temperature plot shown demonstrates how the TGO becomes tensile when subjected to a 64 MPa tensile load. The stress becomes increasingly compressive when held constant at high temperature bringing the TGO back into the compressive region. This transient stress phenomenon is further demonstrated in Figure 7, which displays the TGO in-plane transient stress. Using various creep models, this effect is validated and is a main topic of investigation for single cycle modeling.

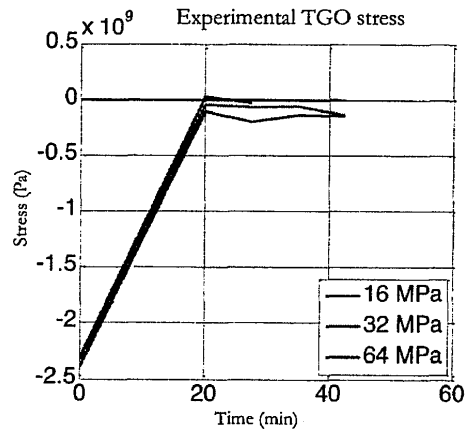


**Figure 6. Experimental In-Plane Strain (Figure from [14])**

are used for comparison due to their very high stresses relative to the other layers. Table 3 below shows the comparison of the finite element results to that of the XRD results.

Figures 8 and 9 then show the transient stress results for both the bond coat and TGO, respectively, throughout the beginning duration of the load cycle. This shows the nonlinear transient behavior of both layers, including a corresponding stress relaxation of the TGO layer. This is largely due to the creep strain experienced in both layers, which is shown in Figures 10 and 11 for the bond coat and TGO respectively.

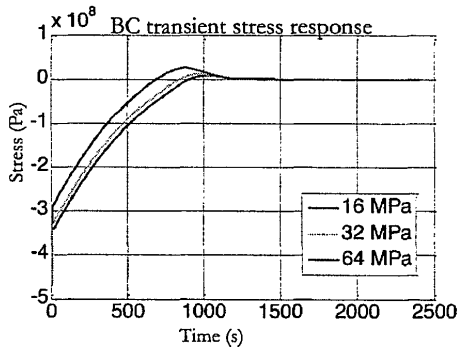
The residual stresses are then used as a form of validation for the finite element model. The TGO stresses, in particular,



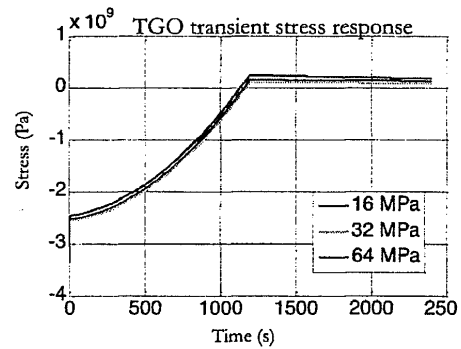
**Figure 7. Experimental TGO In-Plane Transient Stress**

**Table 3 – TGO Residual Stress Comparison**

	FEA (GPa)	Experimental (GPa)
16 MPa	-2.41	-2.39
32 MPa	-2.36	-2.33
64 MPa	-2.25	-2.30

