Weibull-Based Stochastic Simulation of Mud-Crack Damage Formation in an Environmental Barrier Coating

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Abstract:

The integrated Finite Element Analysis–Micromechanics Analysis Code/Ceramics Analysis and Reliability Evaluation of Structures (FEAMAC/CARES) program was used to simulate the formation of mudflat-cracks from thermomechanical loading on a multi-layered Environmental Barrier Coating (EBC) system deposited on a ceramic substrate. FEAMAC/CARES combines MAC/GMC multiscale composite micromechanics code with CARES/Life probabilistic multiaxial failure criteria code and Abaqus finite element analysis. In this work, step function elastic modulus reduction of randomly damaged finite elements was used to represent discrete cracking events. The use of many small-sized low-aspect-ratio finite elements enabled the depiction of crack boundaries and formation of mudflat patterned damage. Demonstrated examples include finite element models of button–sized disk–shaped 3-D specimen, and a 2-D model of through-the-thickness cross-section. All models were subjected to a progressive cool down from 1300^{o} C to room temperature. Mudflat crack damage in the coating system resulted from the buildup of residual tensile stresses between the individual material constituents from thermal expansion mismatch. A 2-parameter Weibull distribution characterized the coating layer stochastic strength response and the effect of the Weibull modulus on the formation of damage was studied here.

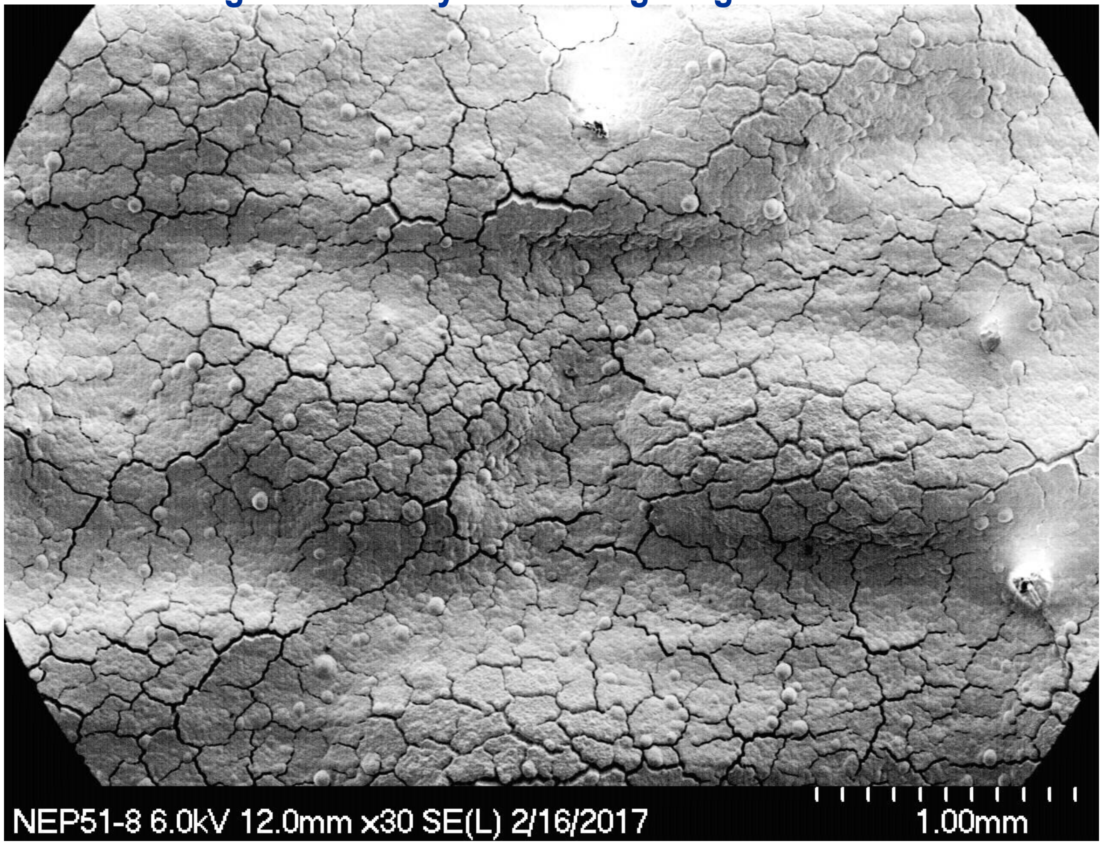
Surface cracking allows environmental penetration, accelerating material degradation. Simulating the process / physics of crack formation is necessary for development of an EBC design & life prediction methodology

Mud-flat cracking examples:

Rare earth silicate EBC after heat flux testing

1

Figure courtesy of Dr. Dongming Zhu



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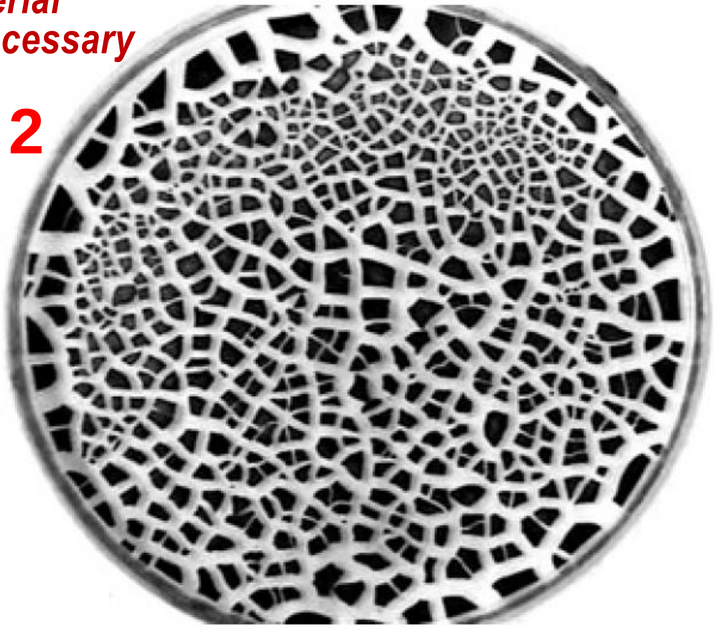


Desiccated layer of synthetic clay suspension on circular petri dish (10 cm in diameter)[a]

3

X-MAS Cookie

Courtesy of Dr. Roy Sullivan

(a) Sadhukhan, et al.: "Desiccation Cracks on Different Substrates: Simulation by a Spring Network Model." J. of Physics: Condensed Matter, Vol. 19, 10pp, 2007.

Objective

1. Demonstrate a generalized life prediction tool for EBC subcomponent subjected to thermomechanical loading that captures some of the salient features of EBC ***mechanical*** failure modes

2. Demonstrate with this tool that a 2-parmeter Weibull distribution describing brittle material failure strength can stimulate spontaneous formation of mud-flat cracking in a multilayered coating system on a rigid substrate when a thermal cool-down load is applied

Outline

1. FEAMAC/CARES code / methodology
2. Applying FEAMAC/CARES to simulate stochastic damage initiation and progression in an environmental barrier coating (EBC) from thermal cool-down from an initial processing temperature
   - Demonstrate methodology and contrast prediction of damage pattern formation for three different values of Weibull modulus (the Weibull “scatter” parameter or “shape” parameter *m*) in an **Ytterbium Monosilicate** multi-layered coating system on a silicon carbide substrate

- 2-D finite element model of EBC coating cross-section
- 3-D finite element model of 1cm diameter EBC coated disk

FEAMAC/CARES:

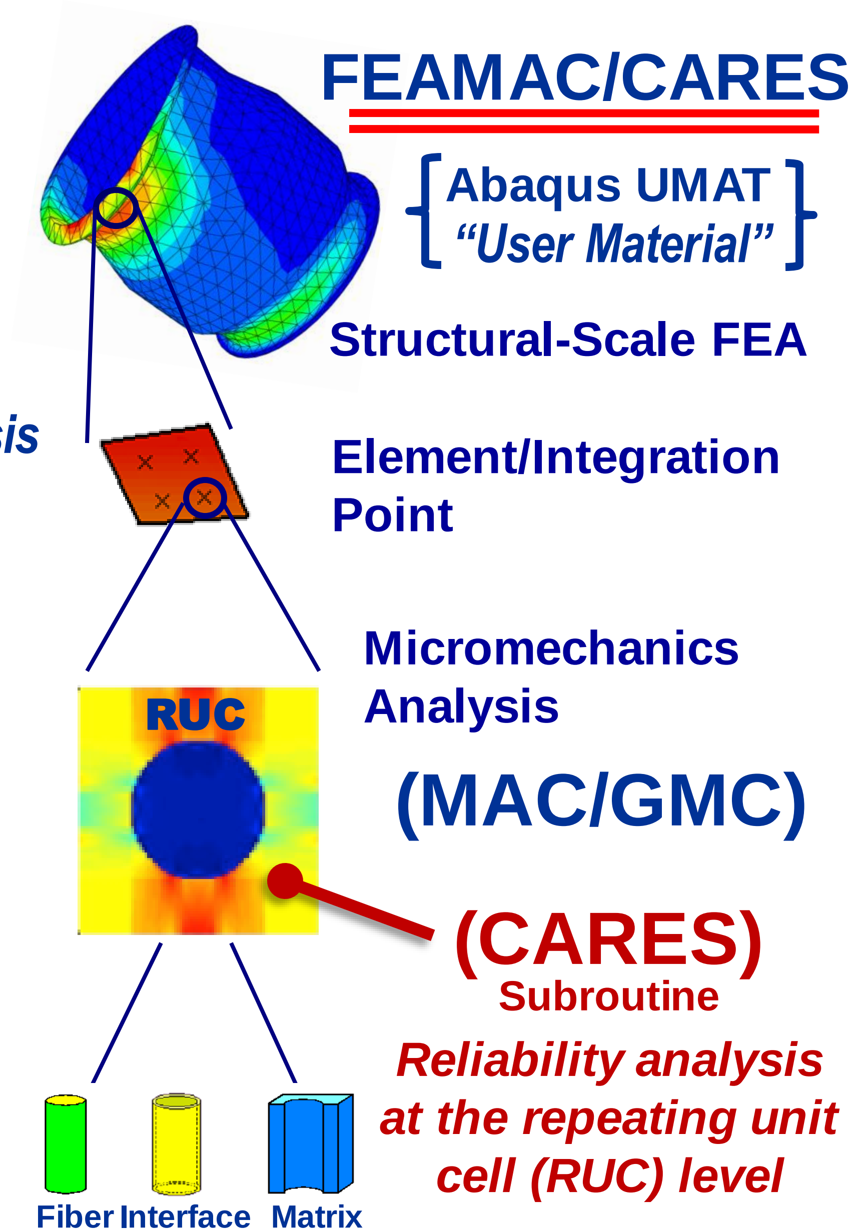
Stochastic-strength-based Life Prediction & Component Design of Composites

Combines codes:

- *MAC/GMC composite micromechanics analysis*
- *CARES/Life ceramics reliability analysis*
- *Abaqus finite element analysis*

❖ FEAMAC/CARES Capability:

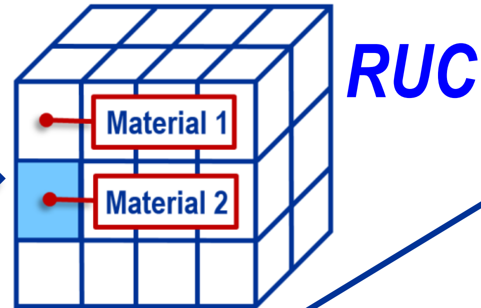
- Individual constituent and component level probability of failure tracked (for failure initiation)
- Progressive damage capability/simulation
  - ➢ Subcells elastic modulus reduced (killed) at random failure thresholds



Stochastic Progressive Damage Criterion

Calculate failure probability, P_f, for each material constituent of the RUC associated with an element integration point

CARES calculated $P_{f\,(CARES)}$ of RUC



Random number generated $P_{f(Random)}$ of RUC

$P_{f\,(CARES)} \geq P_{f\,(Random)}$

Yes → Fail *all* material constituent subcells ➤ *Kill elastic modulus*

No → Don’t fail subcells

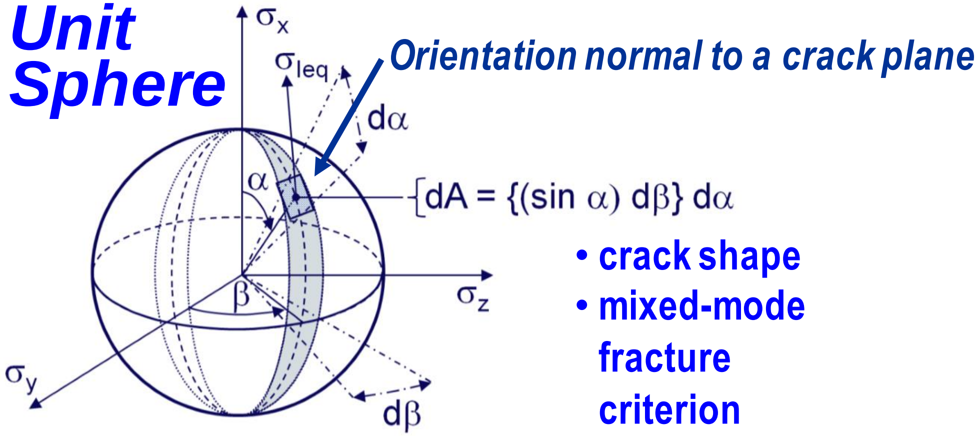
CARES combines Weibull Weakest Link theory with concepts of linear elastic fracture mechanics using the ***Batdorf Unit Sphere model***

Fracture-mechanics-based *multiaxial* failure criteria to predict probability of failure / damage of a material constituent over time

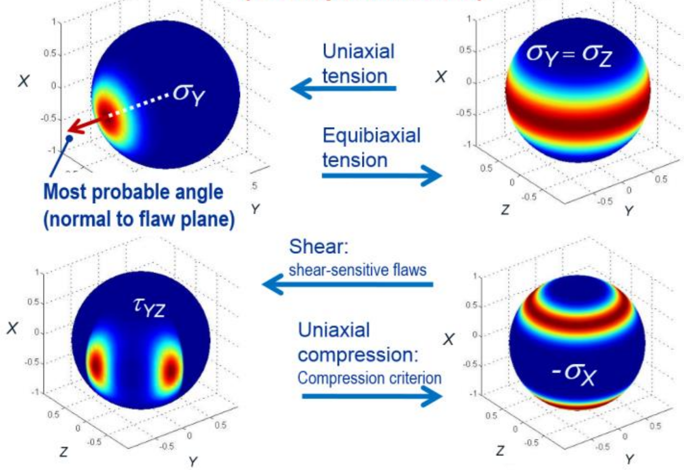
Unit Sphere Probability Density Distribution For Orientation Of Critical Flaws

(Isotropic Material)

Unit Sphere



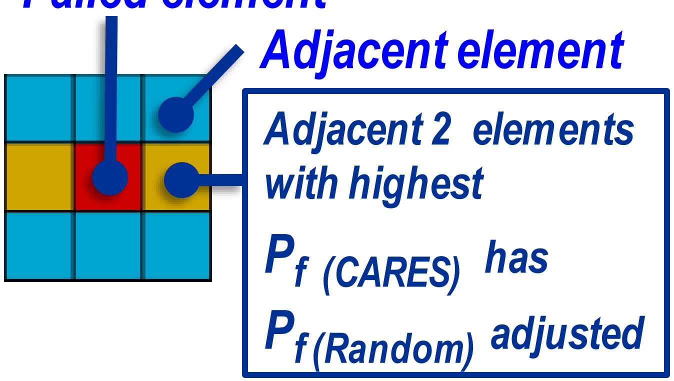
- crack shape
- mixed-mode fracture criterion



Anisotropic material capability also

Cellular Automaton:

Failure probability thresholds of elements adjacent to failed elements adjusted to promote a biased damage direction



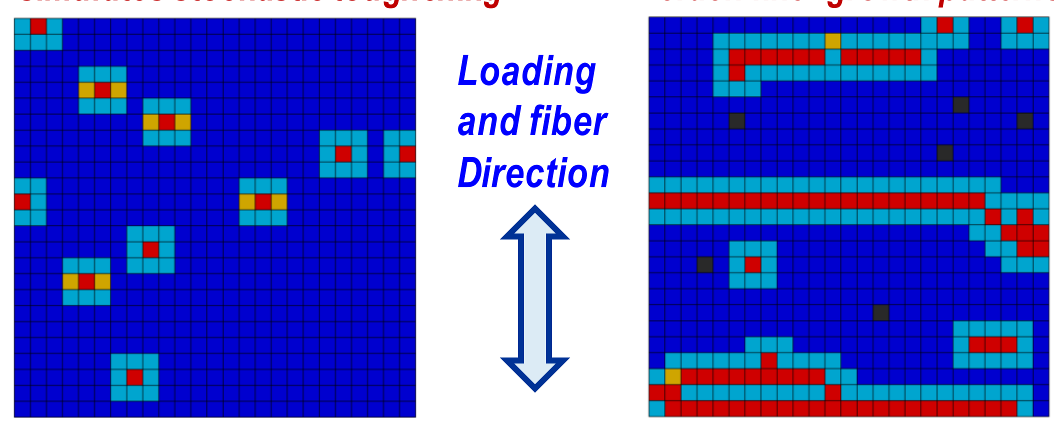
0^{o} Composite ply for 25x25 FEA mesh of shell elements

Random element failure:

- ➢ *simulates stochastic toughening*

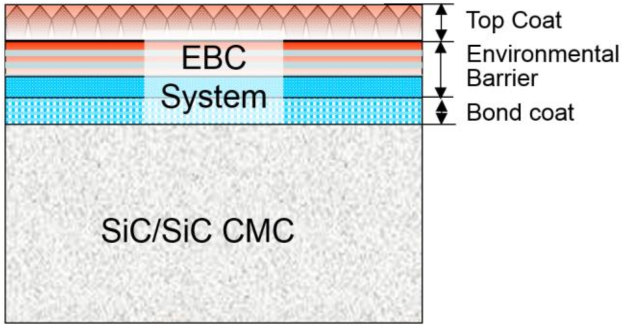
Cellular automaton:

- ➢ *"crack-like" growth patterns*



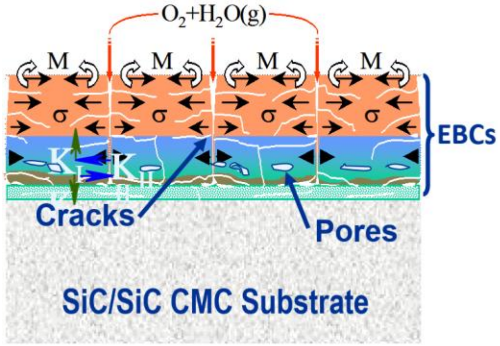
Environmental Barrier Coating Failure/Life Modeling

Environmental barrier coatings (EBCs) display complex failure modes that evolve with time and fluctuating load



APPROACH:

Use FEAMAC/CAREs to simulate stochastic damage initiation and progression in an environmental barrier coating (EBC) from thermal cool-down from an initial processing temperature



Generalized EBC Failure Mechanisms

APPLIED TO:

A Ytterbium monosilicate (YBSM) EBC on a silicon carbide substrate undergoing thermal cool down from an initial processing or annealing temperature of 1300° C to 23° C

DESIRED RESULTS & BENEFITS:

- Predict onset of coating microcracking; crack propagation, delamination, and spallation
- Demonstrate ability to reproduce or simulate formation of mud-flat cracking and create a "parameter space" with which these failure mechanisms can be explored and controlled
- Demonstrate a physically based model that more accurately reproduces progressive damage failure modes under generalized transient loading conditions

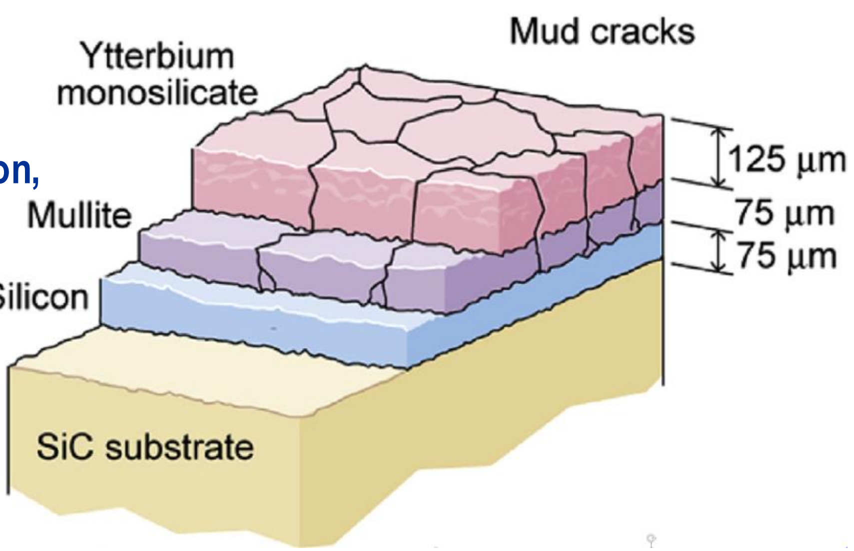


Figure adapted from Richards et al.: Fracture Mechanisms of Ytterbium Monosilicate Environmental barrier coatings during cyclic thermal exposure" Acta Materialia, 103, pp. 448-460, 2016.

