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# Life Prediction Issues in Thermal/ Environmental Barrier Coatings in Ceramic Matrix Composites

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# LIFE PREDICTION ISSUES IN THERMAL/ENVIRONMENTAL BARRIER COATINGS IN CERAMIC MATRIX COMPOSITES

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**ABSTRACT:**

Issues and design requirements for the environmental barrier coating (EBC)/thermal barrier coating (TBC) life that are general and those specific to the NASA Ultra-Efficient Engine Technology (UEET) development program have been described. The current state and trend of the research, methods in vogue related to the failure analysis, and long-term behavior and life prediction of EBC/TBC systems are reported. Also, the perceived failure mechanisms, variables, and related uncertainties governing the EBC/TBC system life are summarized. A combined heat transfer and structural analysis approach based on the oxidation kinetics using the Arrhenius theory is proposed to develop a life prediction model for the EBC/TBC systems. Stochastic process-based reliability approach that includes the physical variables such as gas pressure, temperature, velocity, moisture content, crack density, oxygen content, etc., is suggested. Benefits of the reliability-based approach are also discussed in the report.

**BACKGROUND:**

Computational model development research to predict the behavior and failure of thermal barrier coatings (TBCs) traces back at least 3 decades. However, very little effort has been spent to develop life prediction models accounting for uncertainties in the governing variables. Current efforts in the Ultra-Efficient Engine Technology (UEET) development program at the NASA Glenn Research Center (GRC) are focused not only on protecting components against severe thermal loads but also against the environmental effects due to the moisture, debris, oxygen, etc., in the turbine engine combustor and vanes environment gas [1], [2]. The concept of protecting materials, under development at GRC, against these environmental effects is unique and novel and the protective coating sometimes referred to as the environmental barrier coating (EBC) material system. EBC/TBC material systems developed under GRC sponsored HSCT-EPM (High Speed Civil Transport-Enabling Propulsion Materials) are capable of delivering the expected performance up to 1315 °C gas temperature. However, new EBC/TBCs being developed under the NASA UEET Program are expected to achieve thermal/environmental protection and durability under the operating gas temperature of 1760 °C with coating surface temperature of 1480 °C and bond coat substrate interface temperature of at least 1315 °C with assured reliability.

The current state-of-the-art EBC system consists of CMC (ceramic matrix composite) as substrate, silicon layer as a bond coat, a composite layer of mullite and BSAS (barium strontium aluminum silicate) and pure BSAS layer as EBC at the top was developed under the NASA EPM project. A pictorial representation of this system is shown in the figure 1.

Silicon-based ceramics are excellent candidates for higher temperature applications due to the slow formation of silicon oxide, however, other problems exist related to the degradation and volatilization of the silica scale in the presence of water vapor and alkali salts. Increasing the operating temperature range/magnitudes accelerate problems related to the oxidation of silicon as well as creep, degradation of the strength, and properties of EBC/TBC during the thermal cyclic loads and gradients. These problems result in sintering, creep deformation, cracking in the bond coat, formation of ridges and cavities, surface erosion, and spallation of the coating as well as CMC, etc., ultimately affecting the durability of coatings. Spalling of the coating is induced by the bond coat oxidation accompanied by volumetric expansion during the high-temperature exposure. Generally, the oxidation of the bond coat occurs due to the penetration of water vapor from combustion gases through the EBC/TBC and mullite layers.

Although, the mechanism of spallation has not yet been well understood, many speculative theories supported by some computational results have been proposed specifically for the TBCs on metallic substrate. Due to the differences in thermal expansion coefficients and stiffnesses of the bond coat and the EBC, residual compressive stresses develop under thermal cyclic loads. Additional compressive stresses develop as a result of the oxidation of the bond coat accompanied by the volume change under constrained conditions at the interface. Further growth of oxidation produces ridges and cavities at the interface layer. Also, the wavy and irregular geometry of the interface makes ridges to be sites of stress concentration. These conditions along with the stress relaxation during cooling cycle create normal stresses perpendicular to the interface at defect/ridge sites. Furthermore, the stresses perpendicular to the interface are accentuated due to the effect of the stress concentrations at the ridges. When these normal stresses exceed the tensile strength, cracks form in the EBC as well as the bond coat ultimately leading to spallation. In order to develop an effective coating system it is therefore important to understand its behavior under these loading conditions and other environmental effects from the hot gases.