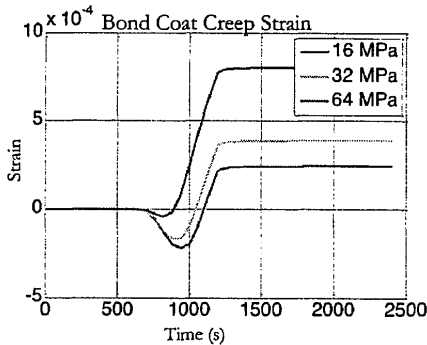


**Figure 8. Bond Coat In-Plane Stress**

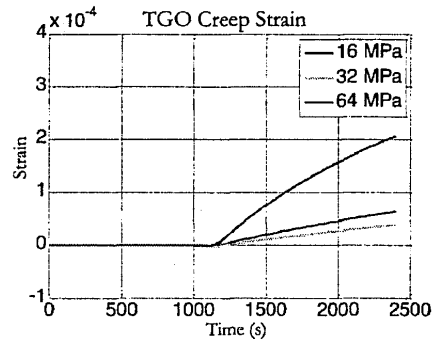


**Figure 9 – TGO In-Plane Stress**

After accurately modeling the material behavior throughout a cycle, the low cycle fatigue effects are then analyzed. The previous load cycle will be replicated for 20 consecutive cycles and higher and the stress progression measured over time. These results will be used to validate the TGO growth stress models with the synchrotron strain measurements of the cycled specimens.



**Figure 10. Bond Coat In-Plane Creep Strain**



**Figure 11. TGO In-Plane Creep Strain**

## V. Conclusion

Results are analyzed and used to develop accurate material models of the coating system, which experiences non-linear behavior such as large temperature variation, creep, and oxide growth. In-situ strain measurements were obtained for various in-cycle loading condition representative of an in-flight load cycle. This has shown that the TGO becomes tensile at operating temperature when exhibiting a 64 MPa tensile load. This tensile condition then relaxes into the compressive region while held at constant high temperature. Finite element models were created and used to compare various nonlinear material models in achieving the stress relaxation realized experimentally. The validated model of this behavior is a significant step towards understanding how the stresses in the interface between layers progress through fatigue cycling. Using these models, simulations can be conducted for stress mapping and crack growth and propagation of fatigued coating systems, which are ultimately used to extend turbine blade life and coating efficiency.

## Acknowledgments

The authors would like to acknowledge Dr. Charles D. Norton, NASA JPL, NASA STTR contract# NNX10CB63C for supporting this research. Experimental studies were supported by the National Science Foundation under Grant No. 1125696. Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

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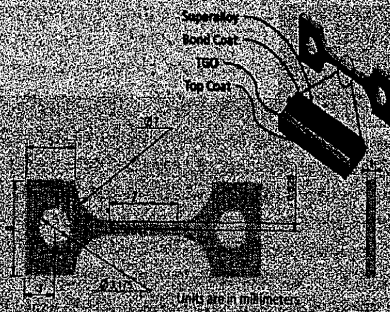


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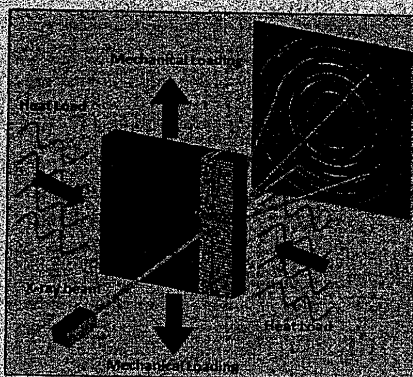
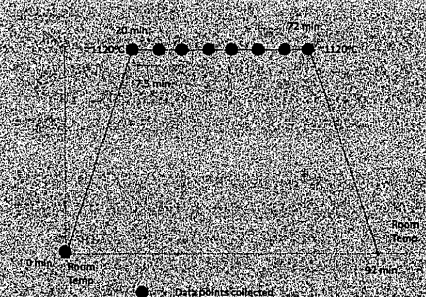


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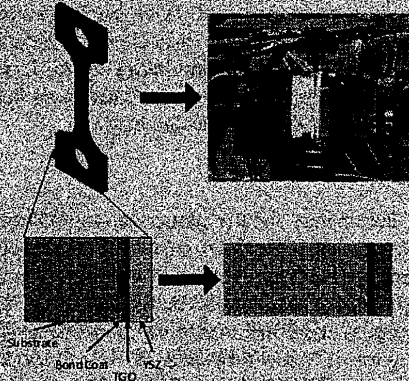
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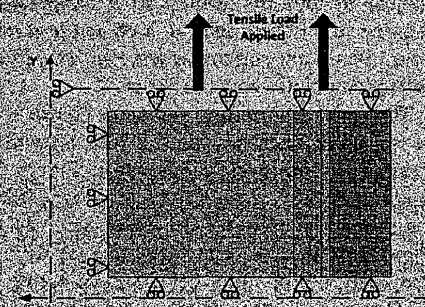
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**Figure 5. Boundary Conditions**