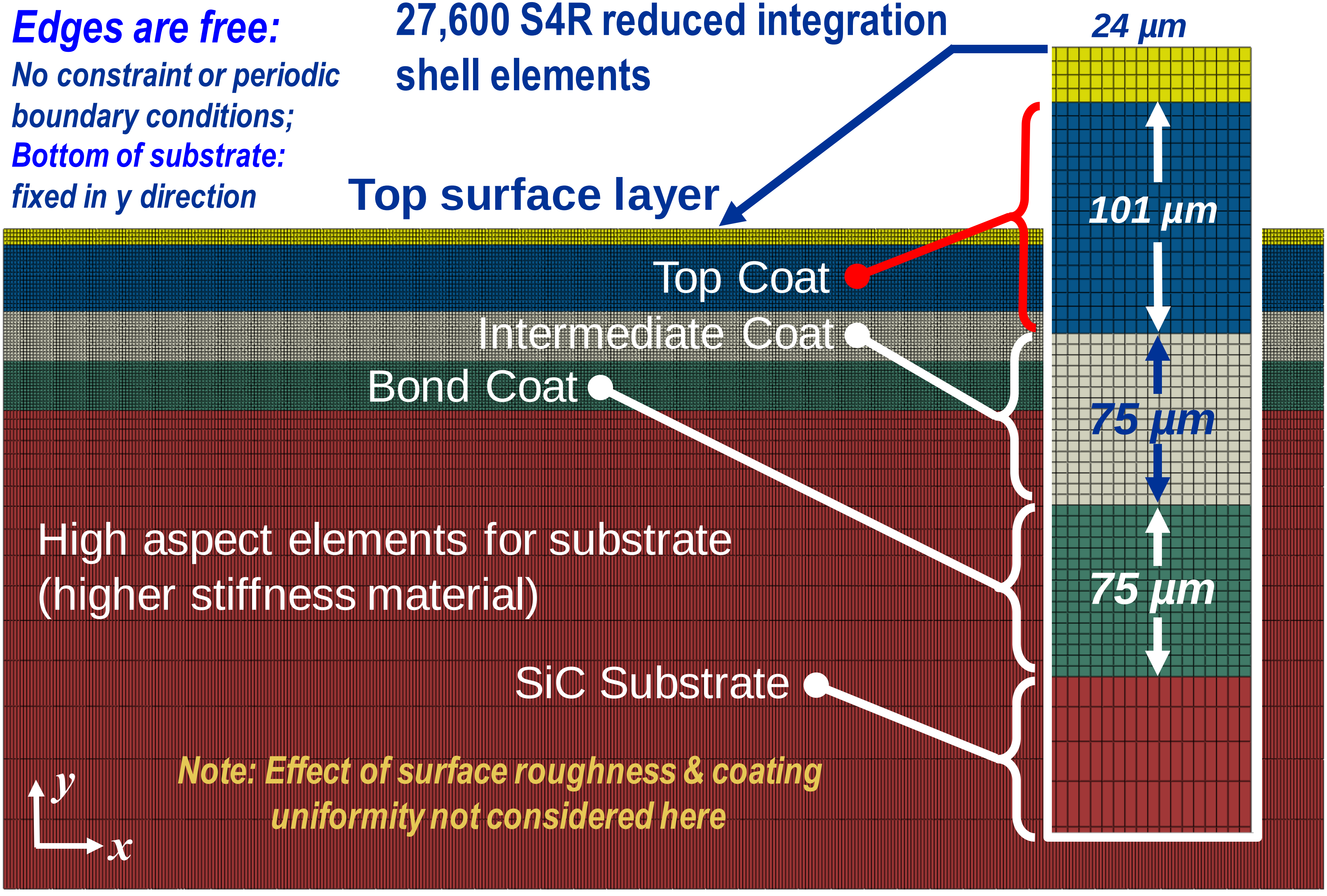
Environmental Barrier Coating Failure/Life Modeling
Our approach…

- **Each coating layer is modeled as a discrete material component in FE model**
- **each coating layer is described by a separate MAC/GMC input file.**
- **A very simple MAC/GMC repeating unit cell (RUC) of a material element:**
  - **RUC consists of only *a single (monolithic) material subcell* representing one of the constituent materials of the EBC material system or substrate.**
- **Damage (defined as failure) for an element or element integration point is an abrupt (99%) step function stiffness reduction**
- **As a consequence; the finite element model uses many small cubic-shaped elements because a failed element is representative of a crack or discontinuity**
- **Irregular top surface (surface roughness) is not initially modeled here with finite elements. Instead a low Weibull modulus top material layer can be optionally substituted to imitate the wide scatter in fracture strength the top surface would induce**

2-D EBC Cross-Section FE model (2mm X 1mm)

Edges are free:
No constraint or periodic boundary conditions;
Bottom of substrate:
fixed in y direction

27,600 S4R reduced integration shell elements



Properties Table

(Tensile strength/Weibull parameters adopted from Abdul-Aziz et al.[2], None listed in Richards et al.[1])

Report	Material	E (Gpa)	Poisson, v	Therm. Expan., α, m/m/°C · 10^{-6}	Weibull modulus, m	Weibull Scale Parameter, σ_o , MPa·mm$^{3/m}$
YBSM **(Richards et al. 2016)[1]** Using 50% reduced properties listed in reference	Top Coat Suface: Ytterbium monosilicate	86	0.27	7.5	2.5 ; 5. ; 10.	14 (assumed)
	Top Coat: Ytterbium monosilicate	86	0.27	7.5	2.5 ; 5. ; 10.	28 (assumed)
	Intermediate Coat: Mullite	110	0.28	5.3	2.5 ; 5. ; 10.	28 (assumed)
	Bond Coat: Silicon	82	0.223	4.1	2.5 ; 5. ; 10.	40 (assumed)
	Substrate: SiC (Monolithic)	430	0.14	4.6	2.5 ; 5. ; 10.	321 (assumed)

[1] Richards et al.: Fracture Mechanisms of Ytterbium Monosilicate Environmental barrier coatings during cyclic thermal exposure" Acta Materialia, 103, pp. 448-460, 2016..

[2] Abdul-Aziz, et al.: "Durability Modeling of Environmental Barrier Coating (EBC) Using Finite Element Based Progressive Failure Analysis" J. of Ceramics, pp. 1-10, 2014

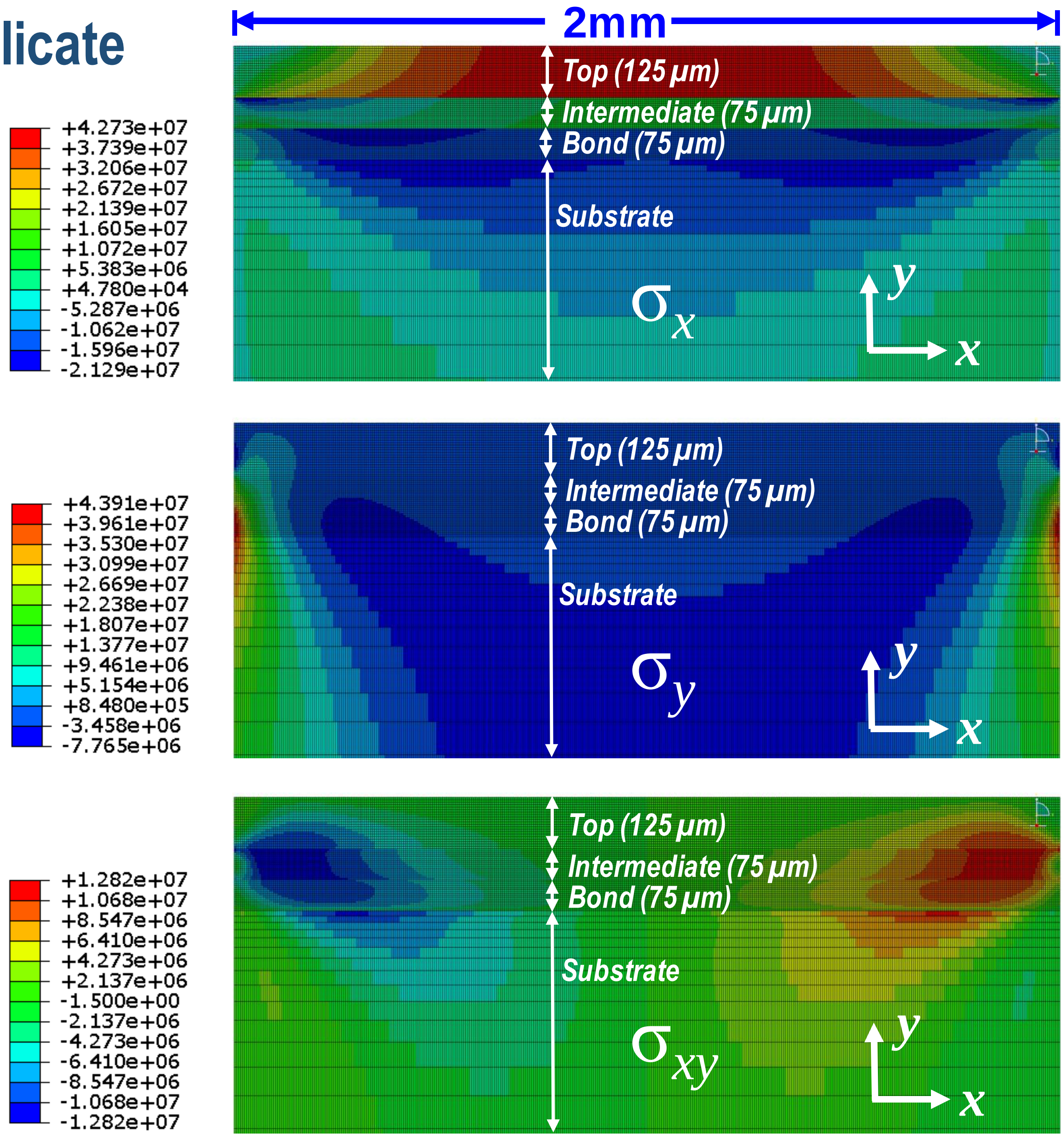
Ytterbium Monosilicate (YBSM)

Stresses (Pa) in undamaged EBC layers :

200° C cool-down from annealing Temp.

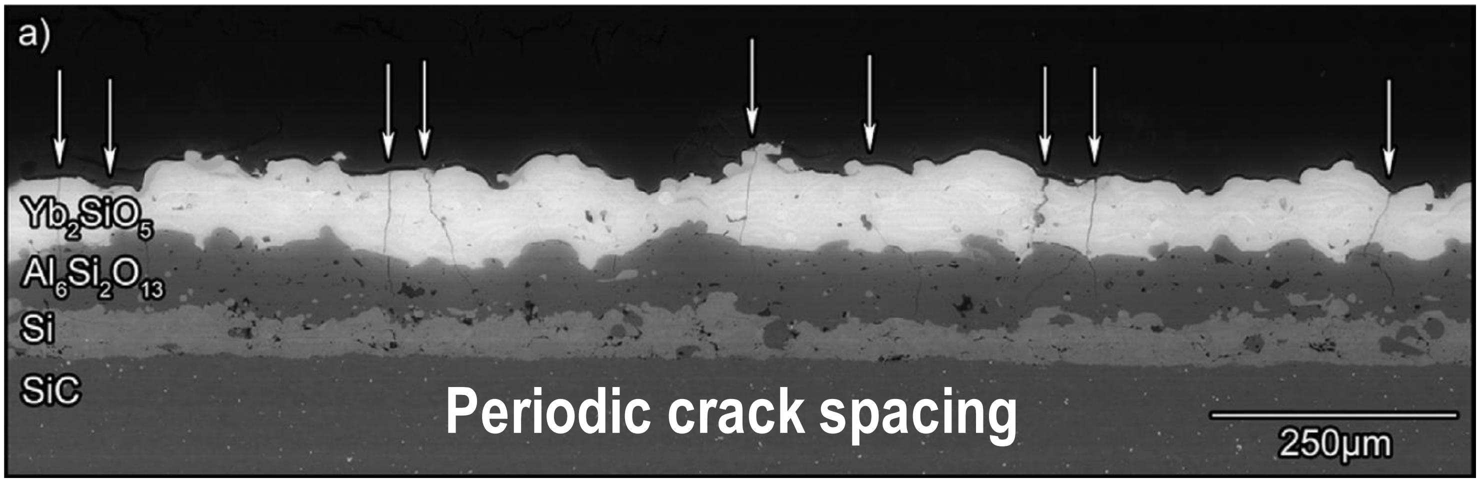
Left & right edges unconstrained

Bottom of substrate fixed in y direction



EBC coating after 1300 C annealing of as processed coating

Figure 6 from Richards et al.



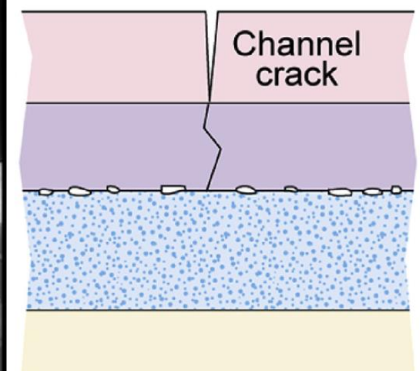
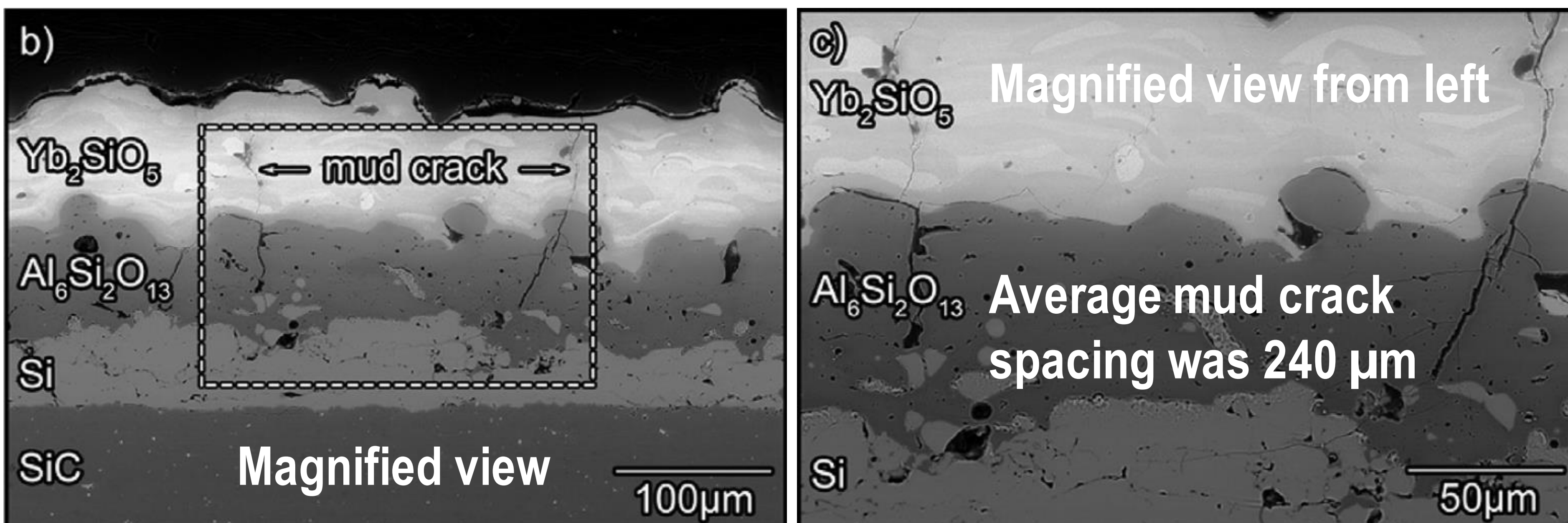


Fig. 1 from Richards et al.