## INTRODUCTION:

With the ever-increasing need for EBC/TBC in more critical applications, the life/durability of coatings has become an important issue. Experimental investigations do lead to understanding its failures and mechanisms to a limited extent. Consequently, analytical modeling of EBC/TBC life/durability is required in order to be able to design an optimum EBC/TBC system to compliment experimental investigations as well as to understand the observed failure mechanisms. These can eventually lead to the development of computational design tools that can be used for optimum design of coating systems for combustor liners. The present report summarizes the relevant literature in the EBC/TBC development and design; key issues involved in the EBC/TBC, and possible ideas on approach and expected results. It is to be noted here that EBC development is generic to GRC and authors are not aware of any literature available on

EBC for CMC outside of GRC sources. Therefore, the described approach focuses heavily on the GRC coating material development design issues.

**LITERATURE SURVEY:**

Since the EBC is a GRC-developed novel material development concept, it appears that research performed or pursued in the life prediction and cracking characteristic of the EBC is very limited. However, many approaches and methodologies pursued or implemented for TBC can be applied to the EBC/TBC as well. Therefore, these procedures can be effectively utilized to develop reliability based life prediction methodology for the EBC/TBC systems.

The consensus among various researchers regarding the cracking behavior suggest that the following failure modes in the TBCs are of significant importance to the life/durability of the coatings as well as the coated components [4]:

| Failure mode: | Definition: |
|---|---|
| Creep | Time dependent, thermally activated inelastic deformation of a material. The rate of creep increases as the temperature increases for constant stress. |
| High-cycle fatigue | Microstructural damage mechanism that results from small stress amplitude cyclic loading such as vibrations; failure will occur after a relatively large number of cycles. |
| Low-cycle fatigue | Microstructural damage mechanism that results from large stress amplitude cyclic loading; failure will occur after a relatively small number of cycles. Very abrupt thermal changes, such as engine start and stop cycles, are the driving force for this failure mode. |
| High-temperature oxidation | Solid-gas chemical reaction that produces the oxide(s) of constituents within the solid. The rate of oxidation increases exponentially with temperature; certain oxides are slow growing and protective of the underlying substrate. |
| Hot corrosion | Electrochemical reaction between substrate and molten salts, typically sodium and potassium sulfates. Two forms of hot corrosion are generally recognized: Type I (high-temperature), which typically occurs between temperatures of 820 °C and 920 °C with a maximum of 870 °C, characterized by the buildup of a nonprotective oxide layer as oxidation and sulfidation destroy the metal substrate; and Type II (low-temperature), which typically occurs between temperatures of 590 °C and 820 °C with a maximum of 700 °C, often exhibiting pitting. |

Several other damage modes can also cause coating loss and accelerate the overall failure mechanism. These are

(1) Mechanical distress to the coating, such as nicks and gouges, which are caused by objects ingested into the engine airstream

(2) Solid-state diffusion of elements between coating and substrate, which can lead to the loss of critical elements from the coating and formation of undesirable phases in the substrate
(3) Spallation caused by differential thermal expansion between the coating and the substrate, which can lead to mechanical failure of the coating
(4) Rumpling of coatings as a result of creep

Cheng *et al*. [5] used conventional finite element analysis methods to quantify the residual stresses in electron beam physical vapor deposited yttria stabilized zirconia TBC system on a Pt-Al bond coat. Elasto-plastic analysis of a circular disk specimen modeled with actual interface surface with ridges and cavities showed significant areas of tensile stresses responsible for cracking. Some of the important conclusions of their study are:

(i) Irregular interfaces lead to large tensile stresses in the thermally grown oxide (TGO) layer. Cracking was observed where these stresses extend more than halfway through TGO layer.
(ii) Elastic analysis did not capture the stresses due to reheating and were found responsible for cracking in the elastoplastic analysis. Elastic analysis is not recommended for wavy surfaces.
(iii) Image processing can be used to obtain more-precise geometry required to generate finite element model (FEMs).
(iv) Use of actual interface geometry is more logical in finite element modeling than the commonly used sinusoidal geometries in the prediction of local stresses.

Brindley [6] conducted experiments to observe the effect of increasing the NiCrAlY bond coat oxidation resistance on TBC life. He showed that although the oxidation is a main driver, the significant difference in the coefficient of thermal expansion (CTE) and stress relaxation of the alloy in the bond coat applied on metallic substrate has a pronounced effect on the life whereas the elastic modulus of the alloy does not. Out-of-plane residual stresses in the bond coats increase during the stress relaxation phase of the plasma-sprayed coatings. These out-of-plane stresses creep more and produce delamination of ceramic layer affecting the life.

DeMasi *et al*. [7] performed an extensive experimental investigation of a two-layer NiCrCoAlY TBC system to study its failure mechanisms and life model development. Their life model used one dimensional constitutive equations developed by Walker [8] and an oxide growth rate that was verified with the experimental data. Important conclusions of their study are:

(i) Spalling results from the progressive damage and oxidation is a significant driver. Bond coat crack oxidation was not conclusively shown to initiate the subcritical cracks.
(ii) Increased coat thickness improves life.
(iii) Plasma-sprayed ceramic exhibits nonlinear stress-strain response in uniaxial tension and compression, a strong creep response, and stress sensitive fatigue behavior.

