Environmental Barrier Coating Fracture, Fatigue and High-Heat-Flux Durability Modeling and Stochastic Progressive Damage Simulation

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Introduction
The environmental barrier coatings and durability model development
• Develop innovative coating technologies, design tool and life prediction approaches
• Help fundamental understanding of failure modes in simulated testing environments, database and design tool development
• Emphasize improving temperature capability, performance, long-term durability

Key model considerations
• Sintering, creep and thermal expansion mismatch induce surface crack propagation
• Surface cracking accelerates coating delamination under mixed mode thermal and mechanical loading ($K_1$ and $K_{II}$)
• Creep, fatigue, environment interactions including oxidation and recession
• Coating interface reactions
• Interfacial pore formation further accelerating coating spallation under heat flux

Generalized EBC Failure Mechanisms

Environmental barrier coatings

Combustion gas

SiO$_2$ + 2H$_2$O(g) $\rightarrow$ Si(OH)$_4$(g)

Cooling gas

EBC-CMC film-cooled recession
Modeling Objectives and Challenges

• Major focuses
  – Develop high-heat-flux thermal gradient EBC degradation and failure models
  – Incorporate coating creep and thermomechanical fatigue models for environmental barrier coatings on SiC/SiC ceramic matrix composites (CMCs)
  – Establish physics-based property and life models with key experimental validations
  – Help multi-scale modeling of environmental barrier coating systems, guiding coating designs for the coating development needs

• Major challenges
  – Evolving coating properties in operating conditions, no general acceptable measurable quantities to describe coating degradations
  – Complex interactions in thermal gradients (temperature and heat flux), thermomechanical loading (creep and fatigue), and environments, lacking understanding of the failure mechanisms
EBC-CMC Systems: Prime-Reliant Coatings Design Requirements

- Emphasize improving temperature capability, performance and long-term durability of ceramic turbine airfoil coatings
  - Increased gas inlet temperatures for net generation engines lead to significant CMAS-related coating durability issues – CMAS infiltration and reactions
  - High heat flux, and highly loaded components


Approach – Experimental Methods and Mechanisms-Based Modeling

• Our Approach
  – Understand the true coating failure driving force and resistance in complex simulated engine testing environments
  – Use combined \textit{Fracture Mechanics} and \textit{Damage Mechanics} modeling approaches for physics based modeling
  – Validate modeling with laboratory high heat flux, environment tests, and measured coating property data

• Our modeling emphasizes integrations of fracture and continuum mechanics
  – Fracture mechanics based approach for failure and life prediction
  – Continuum damage mechanics based approach for quantifying coating property evolutions and environmental interactions
  – In particular, using the stochastic progressive damage simulation successfully predicts mud flat damage pattern in EBCs

• Utilize advanced environmental barrier coating systems, expanding broader ranges of test conditions for experiment assisted model validations
Modeling Environmental Barrier Coating Tensile Creep Rupture and Fatigue Testing Induced Cracking - Delamination Testing

- Fracture Mechanics based models for EBC multi-crack stress intensity modeling: emphasize creep, thermal gradient and stress rupture interactions
- Laser heat flux rig validations

![Diagram of Laser heat flux thermal gradient tensile rupture rig]

- High-heat-flux thermal gradient “Steam” testing rigs
- Laser Rig coupled MTS 810 High Cycle Fatigue – Mechanical test rigs with “Steam” jets capabilities
Modeling Environmental Barrier Coating Tensile Creep Rupture and Fatigue Induced Cracking and Delamination

- Fracture mechanics based models for EBC crack stress intensity modeling: emphasizing creep, thermal gradient and stress rupture interactions

- Benchmark failure modes established in EBC systems:
  - Yb$_2$Si$_2$O$_7$ in steam environments
  - EBC/HfO$_2$-Si bond coat on SiC/SiC CMC in air: more robust

Thermal gradient cyclic fatigue failure of Yb$_2$Si$_2$O$_7$ in steam environments

Thermal gradient thermomechanical fatigue tested failure of EBC/HfO$_2$-Si bond coat on SiC/SiC CMC in air: more robust
CMAS Heat Flux Induced Environmental Barrier Coating Surface Cracking