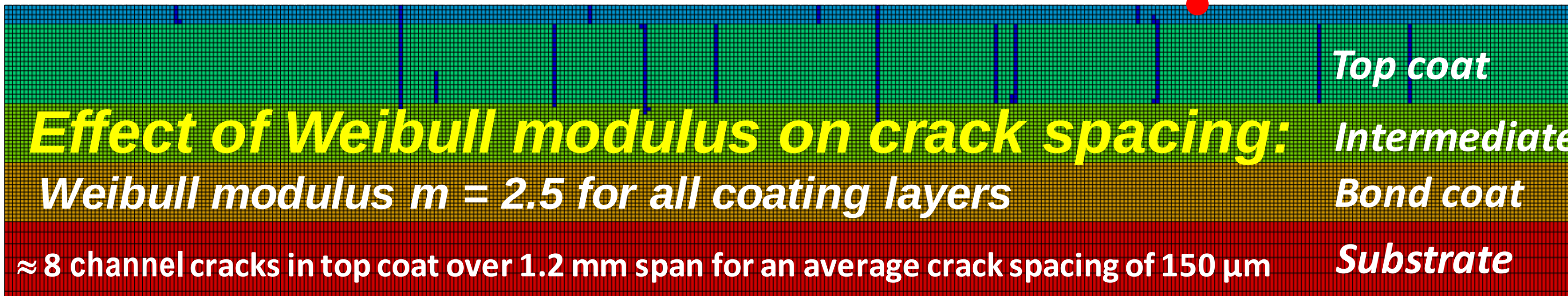


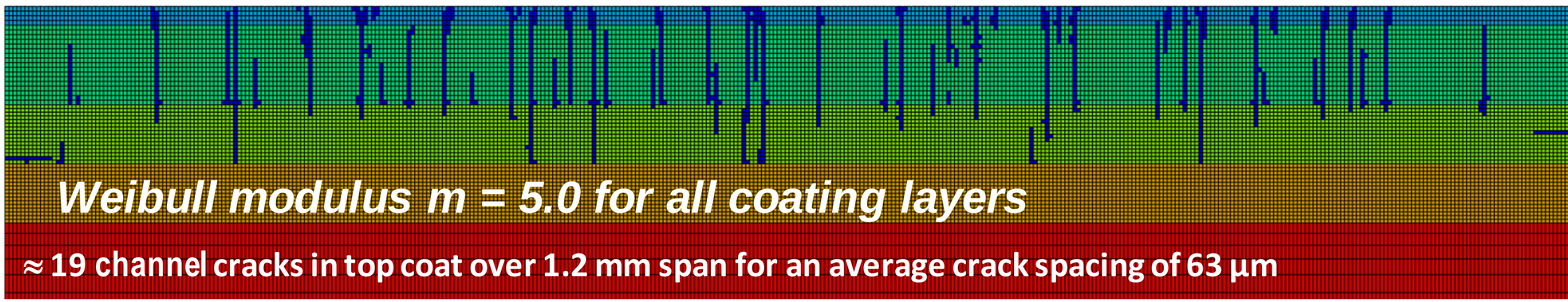
Richards et al.: Fracture Mechanisms of Ytterbium Monosilicate Environmental barrier coatings during cyclic thermal exposure" Acta Materialia, 103, pp. 448-460, 2016.

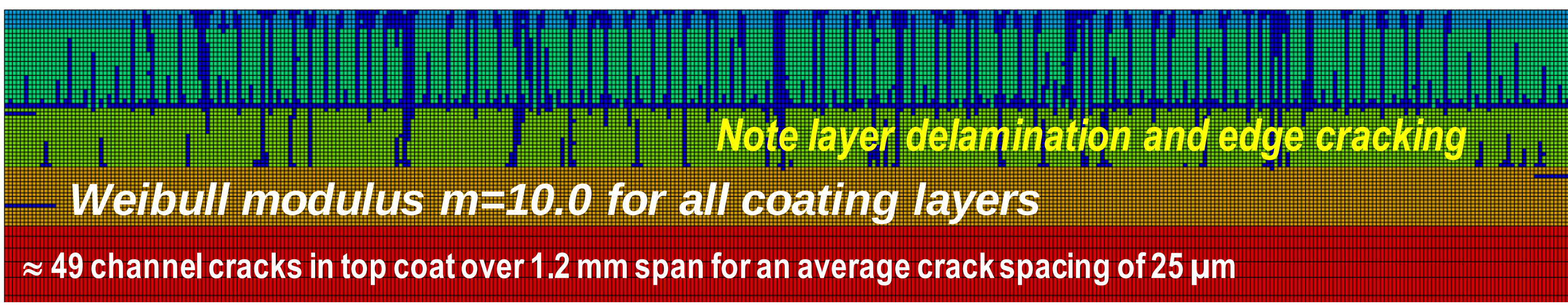
Ytterbium Monosilicate: 2D cross-sectional model

Damage at 23° C increment 810 ***Complete substrate not shown***

Top coat: low strength layer





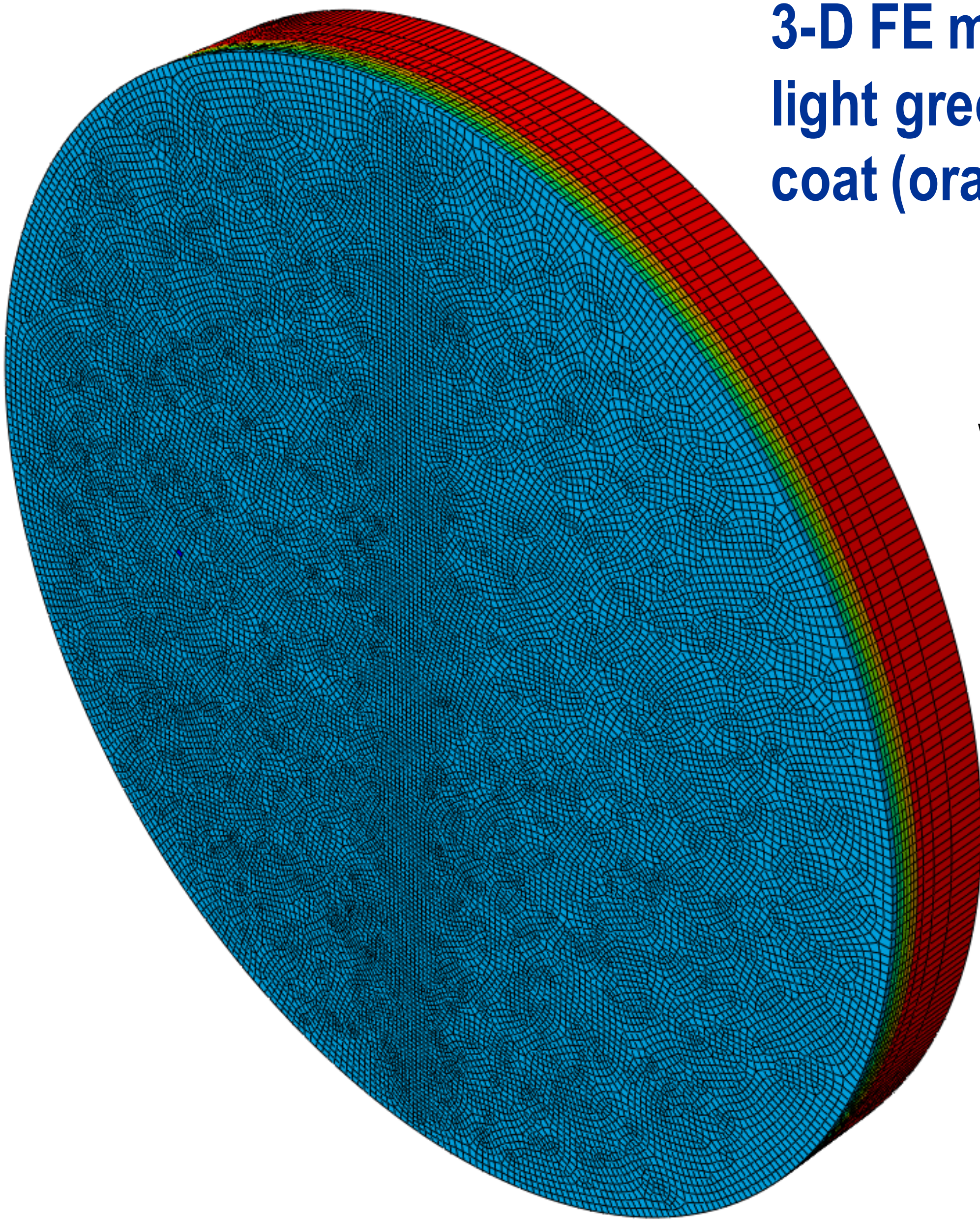


810 load increment steps (ramp load):

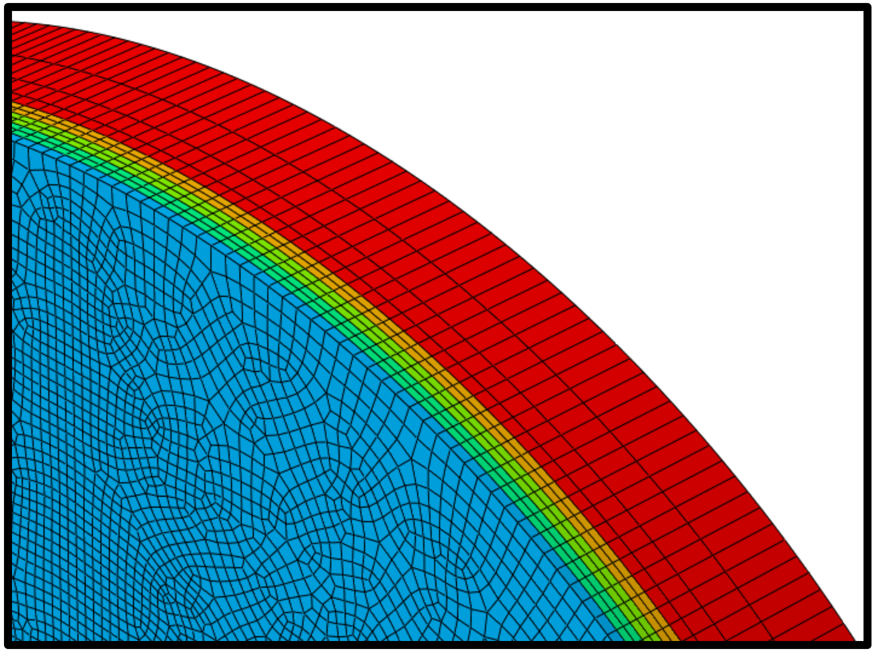
- First 10 early cool-down steps from 1300° C to 1200° C
- 800 increment steps from 1200° C to 23° C

But we don't know the temperature when microcracking initiated !

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



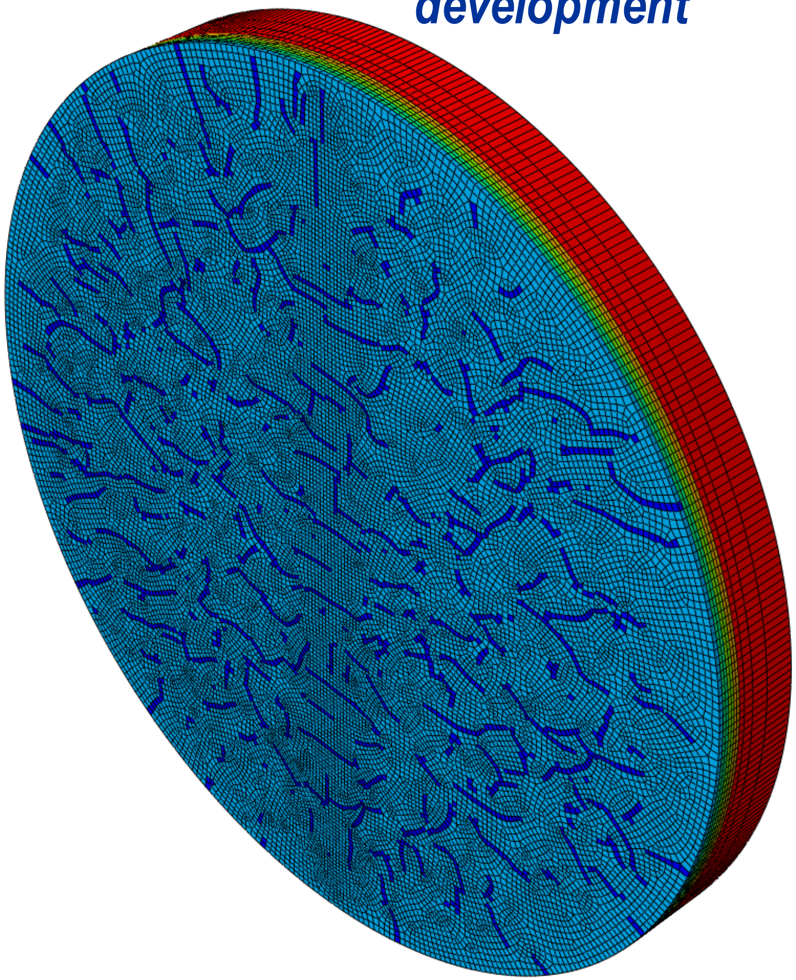
10mm dia. *X* 1mm thick disk model with about 280,000 solid C3D8R reduced integration elements



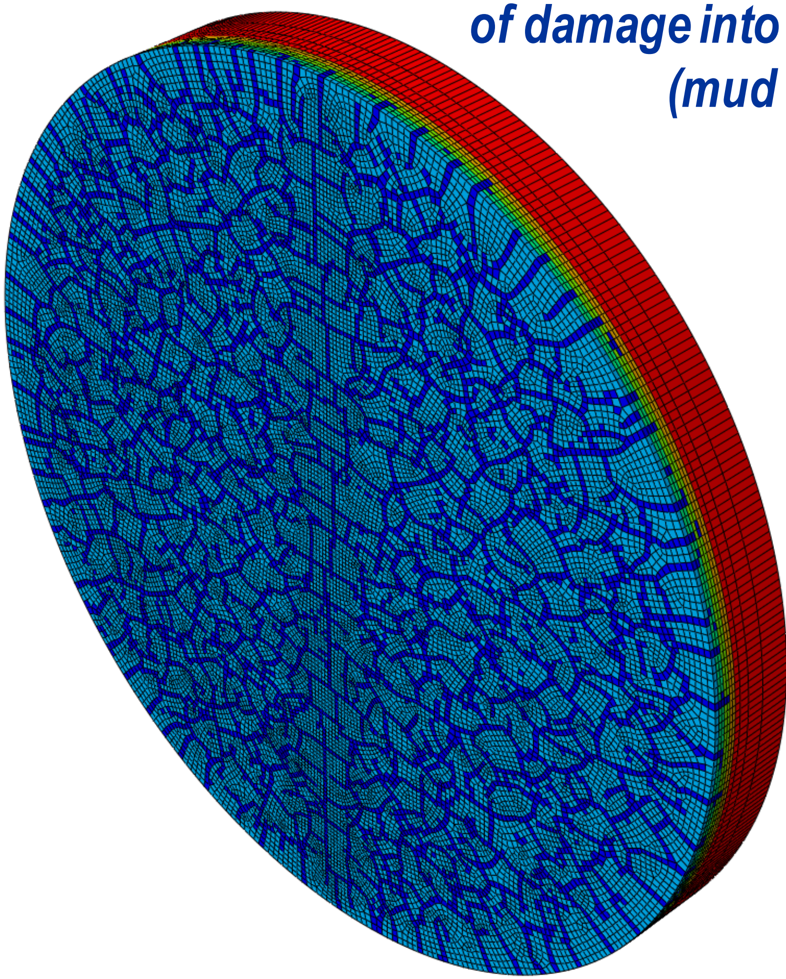
Damage Pattern In 3-D EBC Stochastic Progressive Damage Simulation

Spontaneous development of mud flats fragment into progressively smaller sizes when cooling from 1300° C to room temperature (fractal fracture pattern)

Early damage development



Advanced development of damage into cells (mud flats)



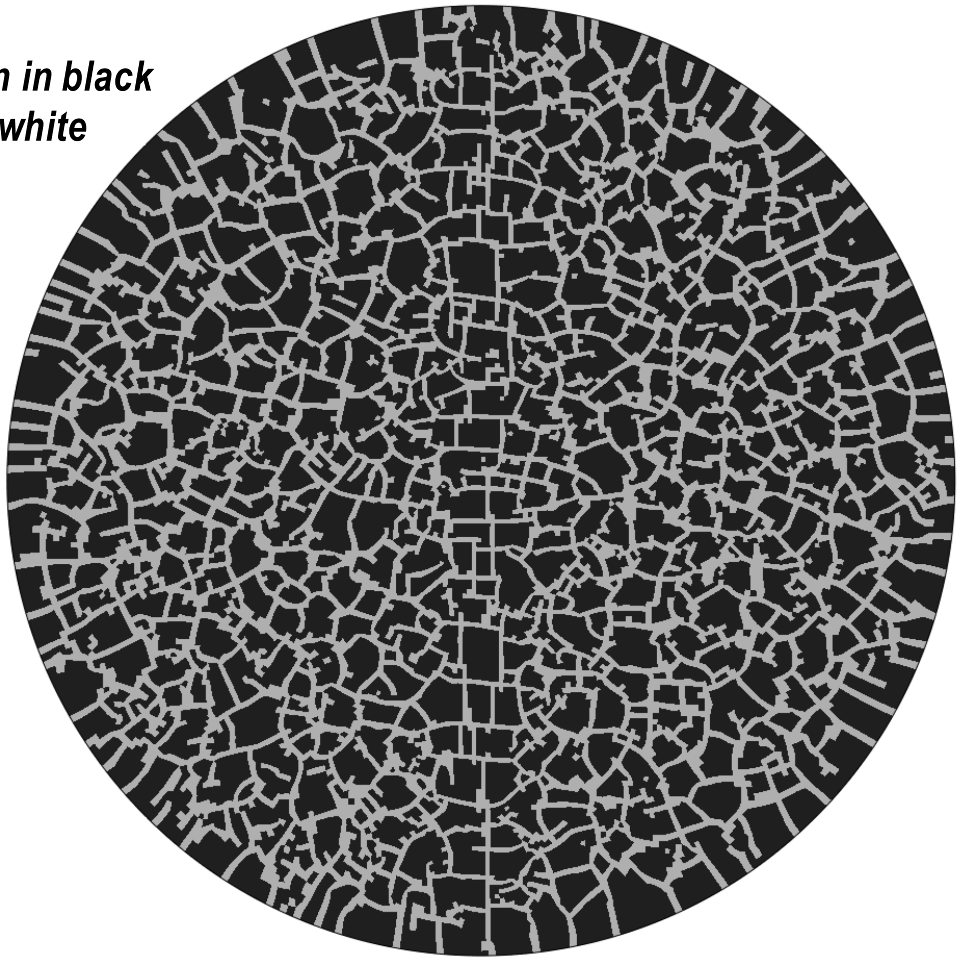
Weibull modulus m = 5

EBC coating cool down from 1300° C annealing/processing temp.