Kokini *et al*. [9] have studied TBC properties and its behavior under high-thermal gradients and thermal cyclic loads. Their initial study focused on fracture mechanisms in TBC and effects of surface temperature as well as thermal gradients. For the CoCrAlY coating, the surface cracking is initiated by the stress relaxation resulting in the tensile stress during the cooling from high temperature to room temperature. Since the edge crack initiation has singular stresses, the stress criterion cannot be used for failure although it shows both opening and shearing modes of cracks. The interface cracking is significantly different from the opening and shearing deformations with different energy release rates. Later they also studied the effects of laser heating, the manufacturing process, and the thickness of coating on the cracking behavior of TBC [10]. Their experimental investigations revealed that the laser heating with sufficient energy could make the microstructure denser. Their study showed that the higher compressive stresses develop with high energy and rapid heating and producing tensile stresses when cooled down to room temperature. As a result of such a rapid heating and cooling cycle, more cracking occurs. Another observation in relation to the manufacturing process is that the sintering and stress relaxation in a continuously manufactured thin ceramic layer lead to multiple surface cracks upon ambient cooling whereas in a thick layer it causes surface and interface cracks. Also, when the stress field developed due to thermal heating is of a high intensity and coincides with the plane of weakness within coating, it can cause delamination at that plane. These experimental investigations greatly help to understand the interface delamination and multiple surface crack formation response of TBCs to the high heat flux, manufacturing process, and transition thickness. However, computational simulation approaches are needed to understand the behavior of EBC/TBCs in order to eliminate the necessity of a large number of complicated experiments.

Lee [1], [2] identified the major issues related to the selection of EBC systems. He indicated that the coating should have the ability to resist reaction with the aggressive environment, and have low oxygen permeability. Also, the CTE of the coating should be close to that of the substrate material along with their chemical compatibility. An additional desired quality is their ability to maintain a stable phase in a thermal environment.

Based on the above requirements, Lee described the evolution of the mullite EBC system being developed at the GRC. Such a system still faces key durability issues such as through-thickness cracking in the mullite, weak bonding of mullite onto silicon-based ceramic, and interface contamination. It is still not known or verified computationally what causes through thickness cracks. However, it is strongly believed that these cracks allow the oxygen transportation that accelerates water-vapor-enhanced oxidation of the bond coat and eventual failure of the system. Additionally, the delamination of the bond coat and precipitation of the second phase such as residual amorphous mullite and alumina in the mullite and the volumetric shrinkage, reduce the durability of the EBC system.

Choules *et al*. [10] performed experimental studies on the effect of high heat flux on the thermal fracture of TBCs on a steel base. However, their study focused primarily on the effect of processing method (plasma spraying) such as interrupted two-pass and continuous spraying, coating thickness, preheat conditions, and laser heating on TBC failures. The schematic of the specimens tested is shown in figure 2.

The effect of the 150 and 200 W laser heating was studied in all specimens with a 1.09-mm-thick coating. The heating was applied at an increment of 50 W until fracture was observed. The substrate temperatures in the tests were kept below 200 °C indicating that the bond coat oxidation was not a factor and the resulting instantaneous gradient obtained was up to 1400 °C. Based on the observation, the following conclusions were made by Choules *et al*.

(i) Laser heating of sufficient energy can change the material leading to denser microstructure.
(ii) Sintering and stress relaxation in a continuously manufactured thin ceramic layer lead to multiple surface cracking upon ambient cooling following laser heating.
(iii) Sintering and stress relaxation in a continuously manufactured thick ceramic layer lead to surface and interface cracking upon ambient cooling following laser heating.
(iv) If the stress field due to thermal heating is sufficiently high and it coincides with a plane of weakness within the coating, it is possible to cause delamination at that plane.

It is clear from the above conclusions on TBC made by Choules *et al*. that the effect of processing, the coating thickness and time dependent behavior of the coating for the EBC/TBC system, must be considered in the design and life evaluation.