- Surface heat flux cracking of EBC in CMAS Environments

CMAS cracking on EBCs

Yb$_2$Si$_2$O$_7$ cracking on EBCs

Multicomponent EBC cracking with CMAS

Multicomponent RE Silicate EBC-1

Multicomponent RE Silicate EBC-2

HfSi(O) bond coat
Modeling Environmental Barrier Coating Tensile Creep Rupture and Fatigue Induced Cracking and Delamination, with Validations

- Fracture mechanics based models for EBC crack stress intensity modeling: emphasizing creep, thermal gradient and stress rupture interactions

- Benchmark failure modes established in EBC systems:
  - Thermal gradient cyclic fatigue failure of \( Yb_2Si_2O_7 \) in steam environments
  - Thermal gradient thermomechanical fatigue tested failure of EBC/HfO\(_2\)-Si bond coat on SiC/SiC CMC in air: HfO\(_2\)-Si bond coat

Side view of tensile specimen as heated. Top=1450° C, Bottom=1200° C, intermediate=1300° C

Microstructures after 1000 hr, 1482°C (2700°F), 103 MPa (15 ksi) testing
FEAMAC/CARES Modeling of Environmental Barrier Coatings (EBCs) on Ceramic Matrix Composites (CMCs): Mudflat Cracking

• Use the newly developed FEAMAC/CARES code \{Composite Micromechanics Code (MAC/GMC) & Ceramics Analysis and Reliability Evaluation of Structures (CARES/Life)\} with finite element analysis
• Simulate the stochastic damage evolution of EBC material system under generalized and transient thermomechanical loading over time and cyclic loading
Modeling Environmental Barrier Coating Surface Crack Evolution

- Reproduce and understand EBC failure modes such as mud flat cracking and delamination which lays the foundation for future enhancements
- Aimed at modeling effect of oxidizing species penetration within mud-cracks over time and the effect of thermally grown oxide (TGO) layer

Stochastic Progressive Damage Simulation Successfully Predicts Mud Flat Damage Pattern In EBCs

Compare to rare earth silicate EBC after heat flux testing showing mud flat damage

FE model of EBC (top coat (blue and light green), intermediate coat (green), bond coat (orange), on a rigid SiC substrate (red))

10mm dia. X 1mm disk model with about 280,000 solid elements
Cooling from a processing temperature of 1300°C

Early damage development

Advanced development of damage into cells (mud flats)

Weibull modulus m = 5

Random Element Failure vs: Neighbor Influenced Failure (Cellular Automaton Enhancement)

Encourage more abrupt failure and “crack-like” damage growth patterns

failure probability thresholds of elements adjacent to failed elements adjusted to promote a biased damage direction according to rules defined for a cellular automaton

Random element failure 
> simulates stochastic toughening

With cellular automaton Rules 
> “crack-like” growth patterns

Example: 0° Ply uniaxial ramp load 25x25 FEA mesh of shell elements
Modeling Environmental Barrier Coating – Viewing Coating Layered Damaged Elements

View damaged elements for individual material layers

View from the top

View from the bottom

Green – Top layer
Yellow – Intermediate layer
Red – Bond layer
Conclusions

Environmental barrier coating modeling strongly depends on the coating material behavior at high temperature and operating conditions

- Physics-based coating degradation and durability models require the understanding of failure driving force and resistance associated with the complex coating failure mechanisms, and their interactions, the modeling is validated with sophisticated and well-thought experiments, along with state-of-the-art environmental barrier coating systems
- The initial modeling focused on thermal cycling, creep rupture and fatigue of environmental barrier coatings on SiC/SiC CMCs

- Physics-based coating degradation and durability models require the understanding of the true failure driving force and resistance associated with the complex coating failure mechanisms, and their interactions, the modeling is validated with sophisticated and well-thought experiments, along with state-of-the-art environmental barrier coating systems

- The stochastic progressive damage simulation predicts mud flat damage, reproducing and helping understand EBC failure modes such as mud flat cracking and delamination, which lays the foundation for future enhancements aimed at modeling effect of oxidizing species penetration within mud-cracks over time and the effect of thermally grown oxide (TGO) layer, in conjunction with environmental degradation under high-heat-flux and environment load test conditions
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