Simulation shows qualitative resemblance to mudflat cracking experiment

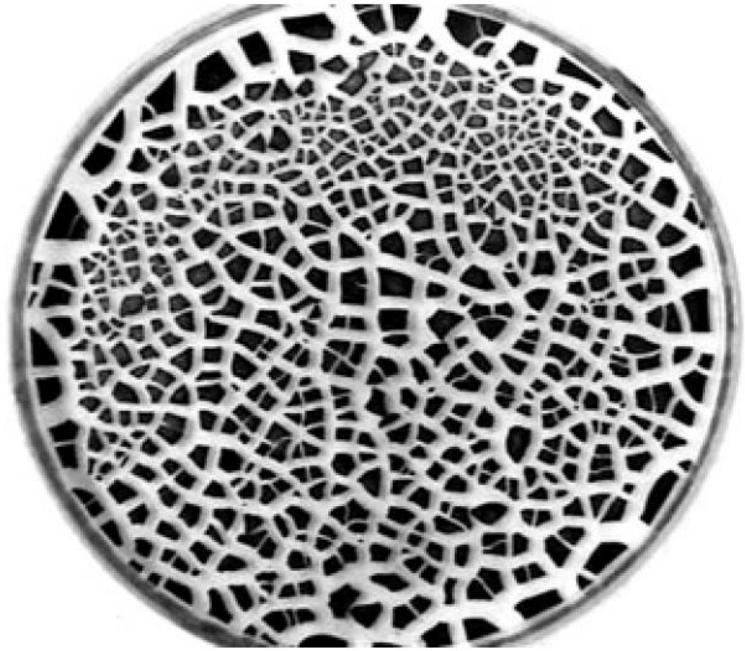
FEAMAC/CARES simulation of YBMS EBC

Shown in black & white



1 cm dia. EBC multilayer coating on SiC substrate
Weibull modulus *m* = 5.0
758.6° C (increment 160)

Real life:
Synthetic clay in petri dish



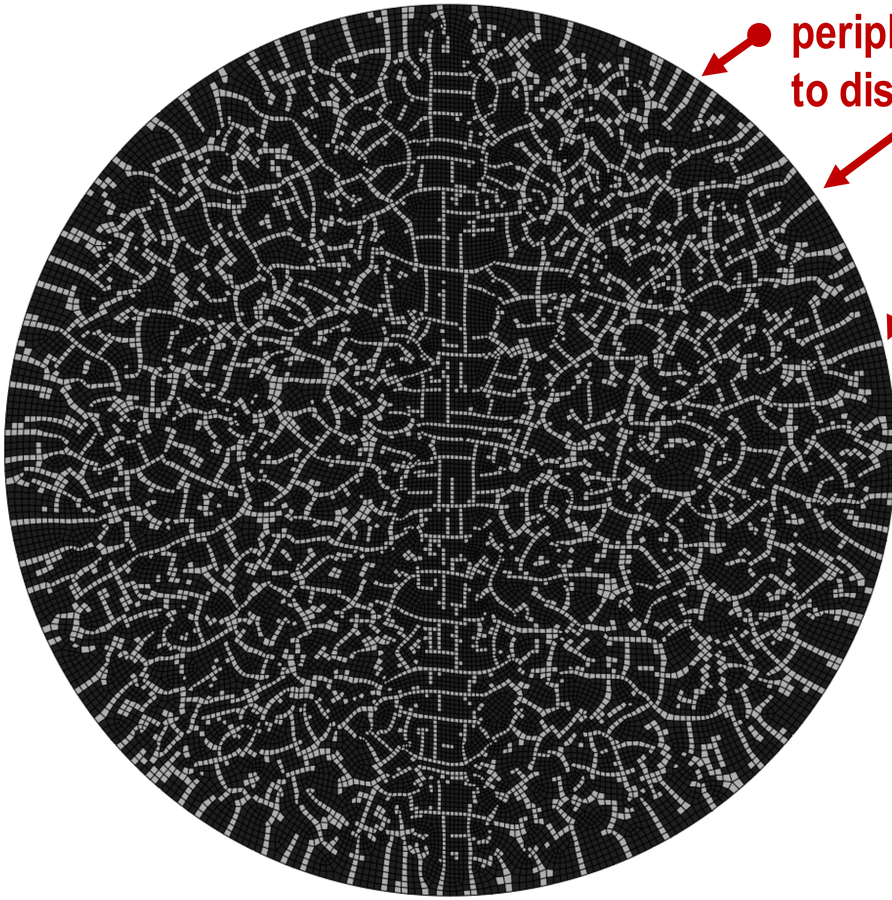
Desiccated layer of synthetic clay suspension on circular petri dish (10 cm in diameter)[a]

Sadhukhan, et al.: "Desiccation Cracks on Different Substrates: Simulation by a Spring Network Model." J. of Physics: Condensed Matter, Vol. 19, 10pp, 2007.

Channel cracks on Periphery :

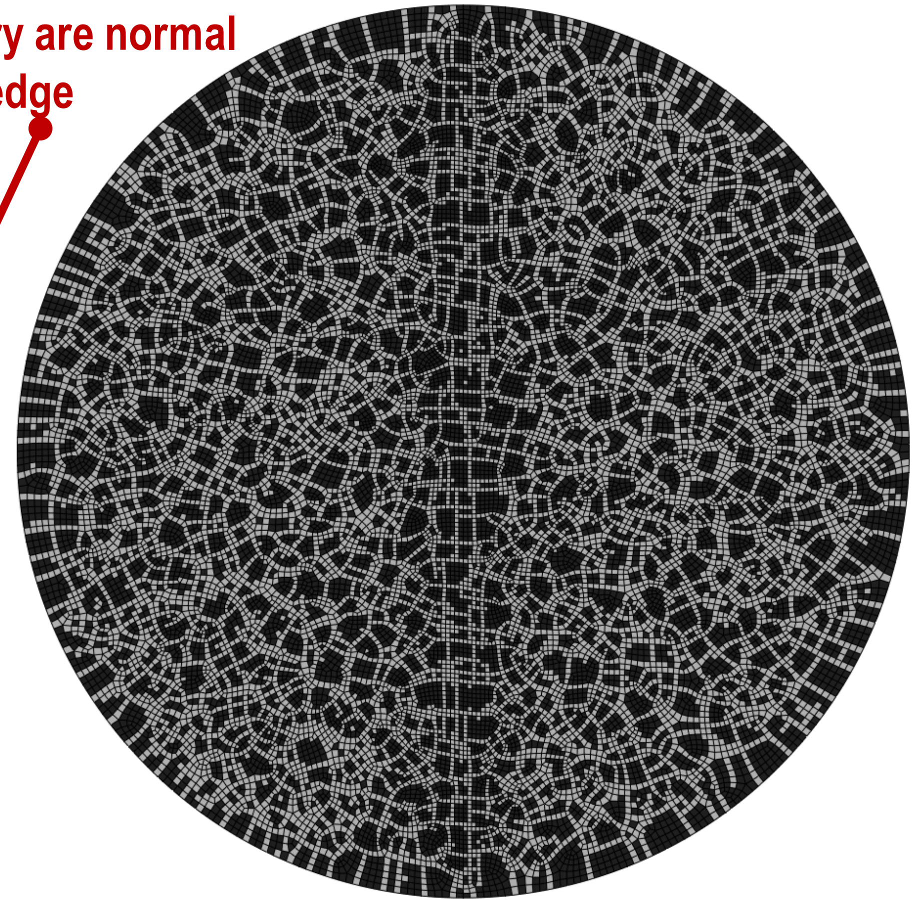
Damage on top surface for EBC coating Cool down from 1300° C to 23° C

Weibull modulus *m* = 2.5



Channel cracks on periphery are normal to disk edge

***m* = 5.0**

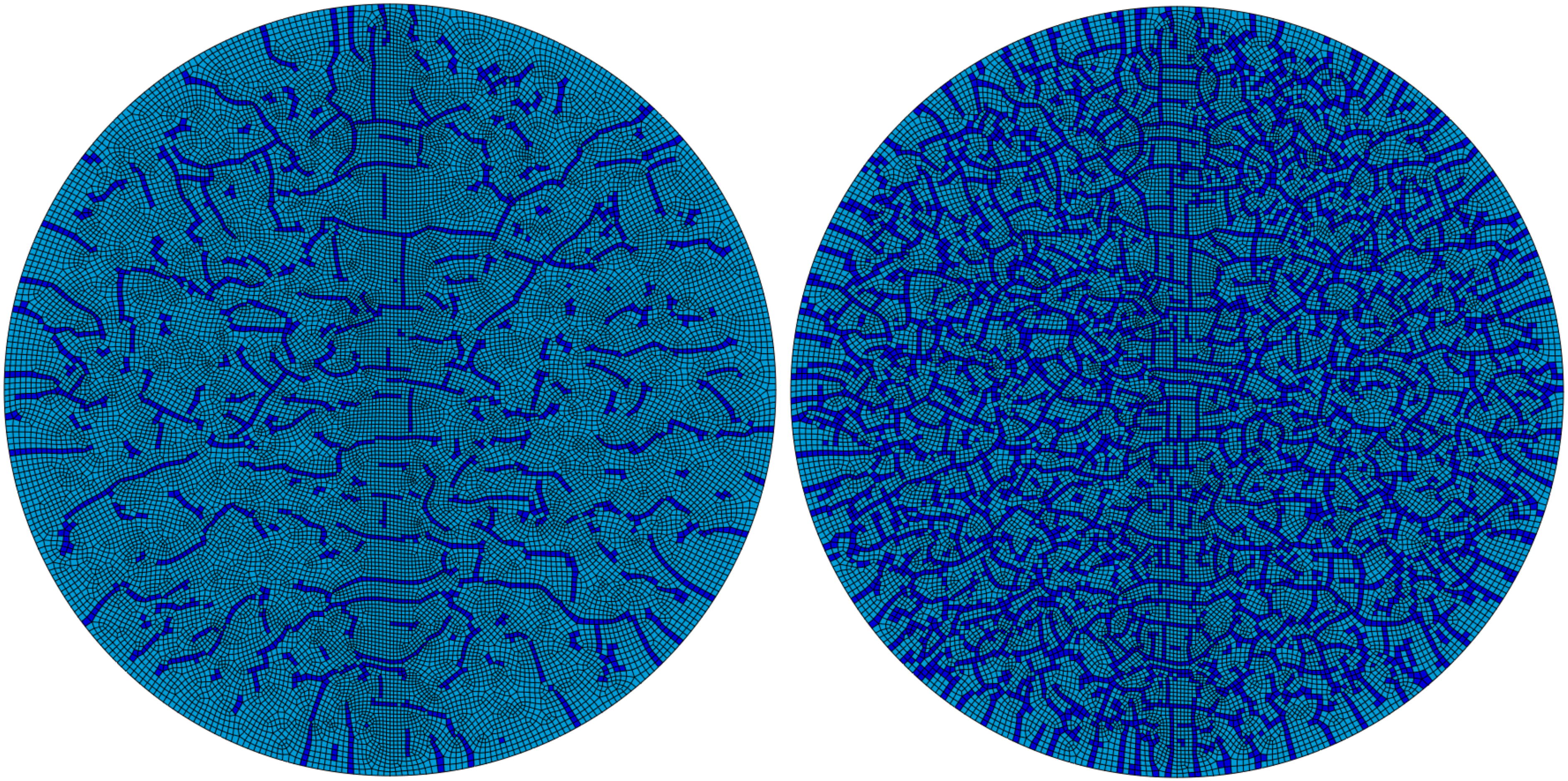


≈ 77 Channel cracks about periphery for 408 *μm average crack spacing*

≈ 102 Channel cracks about periphery for 308 *μm average crack spacing*

Damage of top surface for EBC coating:

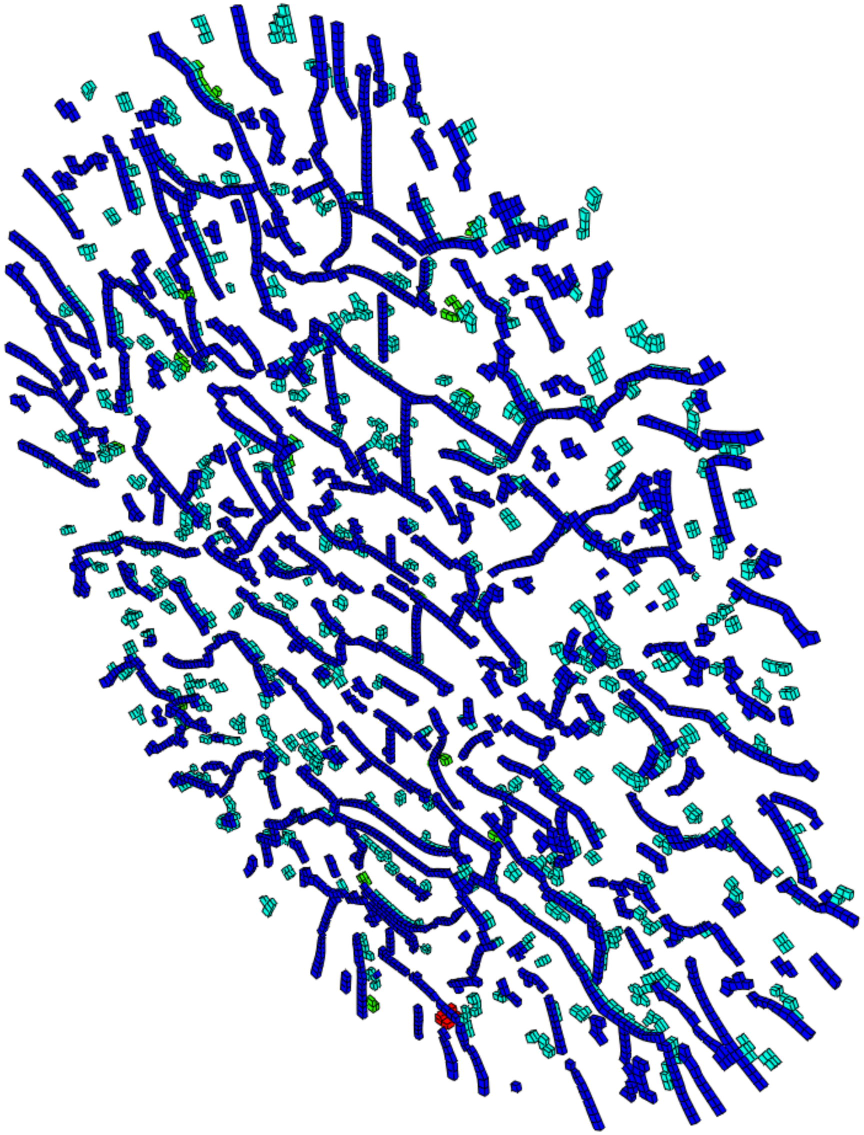
***Weibull modulus m* = 2.5**



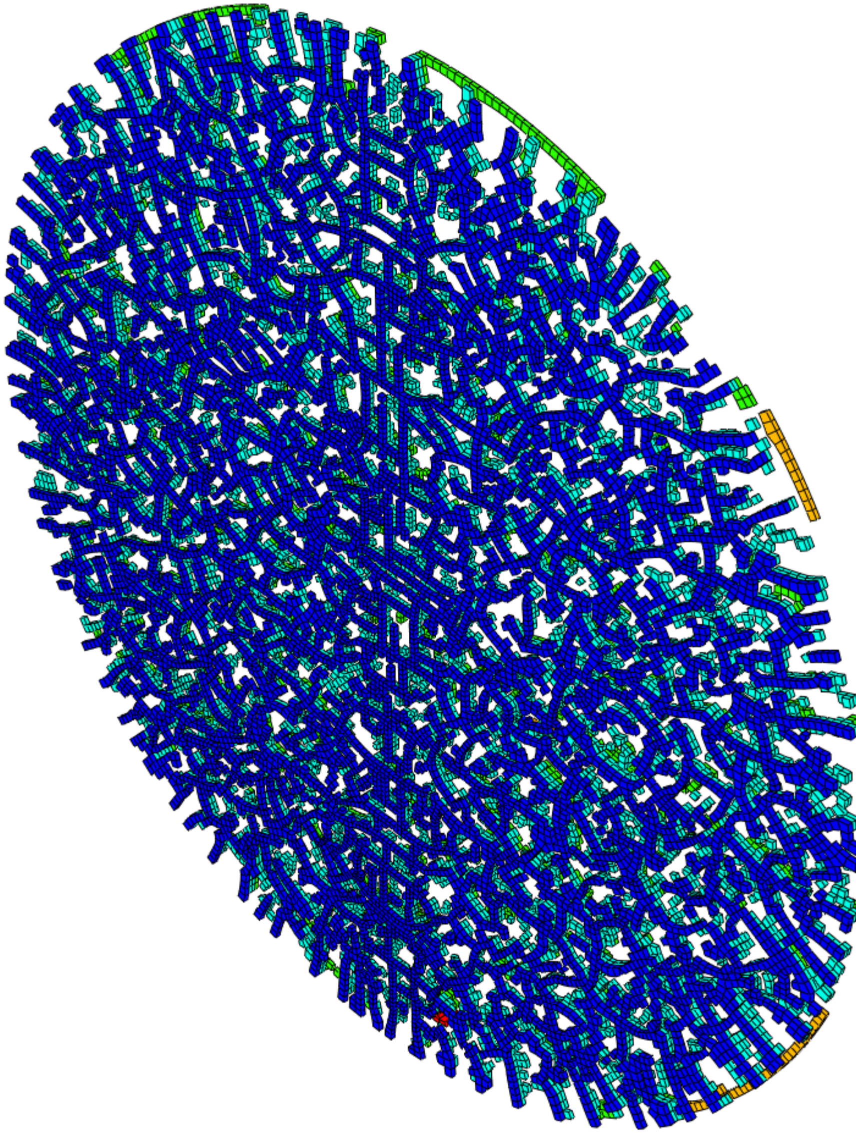
905.8° deg. C (110 steps) **23° deg. C (410 steps)**

Damage through the coating layers:

Weibull modulus m = 2.5



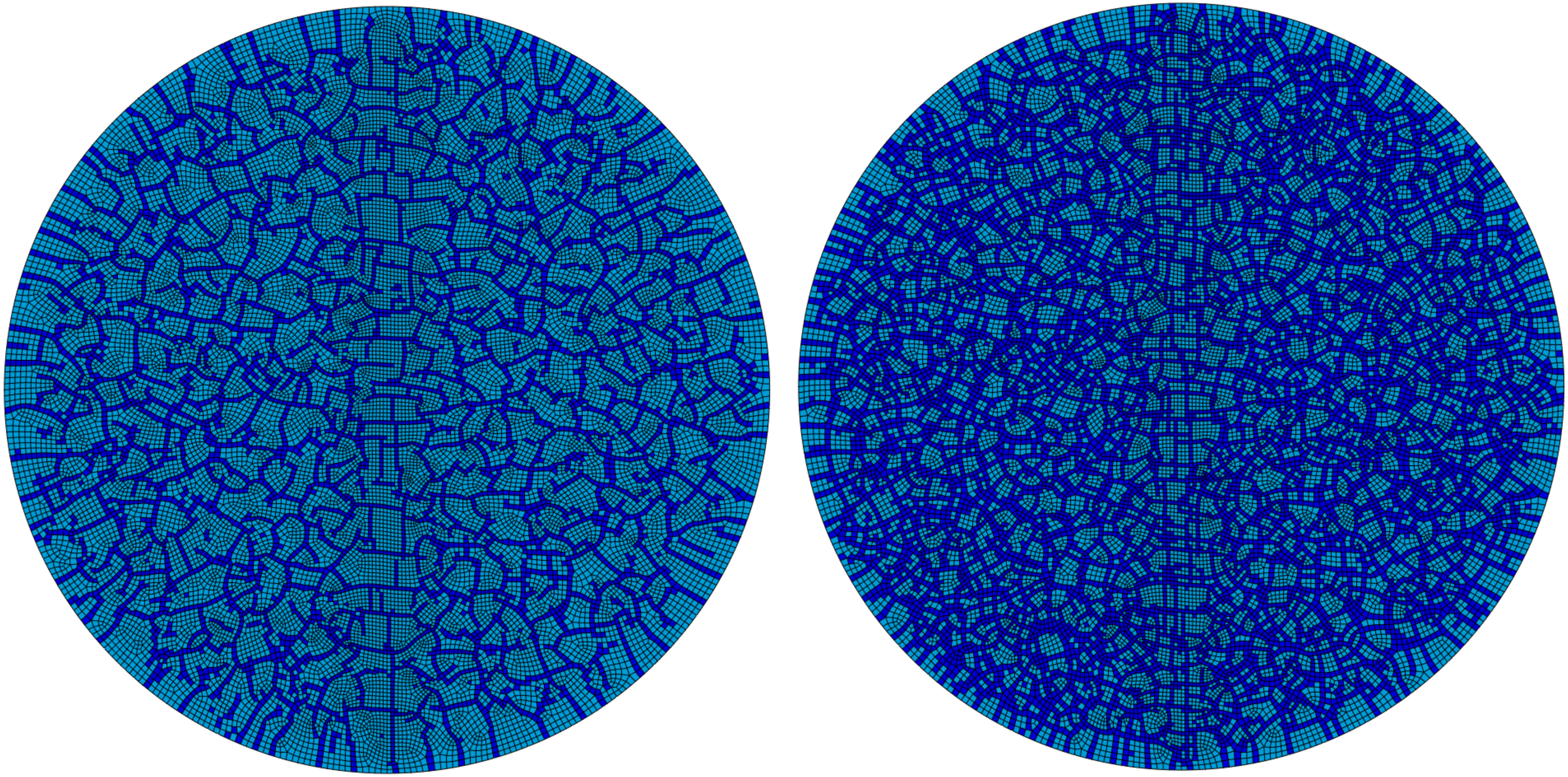
905.8° deg. C (110 steps)



23° deg. C (410 steps)

Damage of top surface for EBC coating:

Weibull modulus m = 5.0

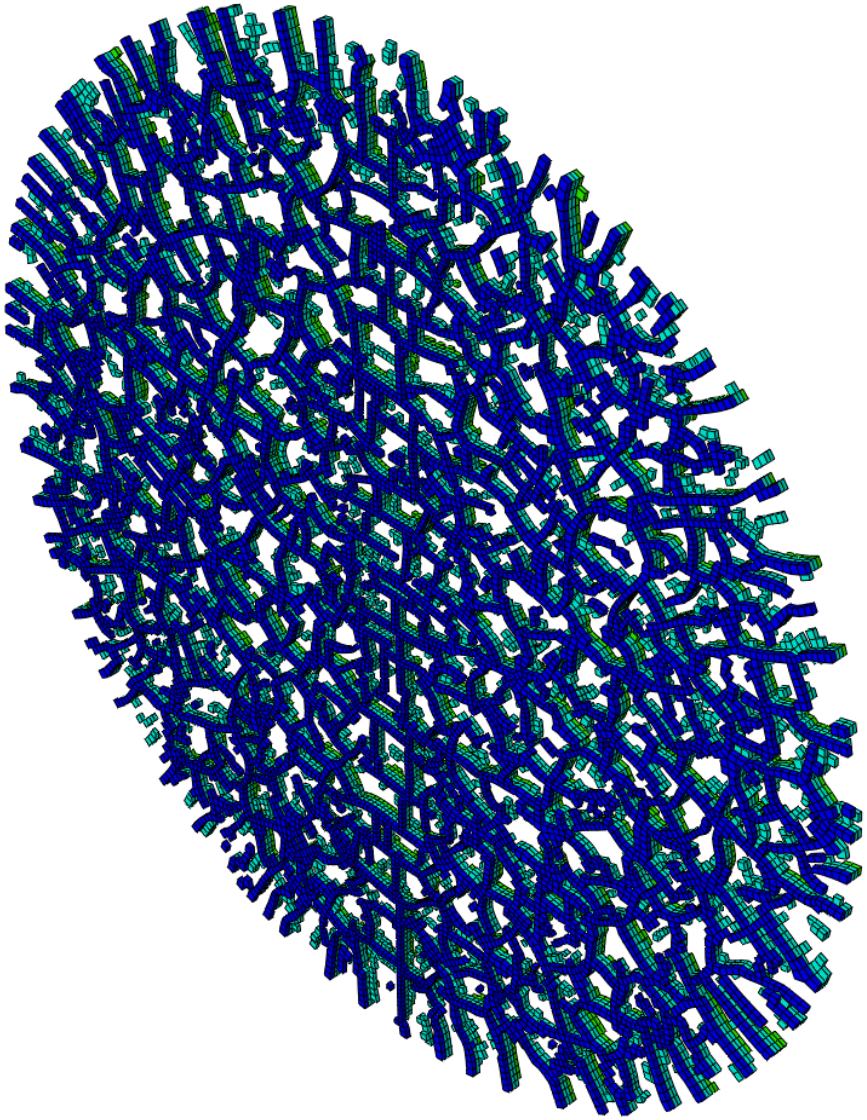


905.8° deg. C (110 steps)

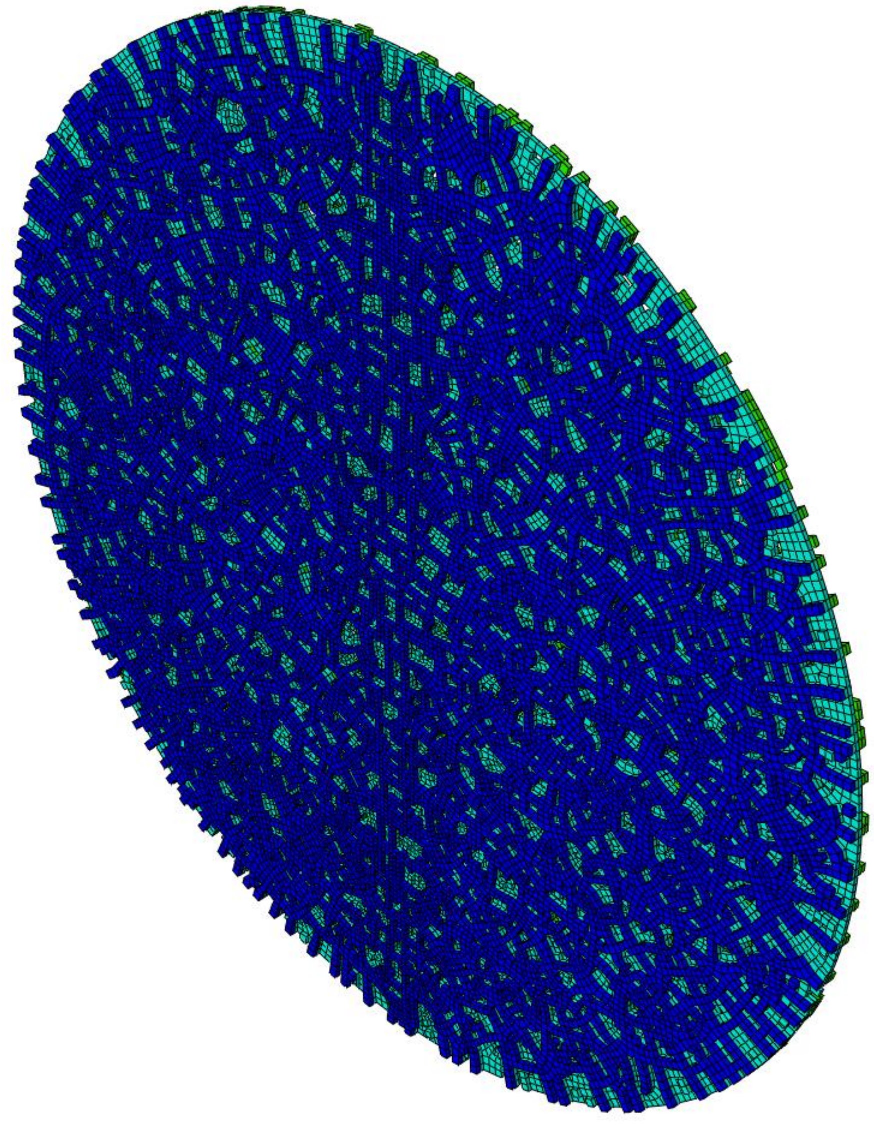
23° deg. C (410 steps)

Damage through the coating layers:

***Weibull modulus m* = 5.0**



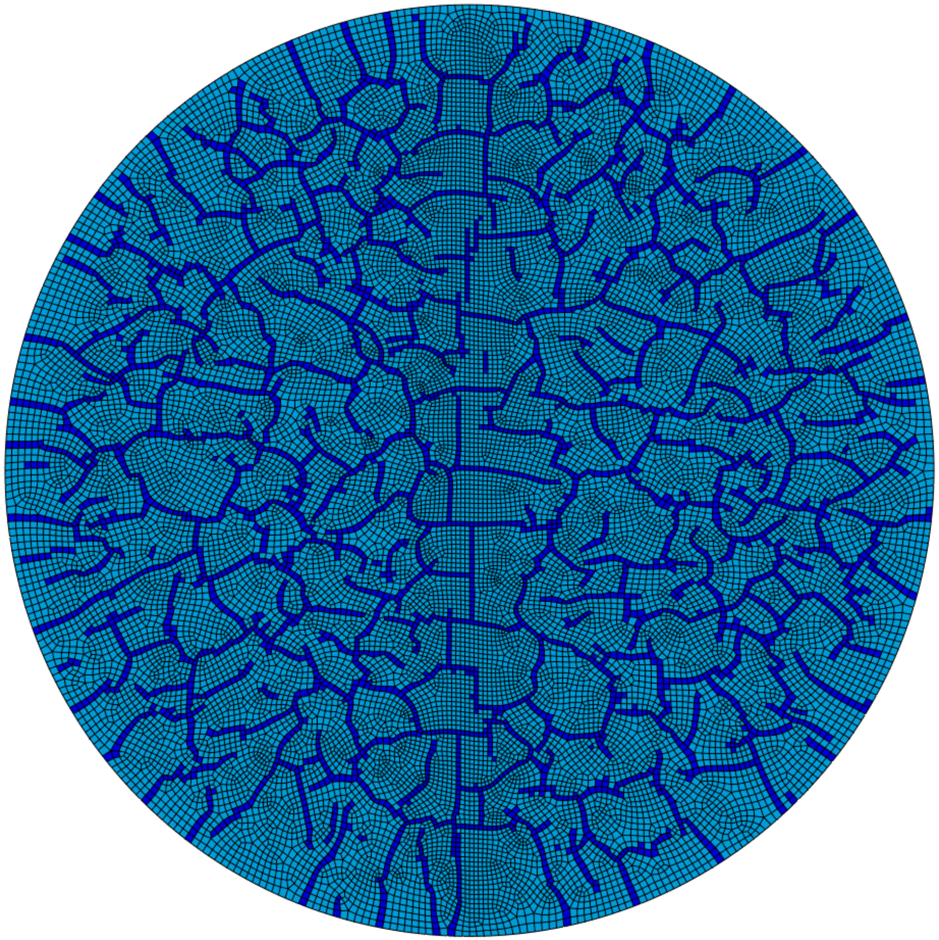
905.8° deg. C (110 steps)



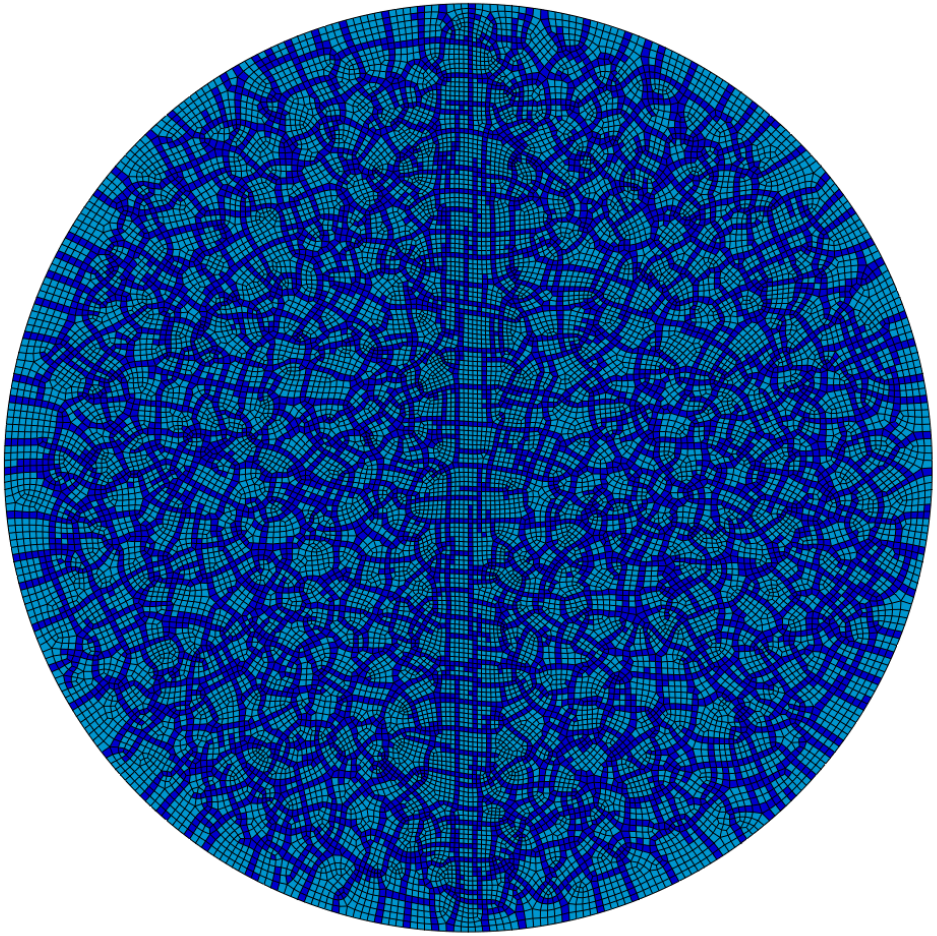
23° deg. C (410 steps)

Damage of top surface for EBC coating:

***Weibull modulus m* = 10.0**



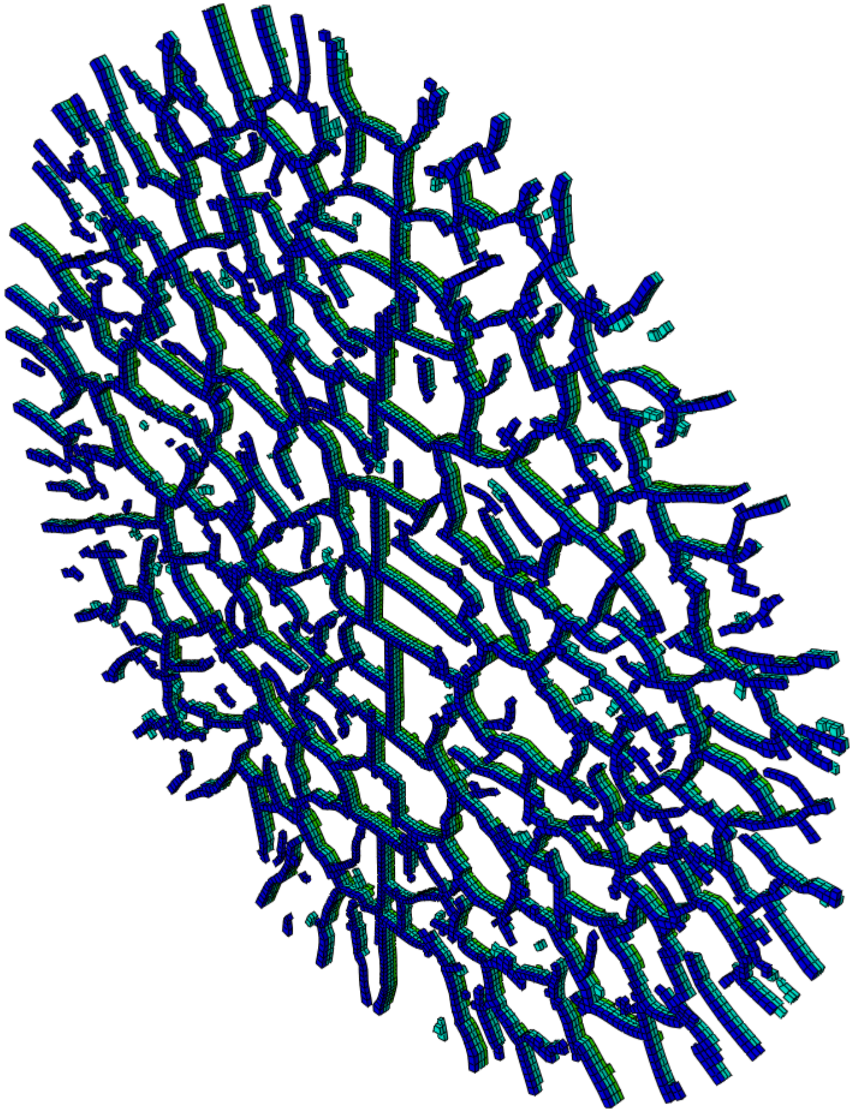
1150.0° deg. C (110 steps)