Andritschky *et al*. [11] studied the mechanics of delamination on the metal-based *thick* ceramic coatings. Delamination initiated by the transverse cracks caused by the sintering process, thermal stresses, and internal oxidation during prolonged exposure to the high temperatures, were experimentally and computationally investigated. Coated samples were tested using four-point bending experiments to study the crack initiation along the substrate-coating interface and subsequent delamination due to tensile stresses. The residual stresses were obtained using the classical elastic theory by equating the average residual stress with the analytically integrated stress distribution. The surface stress thus obtained matched with the observed stress using x-ray diffraction analysis. Force-displacement plots were used to determine the elastic properties of the coating. Analytical expressions based on the elastic theory were used to determine the Weibull distribution of the flexure stress. Since it is difficult to identify the first microcrack and its corresponding stress, the experimentally observed deviation of the flexure stress at the first appearance of the crack was compared with that from the analytically obtained stress in order to determine the critical stress. Analytical equations using the thin-film theory that account for the effect of nearby cracks were used to obtain the stress distribution close to the fracture edge. For thick coatings, linear FEM analysis was performed to obtain the stress intensity factors ($K_I$ and $K_{II}$). The FEM analysis superposed the analytically obtained residual stresses, which were approximate. FEM simulations were used in combination with the analytical classical fracture mechanics to compute stress intensity factors. Their study concludes with the remark that the FEM analysis of the entire coating system can lead to better results due to the complexity of residual stresses, short cracks, multiple cracking, etc.

Teixeira *et al*. [12] quantified the residual stresses induced by the processing and CTE mismatch experimentally and numerically in the plasma-sprayed TBCs. A good agreement between the computed residual stresses and the experimental data was noted. Studies under isothermal and cyclic heat treatment were conducted. Residual stresses developed in the coating lead to the adhesive (delamination of the interface) or cohesive failure (microcracking or spalling within the ceramic coating) due to the CTE mismatch, thermal gradients, and the thermal history. Free edges exhibit large interfacial shear and axial stresses, which promote the microcracking parallel and adjacent to the interface. During rapid thermal cycling, the compressive stresses develop in the coating and cause crack formation at the interface.

Residual stresses in the as-deposited specimen as well as the thermally cycled coatings were computed using a one-dimensional (1-D) heat transfer analysis with the constant boundary conditions followed by an FE analysis. During the rapid thermal cycling the stresses in the oxide layer were assumed to be zero. However, compressive stresses develop in the oxide layer during the cooling cycle due to the CTE mismatch with the substrate. The PVD (plasma sprayed vapor deposition) layer shows compressive stresses during the processing and increases after the thermal cycling. The PS (plasma spray) coating layer was in a tensile state of stress at high temperatures and after thermal cycling due to stress relaxation as a result of microcracking and creep phenomena. Thus, the residual stresses play a significant role in the life prediction model development.

Their observations and inferences of their tests and computations are summarized below:

(1) Residual stresses were not uniform through the thickness in the as-deposited specimen and changed from tensile to compressive when the substrate temperature was increased.
(2) Residual stresses were compressive at the interface and diminished toward the free surface in a linear manner.
(3) Thinner coatings were found to have higher compressive residual stresses at the interface.
(4) Increase in the coating thickness showed surface stress changing from compressive to tensile.
(5) Residual stresses are dependent on the thermal history.
(6) Differences between the computational and experimental results were attributed to the uncertainty in the physical properties of the plasma-sprayed coating.

Bao and Wang [13] focused their study on multiple cracking in the functionally graded materials (FGM). Multiple cracking is the most common phenomena in the coating systems, whether it is a TBC or an EBC. They studied the issue of multiple cracking from the fracture mechanics point of view by computing the crack driving force for multiple cracks. Cracking under mechanical load, thermal load, and combined thermal and mechanical loads was studied. Linear elastic fracture mechanics coupled with the finite element approach was used to compute the energy release rate of the cracks as determined by the coating degradation, crack length, and crack density. In multiple cracking, the crack spacing usually attains saturation due to interaction of the neighboring cracks and relief of the tensile stresses in the coating. Their study, however, assumed the coating to be perfectly bonded to the homogeneous, isotropic metal substrate. This assumption fails to account for the debonding of coatings due to oxidation. Also, the plasticity of metal substrate as well as crack bridging mechanisms was neglected in their study. The functionally graded coating was divided into 100 layers and the equations for the properties of the functionally graded coating were derived as a function of the ratio of the location from the top surface to the thickness of the coating. Subsequently the governing equations for the energy release rates under different load conditions were derived. Energy release rates as a function of the ratio of the crack length to the coating thickness, the crack density and the corresponding stress intensity factors were then computed and plotted for the mechanical, thermal, and combined mechanical and thermal loads. Results showed that the FGM has higher hardness and oxidation resistance at the surface with much lower residual stresses and crack-driving forces compared to that of pure ceramic coatings. The effect of mechanical loads on the crack-driving force is found to be small. However, under thermal loads the effect on crack-driving forces is significant.