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Density, ρ (g/cm <sup>3</sup> )	7.75	7.25	7.80	7.45	4.00	4.00	5.00	4.84
Heat Capacity, C <sub>p</sub> (J/KgK)	400	580	390	700	769	1261	500	630

$$\dot{\epsilon} = C1\sigma^{C2}\exp\left(-\frac{C3}{T}\right) \quad (1)$$

Table 2. Creep Constants

	C1	C2	C3
TGO	1.08e-10	2.3	51,000
Bond	8.96e-15	3.0	35,840
Coat	15		

#### IV. Results

With the model assumptions that each layer is perfectly planar with minimal roughness, only the in-plane stresses and strains are comparable between the model and experimental results. Shown below in Figure 6, from Diaz *et al.*<sup>14</sup> are the in-plane strains resulting from the XRD analysis. The strain profile across the depth of the layers is shown for each mechanical load at the first three data collection points of the cycle. This confirms from previous studies, the highly compressive nature of the TGO layer at room temperature.

The first high temperature plot shown demonstrates how the TGO becomes tensile when subjected to a 64 MPa tensile load. The stress becomes increasingly compressive when held constant at high temperature bringing the TGO back into the compressive region. This transient stress phenomenon is further demonstrated in Figure 7 which displays the TGO in-plane transient stress. Using various creep models, this effect is validated and is a main topic of investigation for single cycle modeling.

The residual stresses are then used as a form of validation for the finite element model. The TGO stresses, in particular,

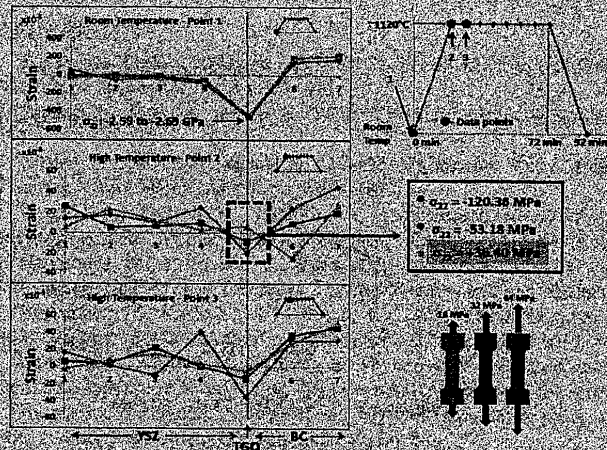


Figure 6. Experimental In-Plane Strain (Figure from [14])

are used for comparison due to their very high stresses relative to the other layers. Table 3 below shows the comparison of the finite element results to that of the XRD results.

Figures 8 and 9 then show the transient stress results for both the bond/coat and TGO, respectively, throughout the beginning duration of the load cycle. This shows the nonlinear transient behavior of both layers, including a corresponding stress relaxation of the TGO layer. This is largely due to the creep strain experienced in both layers, which is shown in Figures 10 and 11 for the bond/coat and TGO respectively.

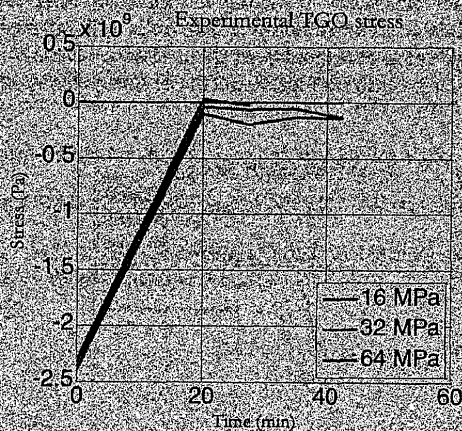


Figure 7. Experimental TGO In-Plane Transient Stress