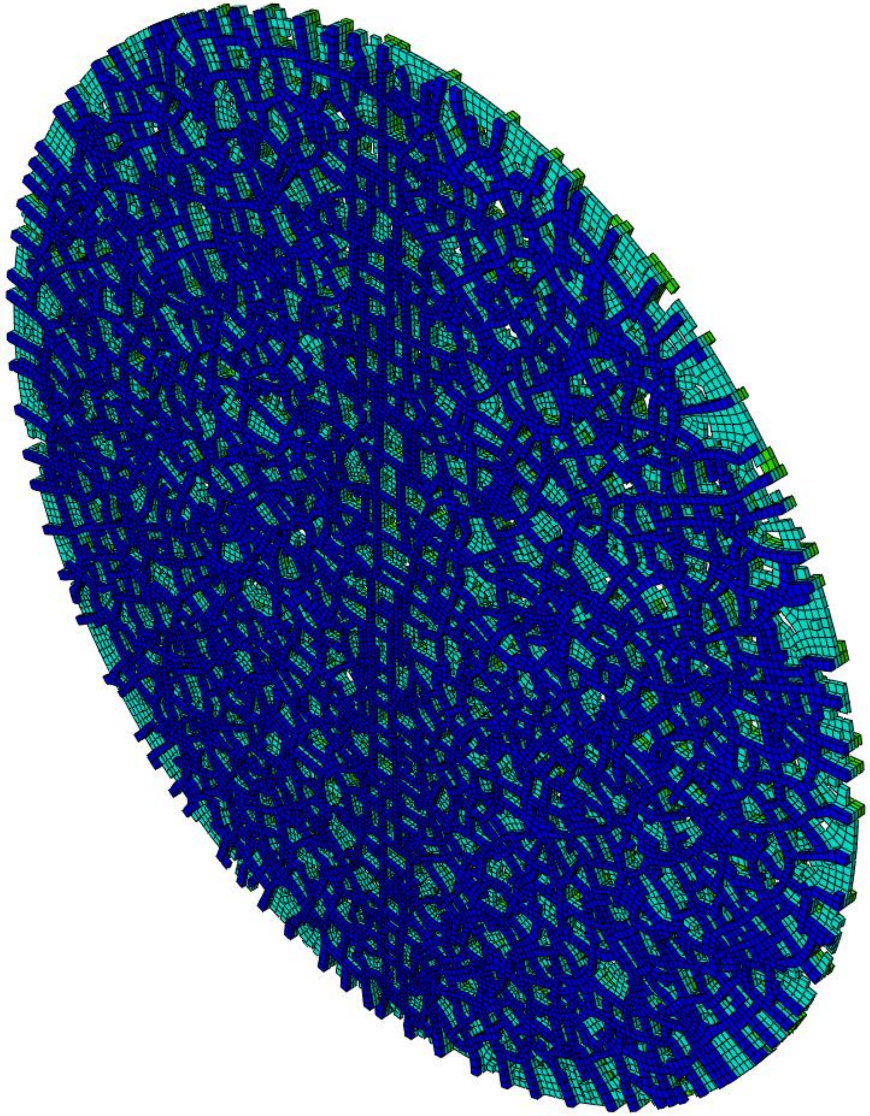
850° deg. C (410 steps)

Damage through the coating layers:

***Weibull modulus m* = 10.0**



1150.0° deg. C (110 steps)



850° deg. C (410 steps)

Conclusions

❖ Progressive damage simulation of EBC coated structure incorporating probabilistic material strength model demonstrated with the FEAMAC/CARES code

Problem investigated:

- Damage development resulting from build-up of residual stresses from thermal cool-down (from processing)
  - 3-D finite element model of disk-shaped specimen
  - 2-D model of material cross-section detailing individual coating layers

Shown was:

- Crack boundaries could be reasonably mimicked with dense mesh of low-aspect-ratio 2-D and 3-D elements and crack growth could be promoted with a cellular automation methodology

Observed was:

- Periodic cracking arose from 2-parameter Weibull distribution describing coating layer stochastic strength response
- (2-D model) periodic channel crack formation observed
- (3-D model) periodic formation of mud cracks on the EBC
  - Mud flat cells became progressively smaller or sub-divided as loading progressed: consistent with fractal-like behavior
- Effect of value of Weibull modulus shown to affect crack spacing density with higher Weibull modulus correlating with higher density
- Channel crack spacing could be analyzed on outside edge of 3-D FE model of disk-shaped specimen
- Could not calibrate model parameters since the temperature where microcracking initiated is not known – *Need to know when microcracking starts when performing an experiment*

Future work:

- reduce fracture path mesh dependency, Incorporation of evolving properties (e.g., thermal conductivity) as a function of damage accumulation, investigating effect of interfacial surface roughness between material layers, creep and environmental effects, TGO layer

Acknowledgement

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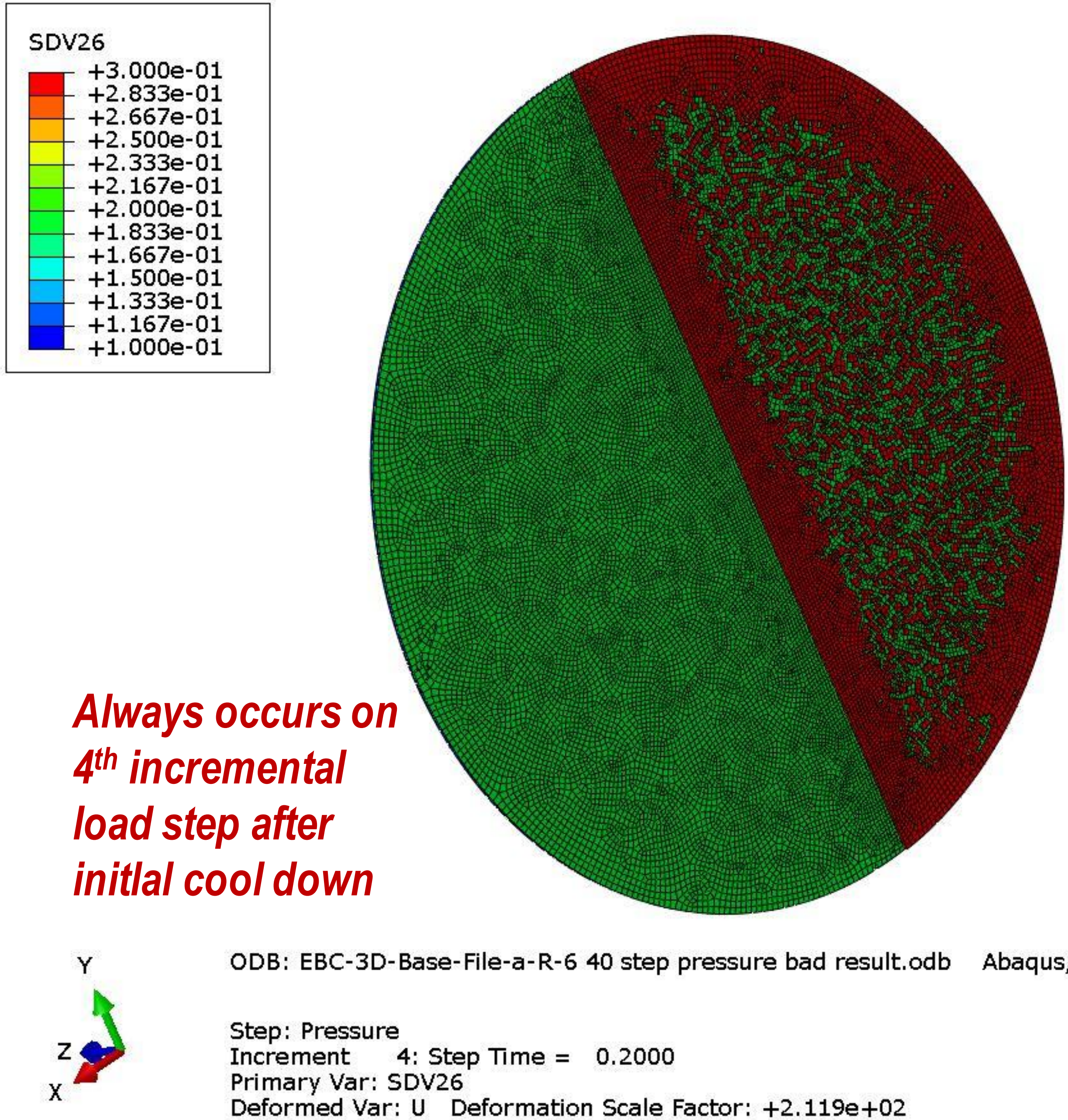
Weird bug…

Attempting to put a pressure load after thermal cool down so as to demonstrate a service loading condition after characterizing initial damage state of material from initial coating deposition



Always occurs on 4th incremental load step after initlal cool down

…yet to be tracked and fixed…

Extra Material

Demonstrate Life Prediction Tool For EBC/CMC Subcomponent Subjected To Thermomechanical Loading

PROBLEM:

Environmental barrier coatings (EBCs) on Ceramic Matrix Composites (CMC) display complex failure modes that evolve with time, fluctuating load, and environmental exposure

APPROACH:

Use the newly developed FEAMAC/CARES code (which combines GRC codes {Composite Micromechanics Code (*MAC/GMC*) & Ceramics Analysis and Reliability Evaluation of Structures (*CARES/Life*)} with finite element analysis to simulate the stochastic damage evolution of EBC material system under generalized and transient thermomechanical loading over time and cyclic loading

INITIAL RESULTS:

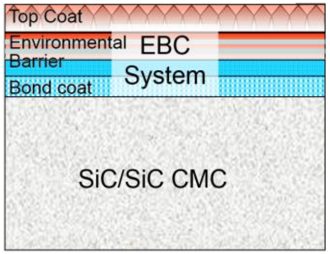
- Established a probabilistic methodology to first damage event and subsequent evolution under multiaxial thermomechanical loading
- Demonstrated the spontaneous formation of mud cracks on an EBC subjected to thermal loads.

SIGNIFICANCE:

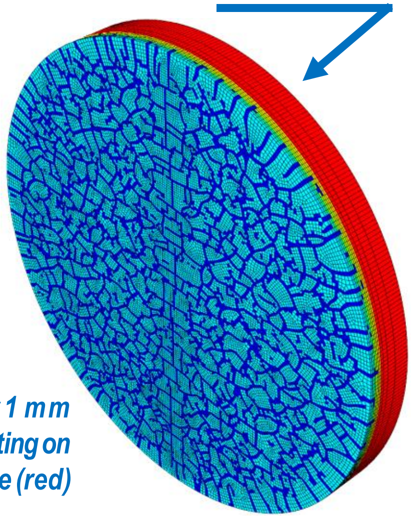
- Provides capability to optimize/design EBC ***mechanical*** performance based on a 2-parameter Weibull distribution of the strength and failure probability of individual brittle material coating layers
- Reproduce and understand EBC failure modes such as mud flat cracking and delamination which lays 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

FOLLOW-ON TOPICS:

- Incorporation of Creep and Environmental effects
- Develop algorithm to reduce fracture path mesh dependency (various means – simple, and more sophisticated)
- Incorporation of evolving properties (e.g., thermal conductivity) as a function of damage accumulation
- Incorporation of interfacial surface roughness between material layers thus inducing stress concentrations and fracture sites



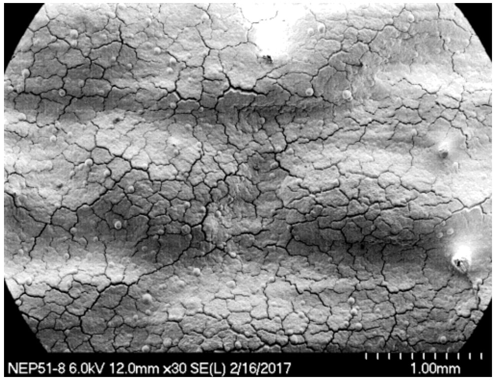
Stochastic Progressive Damage Simulation Successfully Predicts Mud Flat Damage Pattern In EBCs



Spontaneous development of mud flats fragment into progressively smaller sizes when cooling from 1300° C to room temperature (fractal fracture pattern)

10 mm dia. by 1 mm multilayer coating on SiC substrate (red)

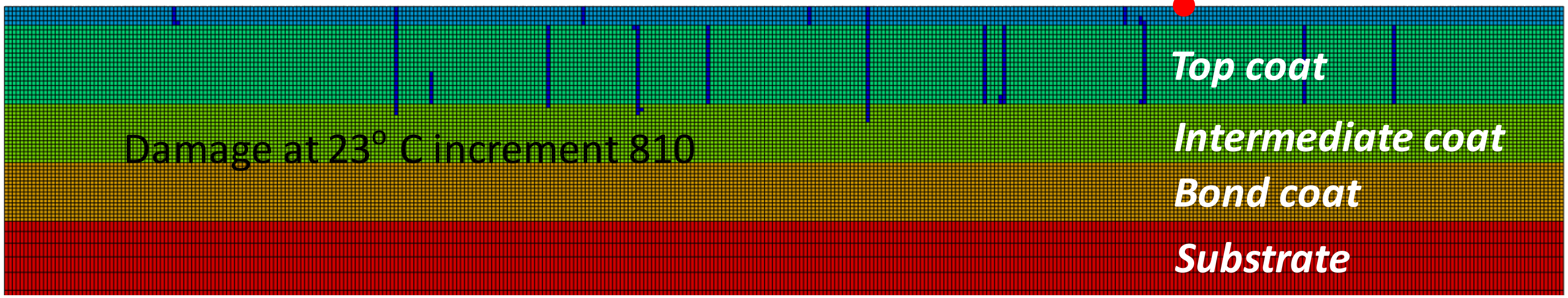
Compare to rare earth silicate EBC after heat flux testing showing mud flat damage

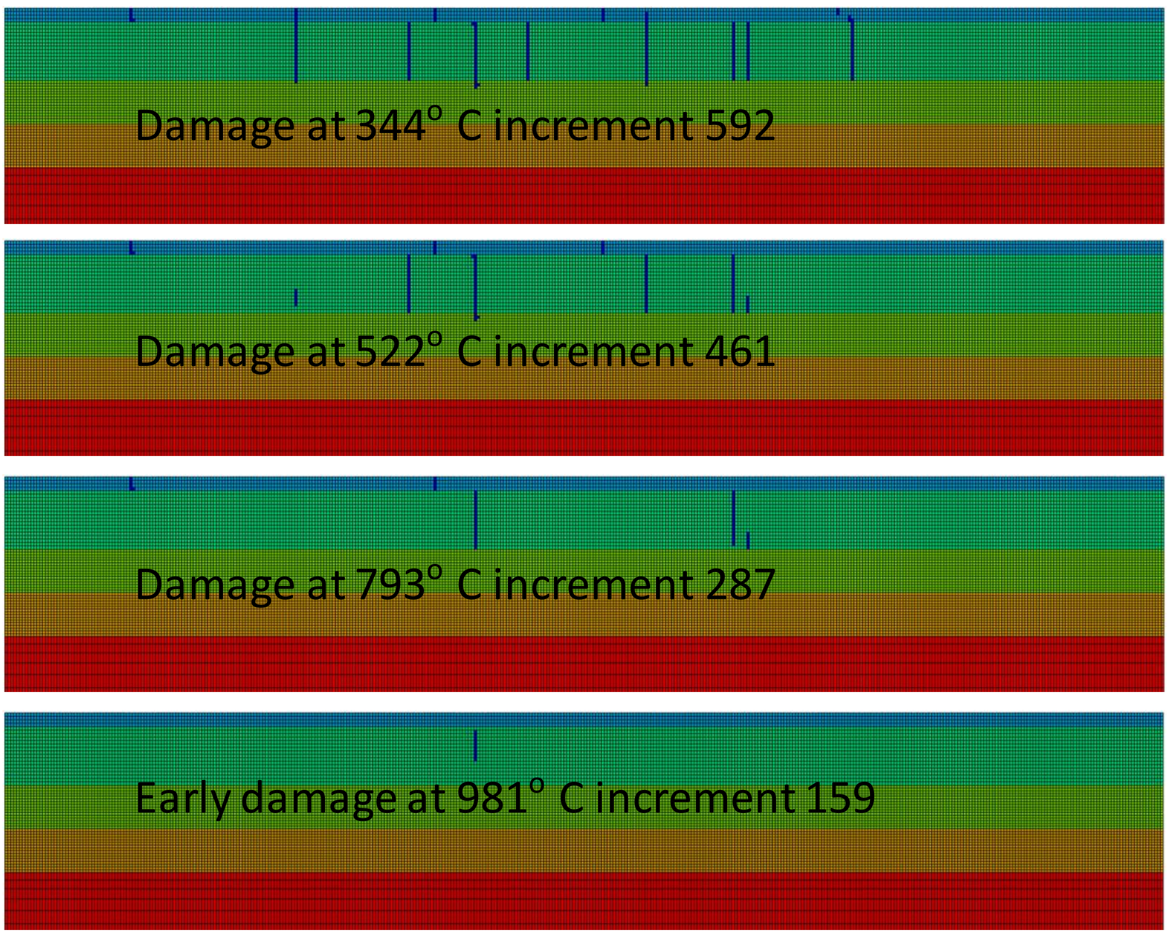


POC: Steven Arnold/ (LMS), Noel Nemeth/ (LMS)

Ytterbium Monosilicate: 2D cross-sectional model
Weibull modulus m=2.5 for all coating layers

Top coat: low strength layer





2 mm X 1 mm specimen

Complete substrate not shown

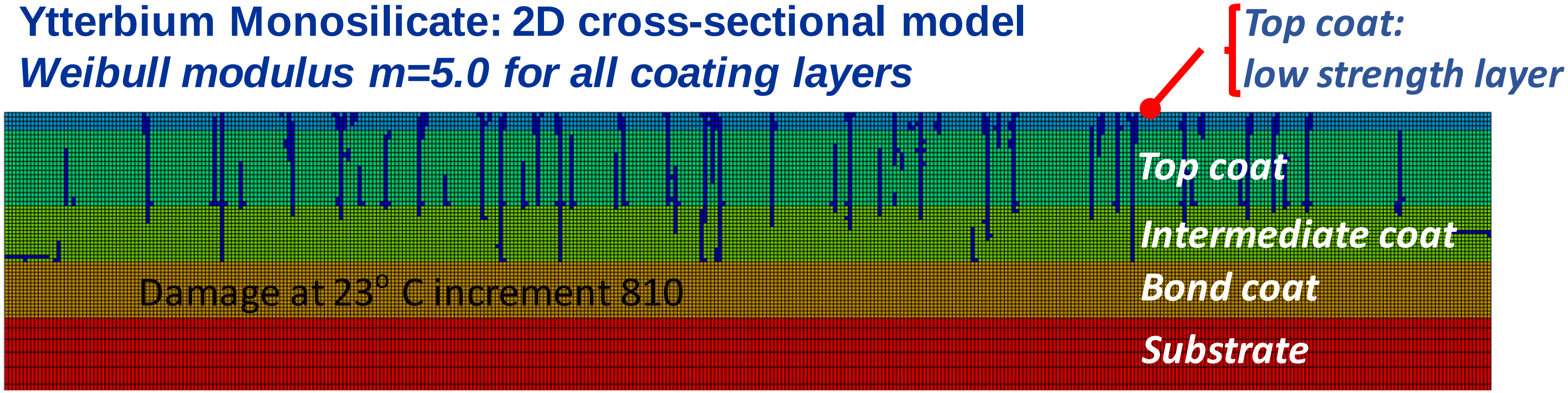
810 load increment steps (ramp load):