Nusier *et al*. [14] performed experimental and analytical investigation of the damage process in the TBCs subjected to different thermal cycle profiles. Attempts were made to describe progressive oxidation and damage evolution mechanistically. The diffusion equation using the Fick's Law was used to compute the oxide growth. However, no conclusions regarding the failure process, life, and bond coat behavior were drawn.

One of the most important problems in the gas turbine engines that affect the TBC life is the erosion due to the foreign object impact (FOI) and moving gas under pressure at high speed. Erosion wears out the surface and may initiate surface cracks or produce nicks and gouges which affect the life. Therefore, understanding the phenomena from a mechanics viewpoint and the effect of the erosion rate is of equal significance for the life assessment. Wellman and Nicholls [15] have performed studies to explain the erosion process mechanism linked with the microstructure of the coatings. Their findings show that the velocity and radius of the impacting object play a significant role in the surface cracking of the coating. Columnar structure of the coating has been shown to accommodate the strain. Three different patterns of microstructures in the columns of material were observed: (i) fern leaf dendrite type on the edges of columns, (ii) striations fanning horizontally across the columns, and (iii) numerous smaller columnar crystallites that are closely packed. The number of cracked columns indicated brittle erosion mechanism and most of the cracks were perpendicular to the direction of column growth. The cracks propagated through the diameter of columns and tensile stresses were responsible for it. Also, cracks did not propagate into the neighboring columns and not more than five columns adjacent to the cracked one were found cracked. Observations showed no correlation with the column diameter and the depth at which crack occurs. Also, no existence of shear cracks was observed. Variations in the Young's modulus and Poisson's ratio of the target have very little effect on the contact radius. The depth at which cracking occurs was a direct function of the impacting particle radius and velocity. Near surface cracking and the dendrite initiated cracking was the most predominant erosion mechanism. All the observations were experimental and were not supported by the computational methods.

Based on the above literature survey it can be concluded that the past work is primarily applicable to TBCs. The research was directed towards understanding of the underlying failure mechanisms of the coating system. Life prediction model development work for TBC was limited, and still remains in a research form. A majority of the TBC life prediction modeling effort was based on linear fracture mechanics and crack propagation methodologies. The fracture mechanics approach has limitations due to its applicability to single dominant crack, and often in thin coatings a multitude of cracks need to be analyzed. Furthermore, accurate experimental determination of the fracture toughness and other parameters for thin coatings required in the fracture mechanics approach is a difficult task. Owing to the difficulties in the experiments, there is a significant variation in these parameters. Some researchers have included the physical aspects of the coating behavior using the diffusion theory and material structure of the coatings. Although, the physical behavior of the TBC is different from that of the EBC, some aspects of the diffusion theory can be useful for the life prediction of EBC. Many researchers have performed computational simulation of the residual stresses and their comparison with the experimental data [11, 12]. The importance of the effect of cyclic loads on residual stresses and ultimate life is yet to be addressed. Another important issue that has been studied is the sintering of TBC and the effect of the manufacturing process. Since the oxidation of the bond coat as well as the crack formation ultimately result into sintering, it is important to simulate physics of sintering in the EBC behavior and life quantification. In summary, the life prediction models and approaches used for TBC are not directly applicable to EBC. The EBC behavior on CMC substrates is quite different from that of TBC on a metallic substrate and additional unique life limiting failure mechanisms need to be identified and addressed.

Further investigation on the failure mechanisms and related modeling aspects for the life prediction of EBC and a possible approach to compute EBC/TBC life and its reliability is reported in the next section.

## PROPOSED APPROACH:

The proposed approach for the life prediction methods development for the EBC/TBC system for ceramic matrix composites (CMCs) being developed at GRC is physics based, compliments the material development process, and lead to the final state-of-the-art computationally efficient design tool development. The following paragraphs describe salient-related features of the approach:

Issues related to EBC/TBC in the UEET Program:

Critical issues [1], [2] that relate to the EBC/TBC system development under the UEET Program are (i) chemical incompatibility between the silica formation, Si-based ceramics and EBC result in the reaction zone that may develop pores and cause interface delamination, (ii) volatilization of the silica under high temperature in the presence of moisture and oxygen, (iii) mismatch between the CTEs of substrate and coating resulting in the residual stresses and surface cracks, (iv) initial flaws due to nicks and gouges as a result of foreign object impacts, (v) through- and surface-crack development in the coating due to thermomechanical loads, (vi) spalling under thermal cycling, and (vii) sintering causing volumetric changes that result in the mudflat cracks.

Perceived preliminary failure mechanism in EBC/TBC:

It is important to understand the underlying physical behavior of the EBC/TBC coating system under thermomechanical cyclic loads in order to understand the issues described above. Based on personal discussions with Lee [1], [2], [3], the perceived preliminary failure mechanism has been described. During the manufacturing process, several passes of the coating are applied under prescribed thermal conditions. Cooling and heating cycles involved in the manufacturing process result in the residual thermal stress buildup. After formation of the coating, micro level cracks in the surface as well as through the thickness have been observed. Additionally, the cracks on the surface form due to the mechanical distress to the coating and nicks and gouges caused by the objects ingested into the engine air stream. Also, thermal gradient between the substrate and coating develops under the operating conditions of thermal shocks and thermal cycles mainly due to the difference in the thermal conductivity and requirement of maintaining substrate temperature within certain magnitude. Under the cyclic nature of thermal loads and mismatch in the thermal expansion coefficients of the coating, mullite, silica, and substrate, residual stresses develop as well as stress relaxation occurs in these layers. These conditions accentuate the crack formation and growth in the coating system layers.

Once the cracks in the coating system form and grow as the components undergo increased operation, the moisture, oxygen, and alkaline salts present in the gas penetrates to the silica layer. Under high-temperature conditions and presence of these agents, the silica oxidation starts and silica scale formation begins/continues. Continued formation of the $SiO_2$ results in the volumetric changes involving shrinkage and swelling. Furthermore, the oxidation results in sintering and spalling of the coating. Volumetric changes accompanied by the cyclic nature of stresses, the crack formation, growth, and silica oxidation continues until the coating system fails.

Approach objectives:

Having described the issues and perceived failure mechanism in the EBC/TBC system, the objectives of the current effort are to

(i) Develop a generic reliability based EBC/TBC life prediction methodology
(ii) Capture uncertainties associated with the EBC/TBC life
(iii) Identify and quantify the sensitivity of variables governing the EBC/TBC life
(iv) Quantify the reliability of EBC/TBC life
(v) Develop generic and general-purpose computational design tool for EBC/TBC life prediction.

Approach description:

The approach consists of (i) heat transfer and stress analysis, (ii) physics-based deterministic life prediction model development, and (iii) reliability-based life prediction method development.

Heat transfer (HT) analysis:

- Perform steady state and transient heat transfer analysis to calibrate the experimentally obtained thermal properties/response
- Establish thermal design guidance for 2-D and 3-D finite element thermal analysis

Physics-based deterministic life prediction method development:

Life prediction methods development of EBC/TBC system is a formidable task. In order to assess the life of coatings, a reasonably accurate stress analysis and long-term behavior of the coating based on the real physical aspects need to be simulated. Therefore, a transient analysis that couples the heat transfer and stress analyses in a probabilistic sense forms a core of a possible approach. To achieve this objective, the approach planned is outlined in Figure 3.

The approach aims at computing the useful life of the coating and not until its complete failure. Since the design procedures aims mainly at the functional behavior of the coating and also the fact that the continued life after the exposure of the substrate to the thermal effects of the gas is very little, simulation of a complete failure of the coating is not needed. The approach consists of simulation of the following:

(1) Residual stress development due to the CTE mismatch between substrate, bond coat, mullite, and coating
(2) Penetration of the moisture and oxygen to the bond coat through the existing pores and cracks (Figure 4)
(3) Oxide growth formation
(4) Shrinkage and sintering effects
(5) Material degradation especially that of the bond coat
(6) Failure of coating

Reliability-based EBC/TBC life prediction method development:

Due to the variations in the manufacturing and application processes, chemical conditions, thickness, initial crack density, interface geometry, and material properties of the coating system, the behavioral characteristics of the EBC/TBC vary considerably. Additionally, the inherent uncertainties in the gas temperature, pressure, velocity, moisture, oxygen, and alkali salt contents, thermal shocks during the engine startup, etc., affect the performance of the coating. Continued exposure in combustion environment with these uncertainties can lead to significant variation in the actual life. A thorough understanding of the structural characteristics of EBC/TBC from the life and durability point of view therefore becomes a complicated task due to the above-described uncertainties. Initial survey of the literature suggests that very little and perhaps no research effort is going on at present in the government, industry, as well as academia to predict EBC/TBC life with assured reliability using the probabilistic approaches. Probabilistic approach enables the simulation of uncertainties and quantifies the sensitivity of the basic design variables to the life reliability. The majority of the probabilistic approaches are random variable based which are applicable to static and linear problems. EBC/TBC life model development is a time domain problem and involves material non-linearity with time. Therefore, a stochastic process-based approach that integrates thermal, structural, and nonlinear behavior uncertainties to simulate the long-term behavior need to be developed/adopted.