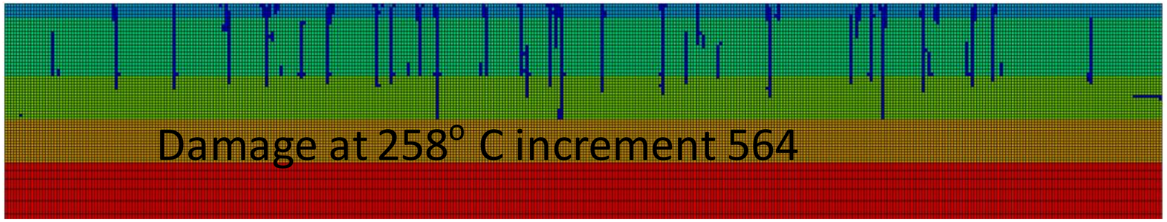
- First 10 early cool-down steps from 1300° C to 1200° C
- 800 increment steps from 1200° C to 23° C

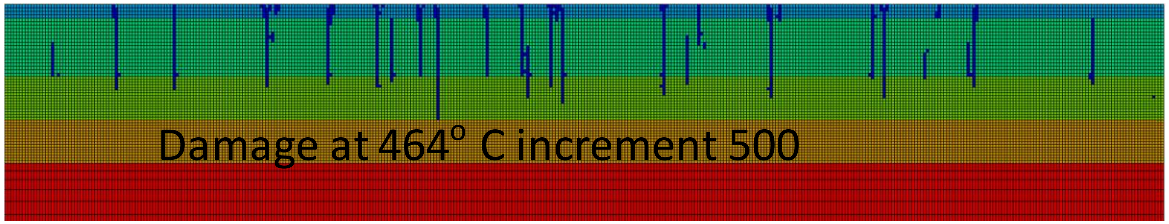
≈ 8 channel cracks in top coat over 1.2 mm span for an average crack spacing of 150 µm

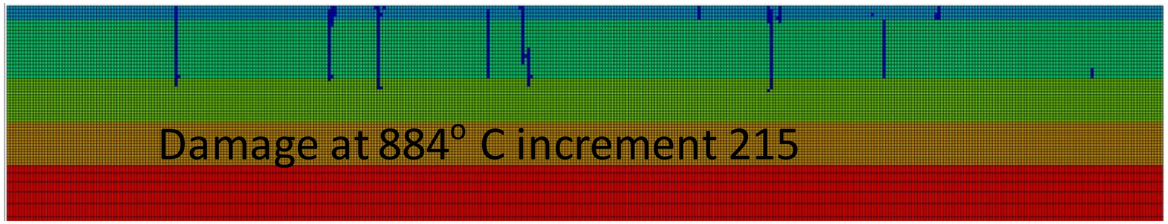
Ytterbium Monosilicate: 2D cross-sectional model

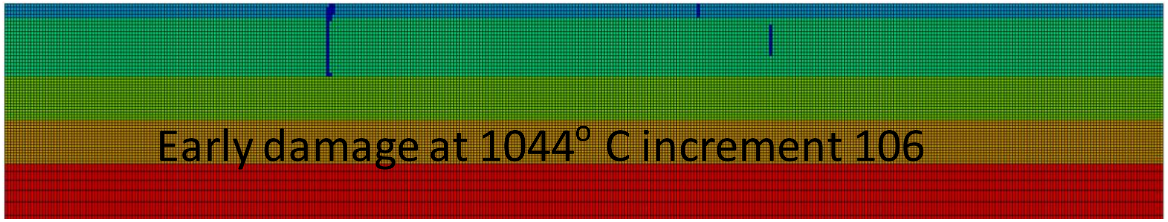
Weibull modulus m=5.0 for all coating layers











2 mm X 1 mm specimen

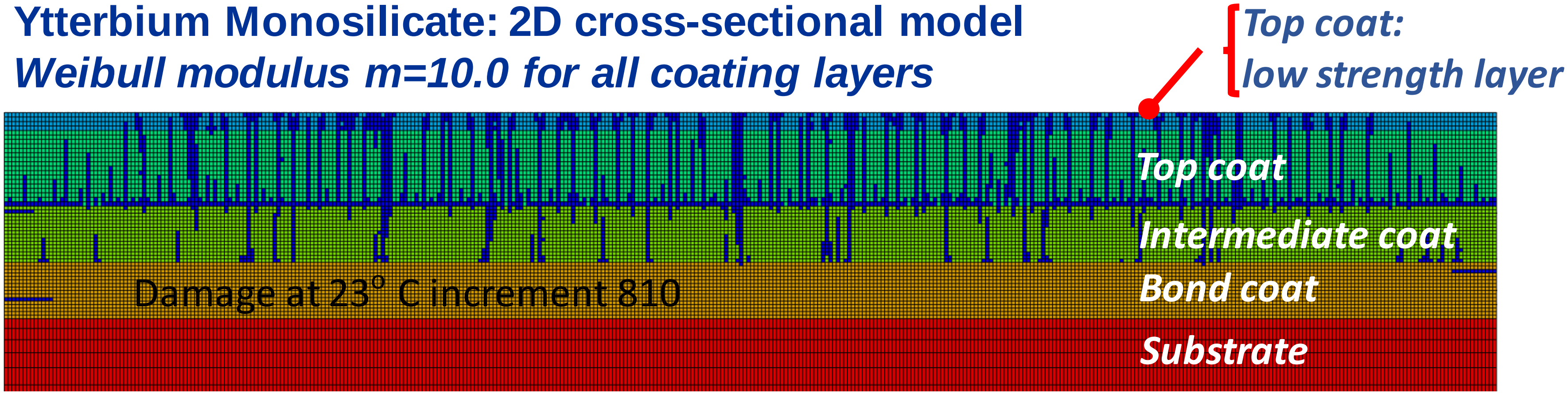
Complete substrate not shown

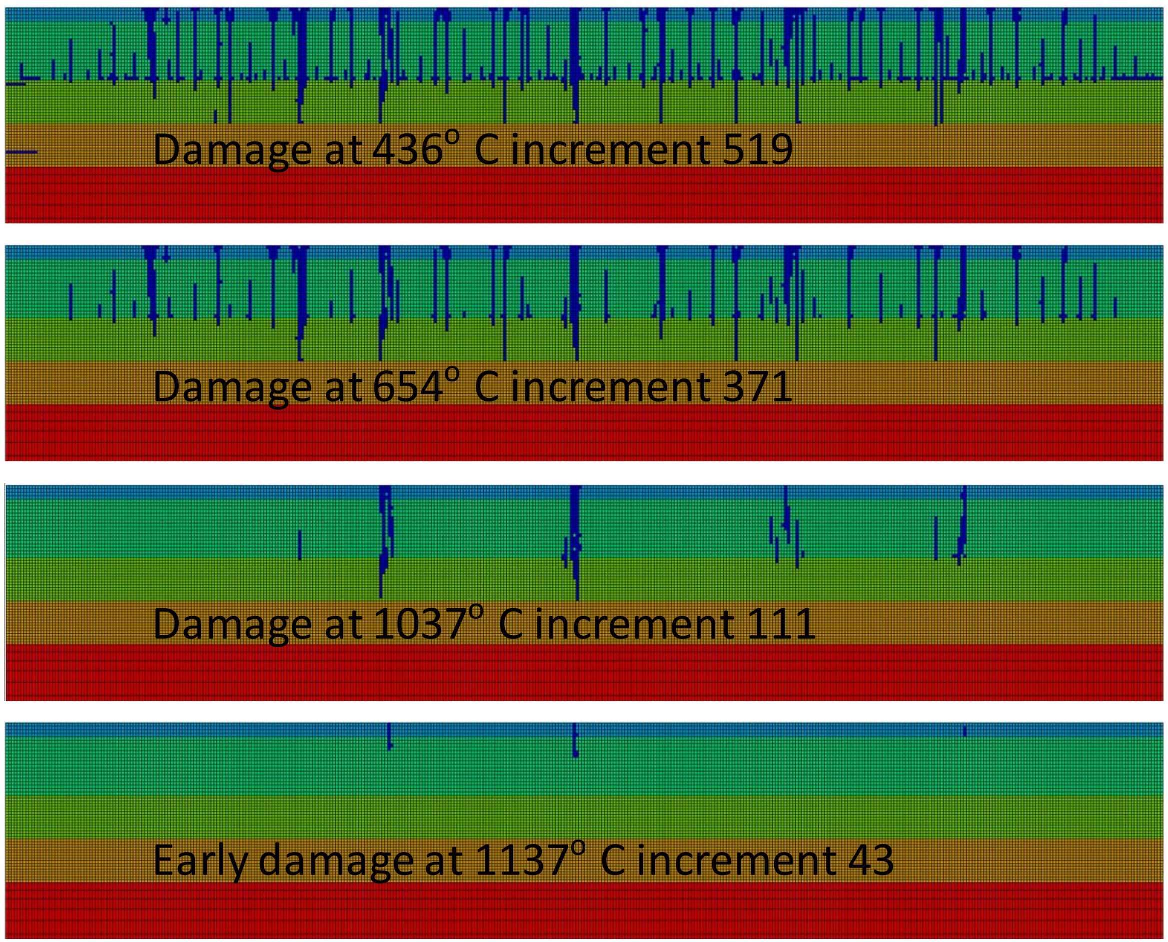
810 load increment steps (ramp load):

- First 10 early cool-down steps from 1300° C to 1200° C
- 800 increment steps from 1200° C to 23° C

≈ 19 channel cracks in top coat over 1.2 mm span for an average crack spacing of 63 μm

Ytterbium Monosilicate: 2D cross-sectional model
Weibull modulus m=10.0 for all coating layers





2 mm X 1 mm specimen

Complete substrate not shown

810 load increment steps (ramp load):

- First 10 early cool-down steps from 1300° C to 1200° C
- 800 increment steps from 1200° C to 23° C

≈ 49 channel cracks in top coat over 1.2 mm span for an average crack spacing of 25 μm

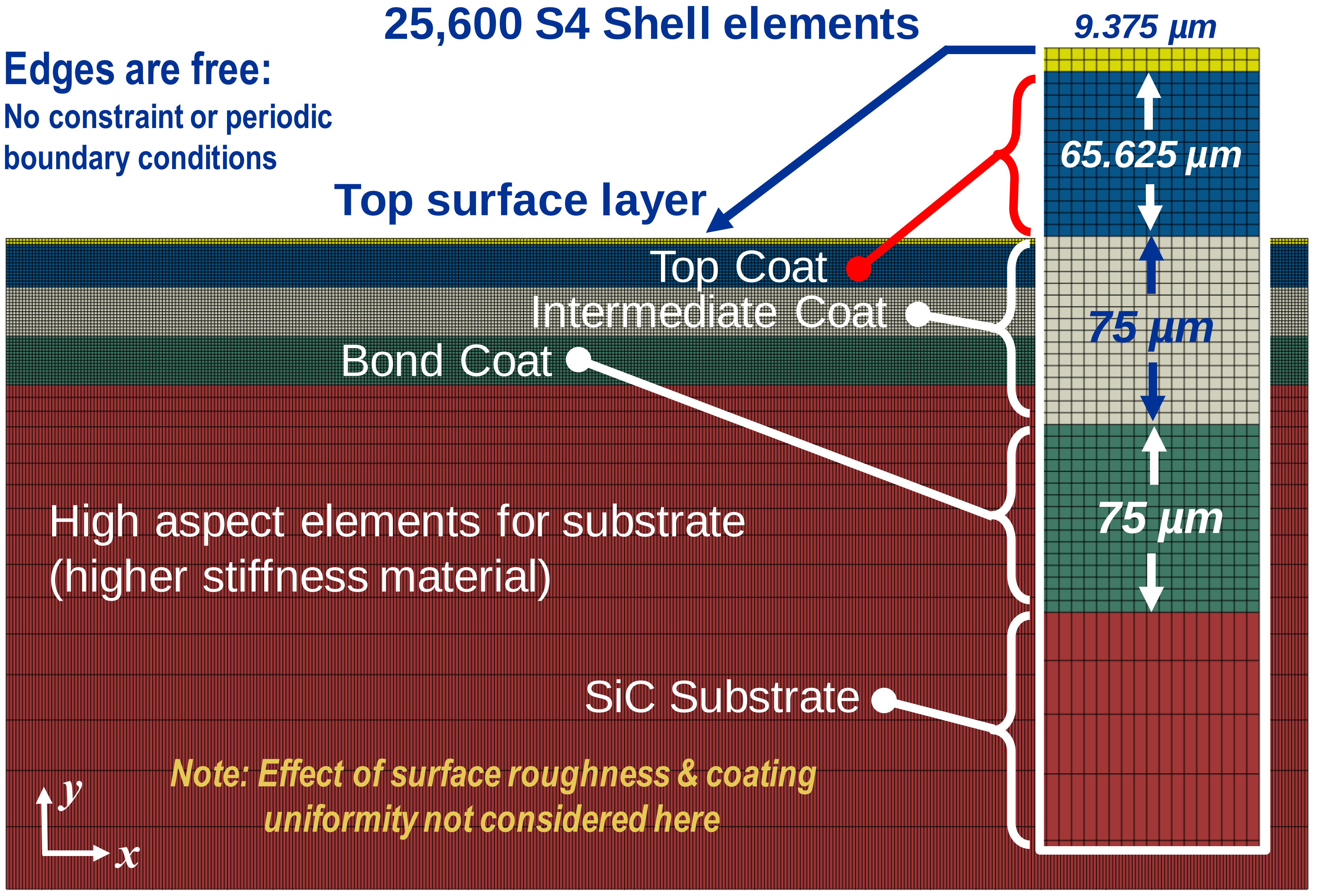
Properties Table (Tensile strength/Weibull parameters adopted from Abdul-Aziz, None listed in Richards)

Report	Material	E (Gpa)	Poisson, v	Therm. Expan., α, m/m/°C · 10^{-6}	Weibull modulus, m	Weibull Scale Parameter, σ_o, MPa·$mm^{3/m}$
YBSM (Richards et al. 2016)[1] Using 50% reduced properties listed in reference	Top Coat Suface: Ytterbium monosilicate	86	0.27	7.5	5	14 (assumed)
	Top Coat: Ytterbium monosilicate	86	0.27	7.5	5	28 (assumed)
	Intermediate Coat: Mullite	110	0.28	5.3	5	28 (assumed)
	Bond Coat: Silicon	82	0.223	4.1	5	40 (assumed)
	Substrate: SiC (Monolithic)	430	0.14	4.6	5	321 (assumed)
BSAS (Abdul-Aziz et al. 2014)[2]	Top Coat Surface: BSAS	32	0.19	5.6	5	14
	Top Coat: BSAS	32	0.19	5.6	5	28
	Intermediate Coat: BSAS+Mullite	37.4	0.179	5.7	5	28
	Bond Coat: Silicon	97	0.21	4.5	5	40
	Substrate: SiC (CMC)	285	0.17	2.71	5	321

[1] Richards et al.: Fracture Mechanisms of Ytterbium Monosilicate Environmental barrier coatings during cyclic thermal exposure" Acta Materialia, 103, pp. 448-460, 2016..

[2] Abdul-Aziz, et al.: "Durability Modeling of Environmental Barrier Coating (EBC) Using Finite Element Based Progressive Failure Analysis" J. of Ceramics, pp. 1-10, 2014

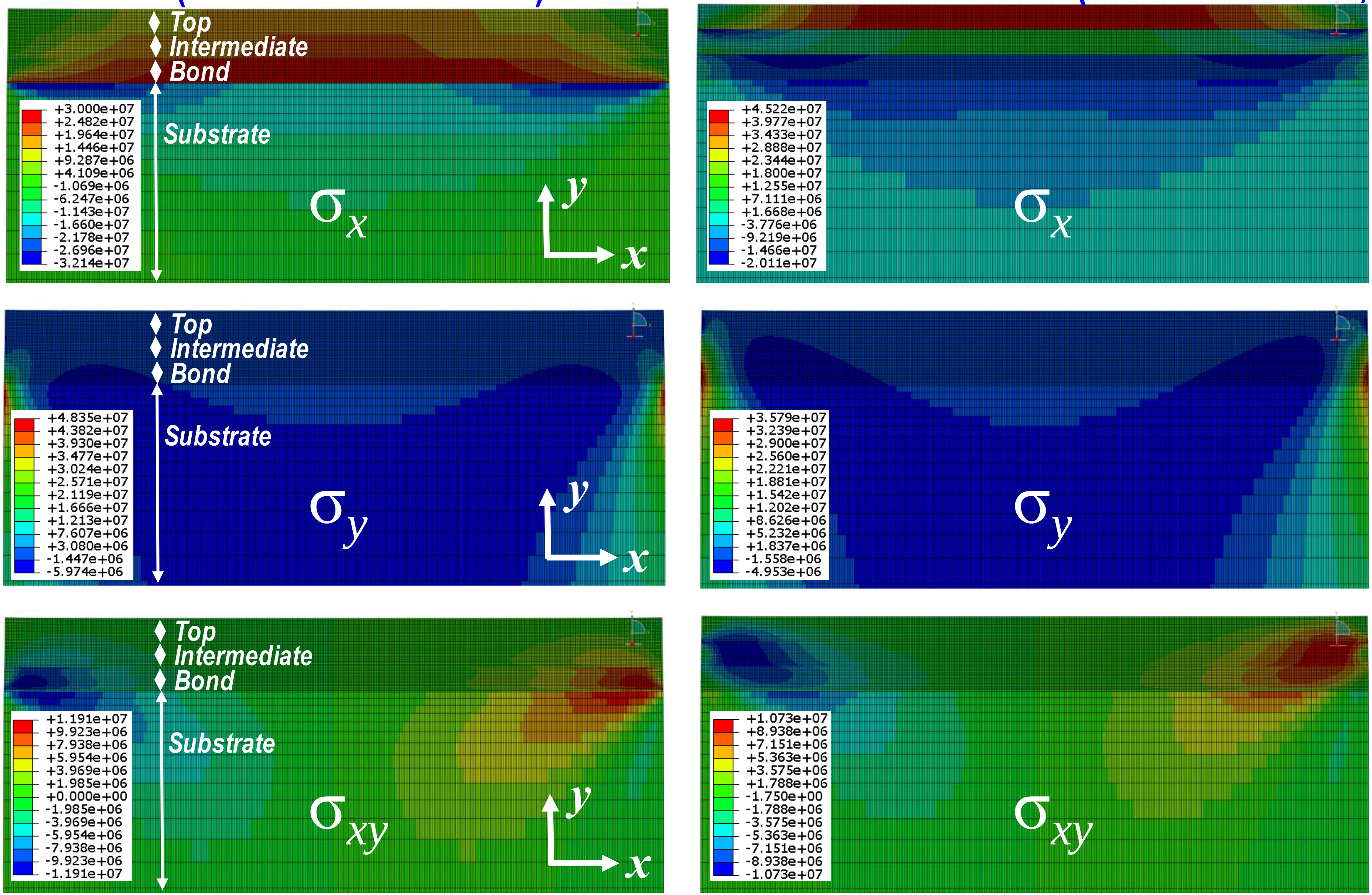
2-D EBC Cross-Section FE model (2mm X 1mm)



Stresses in undamaged EBC layers : 200° C cool-down from annealing Temp.