As a byproduct of the probabilistic analysis, importance ranking of the design variables can be obtained, which provides useful insight to design engineers as well as test/fabrication engineers. As mentioned earlier, in the physics-based methods development, the sensitivity information can be used to compute the non-measurable properties of the coating system as well as the material development process. Using the probabilistic analysis results, the guidelines for the maintenance and inspection intervals can be developed.

Typical results that can be computed for the reliability-based EBC/TBC life development effort is, e.g., reliability-based thickness of the coating system versus life curve (Figure 5), thermal gradient versus life for a given coating system, etc.

Design tool development and objective:

The ultimate objective of the described effort is not to just develop the EBC/TBC life prediction methodology, but also to develop a software tool to design the EBC/TBC systems. The objectives of the design software tool should be: (i) user friendliness (ii) easy link with any commercial FEM package, (iii) ease of identifying input parameters, (iv) to enable the user to configure a coating system, (v) to provide design improvement guidelines to the user, and (vi) to develop reliability-based life curves.

**SUMMARY:**

Failure mechanism and life issues, general and specific to the Ultra-Efficient Engine Technology (UEET) Program, for the environmental barrier coating (EBC)/thermal barrier coating (TBC) systems material development/characterization have been discussed and the relevant current trend of the research in the industry, academia, and government has been identified. The literature survey suggests that the EBC is a new concept of material development initiated at GRC to protect the components from the detrimental effects of the aggressive environment and temperatures. Many researchers have developed several models to characterize the TBC behavior. However, life prediction models that can be used directly for design purposes have not been developed yet. Perceived failure mechanisms specific to EBC/TBC have been reported. Accordingly, penetration of the moisture content to the bond coat; through the micro cracks existing in the EBC layer, either as a result of the manufacturing process or formed by the debris impact, causes it to oxidize in the presence of oxygen. Continued oxidation of the bond coat results in the volumetric change due to shrinkage/swelling and thus produces extra internal forces that expand and propagate the cracks in the EBC/TBC and mullite composite layers. Progressive oxidation results in degradation of the bond coat, delamination, cracking in the coating layers and ultimately results in failure and affects the life. A physics-based approach, using Arrhenius oxidation kinetic model, has been proposed to compute the volumetric change and external forces. Coupled structural thermal time-dependent analysis using an adaptive meshing and material degradation model based on oxidation kinetics has been proposed to develop life prediction models. Uncertainties in the basic governing variables have to be considered in the probabilistic simulation based on the stochastic process approach to compute the reliable life and its sensitivity. Ideas and thoughts to use the existing experimental data as well as design new experiments to generate the test data required to validate/verify the proposed life prediction model development have been discussed. Significant objectives for the design tool development for the structural components using EBC/TBC coating systems have been laid out and a road map has been outlined.

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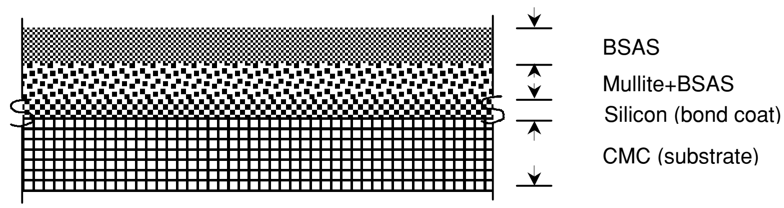


Figure 1. The current state-of-the-art Enabling Propulsion Material (EPM)/ environmental barrier coating material system.

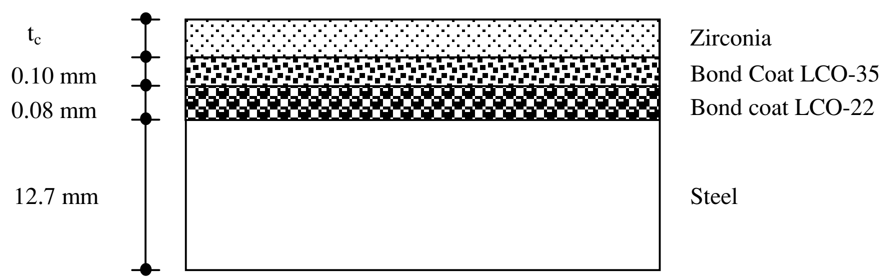


Figure 2. Thermal barrier coating for a steel substrate.

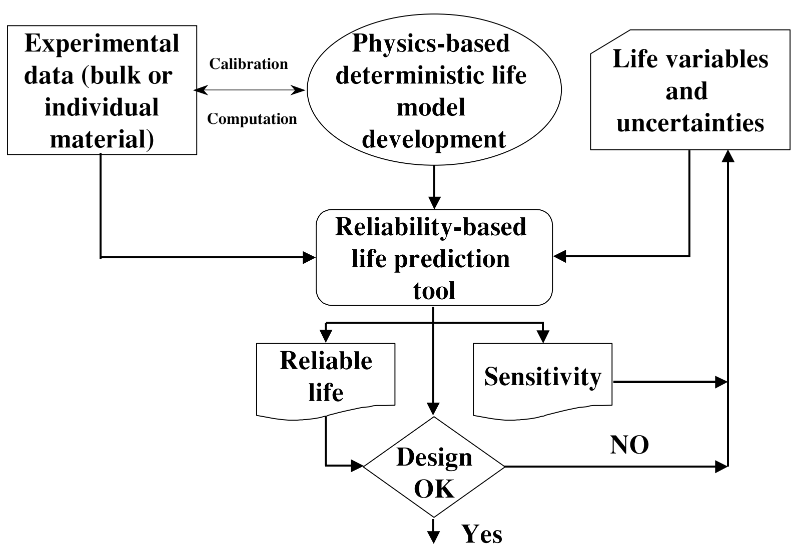


Figure 3. Environmental barrier coating/thermal barrier coating life development approach outline.

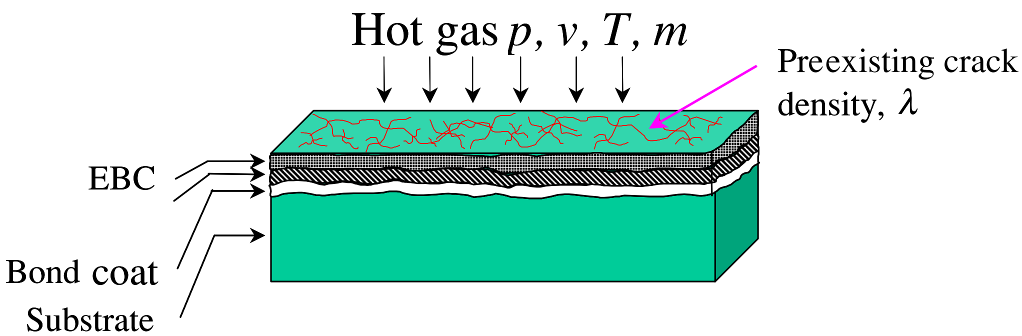


Figure 4. Bond coat degradation mechanism.

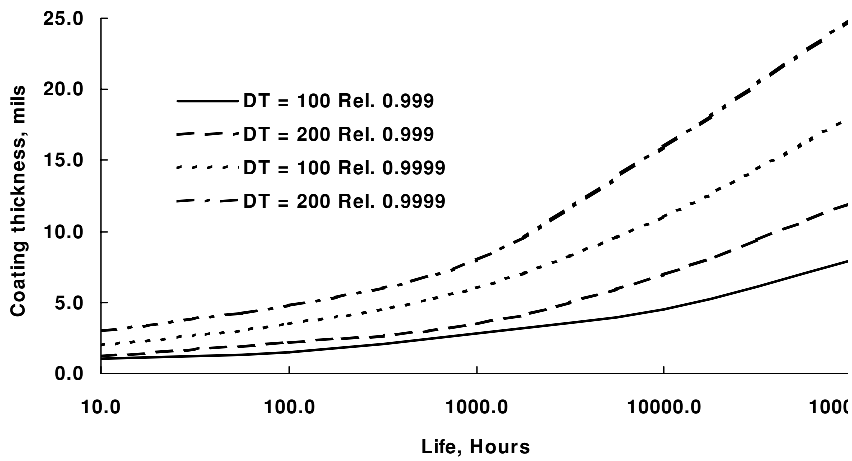


Figure 5. Typical EBC/TBC reliability-based life curve results.

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**13. ABSTRACT** ***(Maximum 200 words)***

Issues and design requirements for the environmental barrier coating (EBC)/thermal barrier coating (TBC) life that are general and those specific to the NASA Ultra-Efficient Engine Technology (UEET) development program have been described. The current state and trend of the research, methods in vogue related to the failure analysis, and long-term behavior and life prediction of EBC/TBC systems are reported. Also, the perceived failure mechanisms, variables, and related uncertainties governing the EBC/TBC system life are summarized. A combined heat transfer and structural analysis approach based on the oxidation kinetics using the Arrhenius theory is proposed to develop a life prediction model for the EBC/TBC systems. Stochastic process-based reliability approach that includes the physical variables such as gas pressure, temperature, velocity, moisture content, crack density, oxygen content, etc., is suggested. Benefits of the reliability-based approach are also discussed in the report.

**14. SUBJECT TERMS**
Life prediction; EBC (Environmental Barrier Coating); TBC (Thermal Barrier Coating); Spalling; Cracking; Failure; Oxidation; Random variable; Reliability; Sintering

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