Comparison for 75 µm thick top coat

BSAS (Abdul-Aziz et al. 2014) | **Ytterbium Monosilicate (Richards et al. 2016)**



Unit Sphere Multiaxial (Batdorf) Model:

Puts linear elastic fracture mechanics into Weibull weakest-link theory

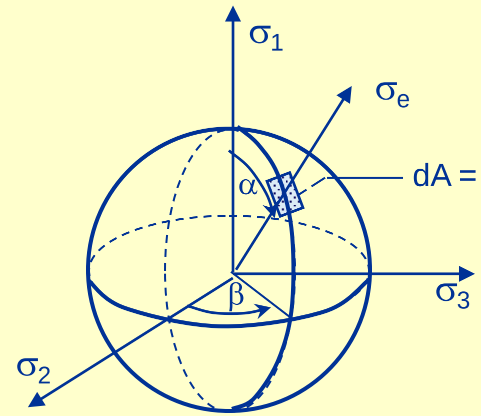
- **Incremental failure probability is the product of two probabilities:**

$$\Delta P_f = P_1 \cdot P_2$$

P_1 = Probability of the existence of a crack having a critical strength between σ_c and $\sigma_c + \Delta\sigma_c$ in the incremental volume ΔV

P_2 = Probability a crack having a critical strength of σ_c will be oriented in a direction such that it will fail under the applied multiaxial stress state

P_2 involves Integration of an equivalent stress σ_e, where $\sigma_e \geq \sigma_c$, over the surface of a unit radius sphere (all possible flaw orientations) divided by the total surface area of the unit radius sphere



σ_e is a function of an assumed crack shape and multiaxial fracture criterion

- **Component failure probability:**

$$P_f = 1 - \exp\left\{ -\int_V \left[\int_0^{\sigma_e} P_1(\sigma_c)\, P_2(\sigma_c)\, d\sigma_c \right] dV \right\}$$

Mixed-Mode Fracture Criteria:

- Normal stress (shear-insensitive cracks)
- Maximum tensile stress
- Total coplanar strain energy release rate
- Noncoplanar (Shetty)

Flaw Shapes:

- Griffith crack
- Penny-shaped crack

Modeling flaw planes/texture anisotropy

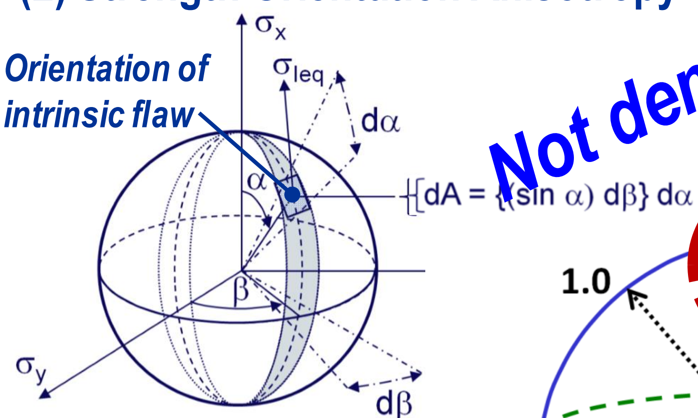
Coating layers have complex microstructures with defect/flaw populations that can have orientation bias of pores, voids, and cracks

This can be accounted with the Unit Sphere stochastic-strength multiaxial criterion model

- **Two models for transverse isotropy**

(1) Flaw / Fracture-Plane Orientation Anisotropy

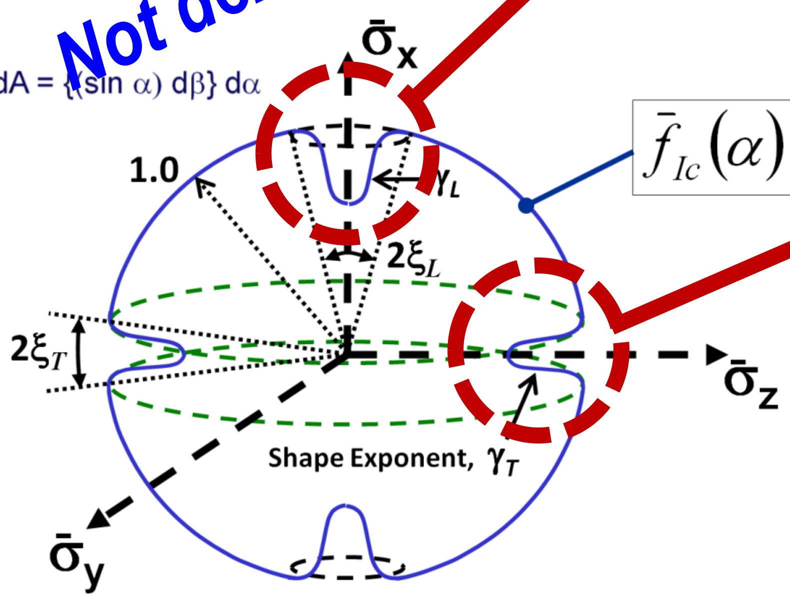
(2) Strength Orientation Anisotropy

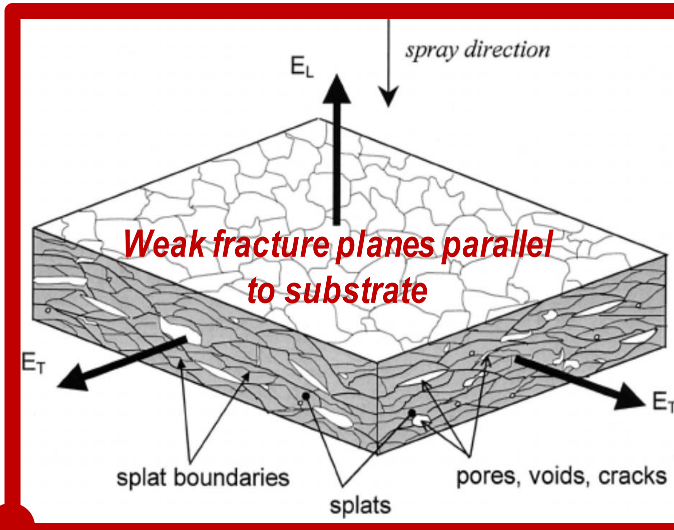


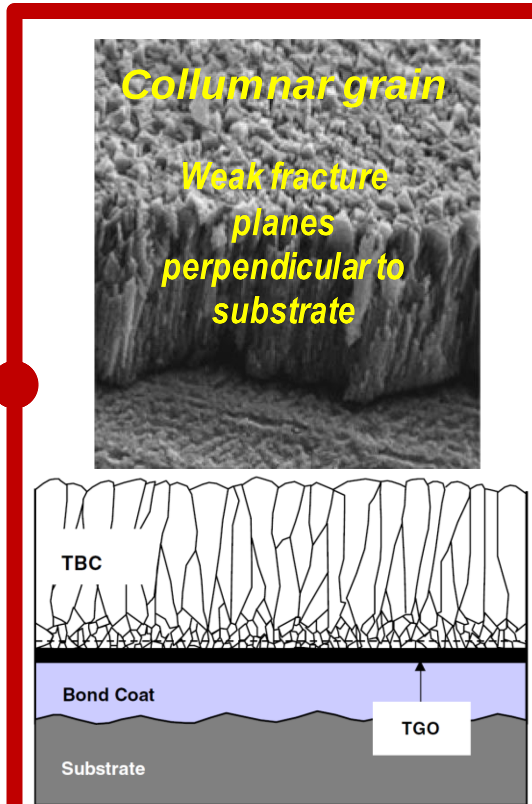
Unit Sphere

- crack shape
- mixed-mode fracture criterion

Not demonstrated here





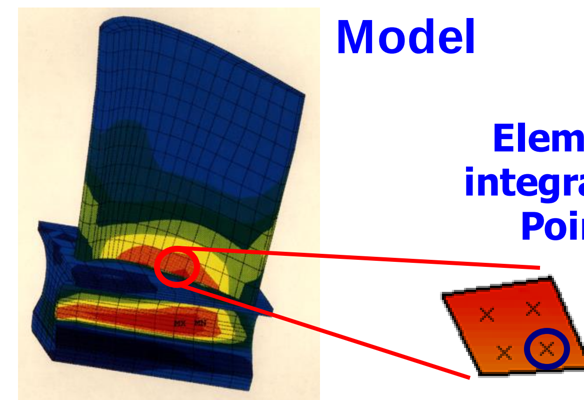


CARES: *Ceramics Analysis and Reliability Evaluation of Structures*

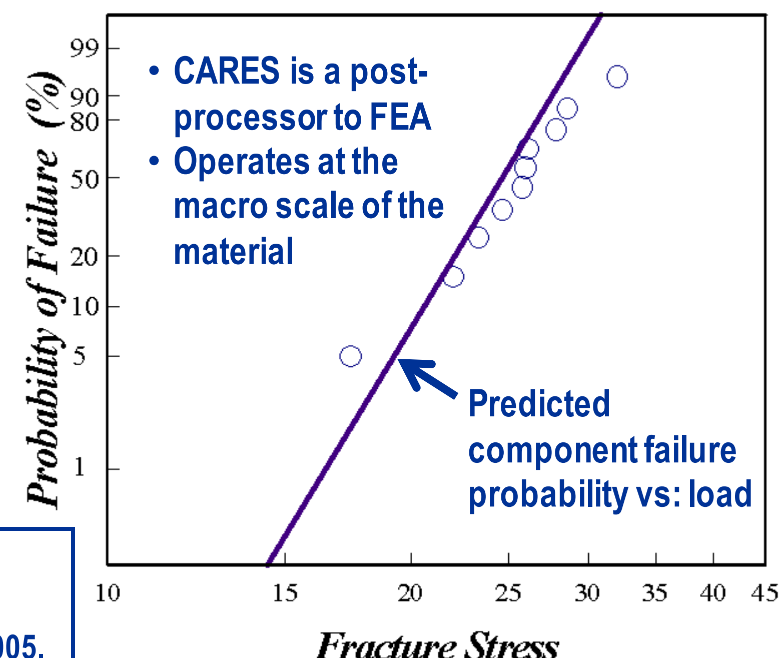
Life Prediction & Component Design Code For Advanced Ceramics

- Developed to predict the probability of failure of ceramic components under complex thermomechanical loading
- Combines Weibull & Weakest Link theory with concepts of linear elastic fracture mechanics (the ***Batdorf Unit Sphere*** model)

Structural Model



(CARES) reliability analysis



Component Reliability Analysis Capability:

- Transient loads and temperatures
- Fast-Fracture Rupture
- Time-dependent (da/dt) crack growth
- Cycle-dependent (da/dn) crack growth
- Multiaxial stress failure models
  *(PIA & **Unit Sphere** & Tsai-Wu & Tsai-Hill)*
- Proof test

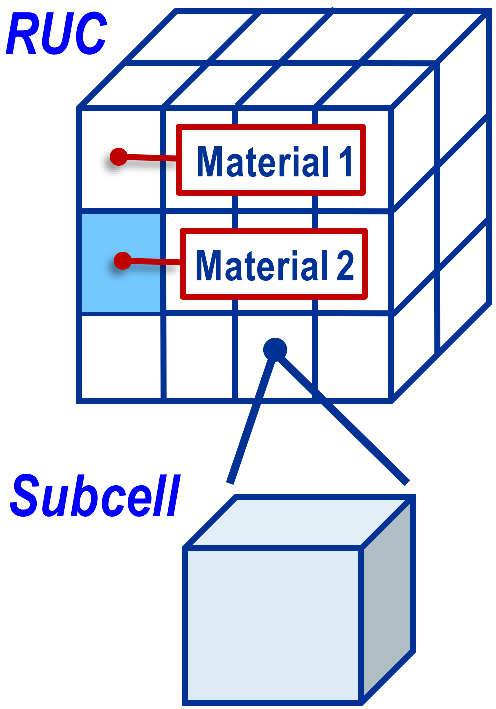
Nemeth, Jadaan, Gyekenyesi.: "Lifetime Reliability Prediction of Ceramic Structures Under Transient Thermomechanical Loads." NASA/TP-2005-212505, 2005.

MAC/GMC Micromechanics Analysis Code

Repeating Unit Cell (RUC) of composite material

❖ RUC made of material subcells

❖ Multiscale capability



- ***FEAMAC:*** *MAC/GMC embedded in FEA as constitutive material*

CARES/Life: Life Prediction Code For Advanced Ceramics

- Predicts the probability of failure of ceramic components under thermomechanical loading
- Combines Weibull & Weakest Link theory with concepts of linear elastic fracture mechanics (the *Batdorf Unit Sphere* model)
- CARES is a post-processor to FEA

Component Reliability Analysis Capability:

➢ Transient loads and temperatures

➢ Fast-Fracture Rupture

➢ Time-dependent (da/dt) crack growth

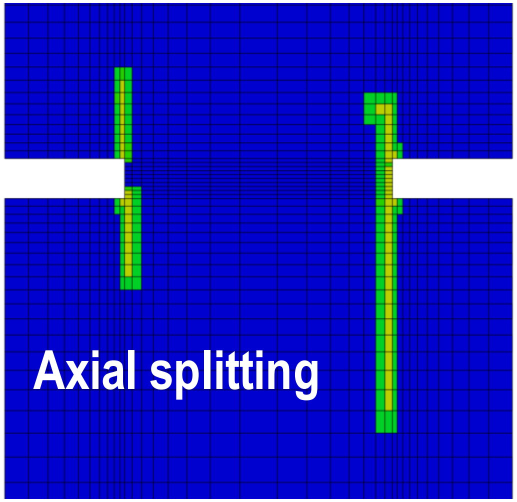
➢ Cycle-dependent (da/dn) crack growth

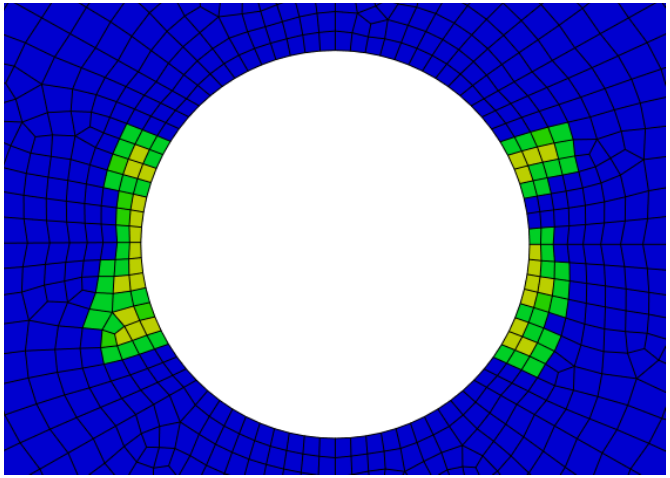
➢ Multiaxial stress failure models *(PIA & Unit Sphere & Tsai-Wu & Tsai-Hill)*

➢ Proof test

0^o CMC Double-Notched vs: Central-Hole Tensile Specimen

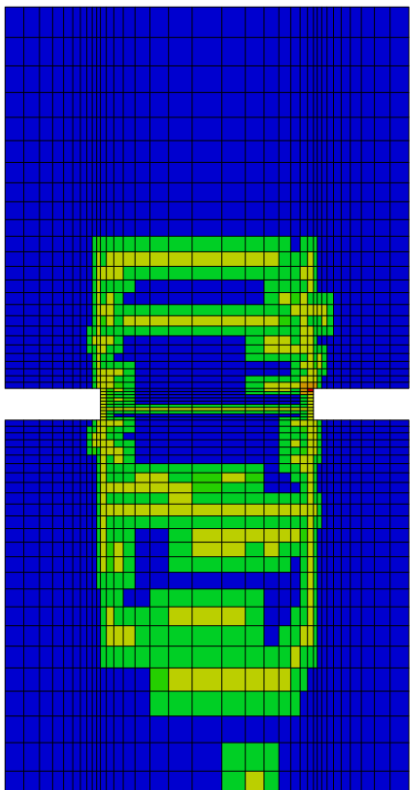
FEAMAC/CARES damage simulation:

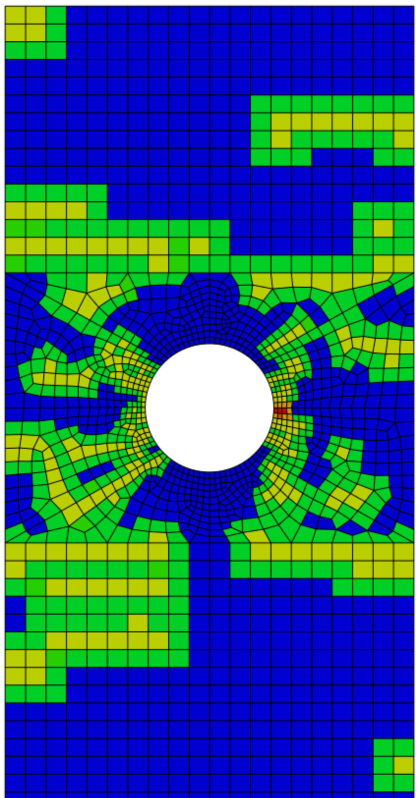




Loading and fiber Direction

Early matrix damage





Matrix damage progression

- Matrix failure
- Adjacent to failed matrix
- Fiber failure
- Adjacent to failed fiber
- No failure