Chemical and Mechanical Instabilities at Thermal Barrier Coating Interfaces

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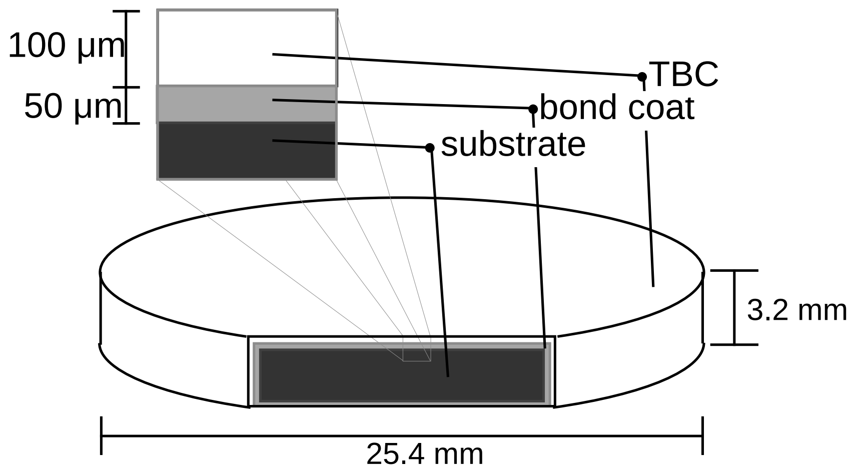
Objectives:

Generate a detailed understanding of the compositional, microstructural, oxidation, and fracture mechanics issues at TBC interfaces that control coating life

- -Characterization of the TBC system in regard to compositional and microstructural developments arising from oxidation.
- -Experimental Measurement and Modeling of the Interfacial Fracture Toughness
- -Finite Element Modeling of Stresses in the TBC System

TBC CHARACTERIZATION

Schematic of Coated Samples



◎**TBC: EB-PVD 7wt% Yttria Partially Stabilized Zirconia (PSZ)**

◎**Bond Coat: Pt Modified Diffusion Aluminide**

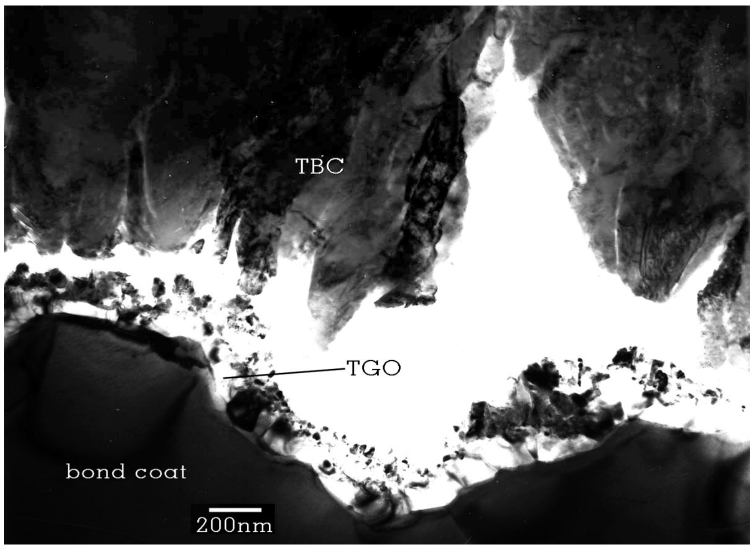
◎**Substrate: N5 Ni Based Single Crystal Superalloy**

N5 Alloy Composition (wt%)

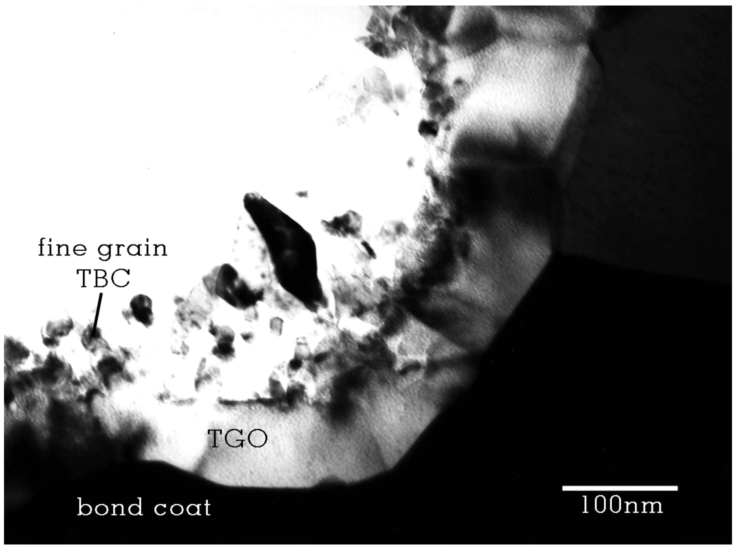
Co	Cr	Mo	W	Re	Ta	Al	Hf	C	B	V
7.5	7.0	1.5	5.0	3.0	6.5	6.2	0.15	0.05	0.004	0.01

As Processed Structure of EB-PVD TBC

- ◎ **TBC has Characteristic Columnar Structure from Vapor Deposition with Channels between each Grain**
- ◎ **A ContinuousAlumina Layer Exists Between the TBC and Bond Coat**
- ◎ **A Fine Grain TBC exists Adjacent to Alumina Layer**



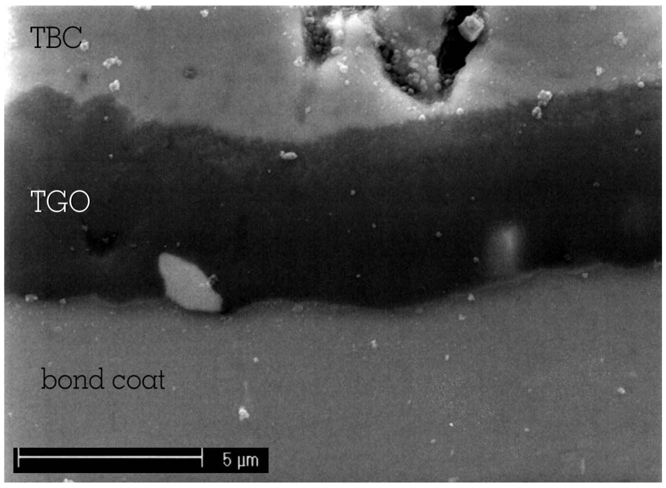
TEM brightfield micrograph showing the TGO layer in the As Processed coating to be continuous.



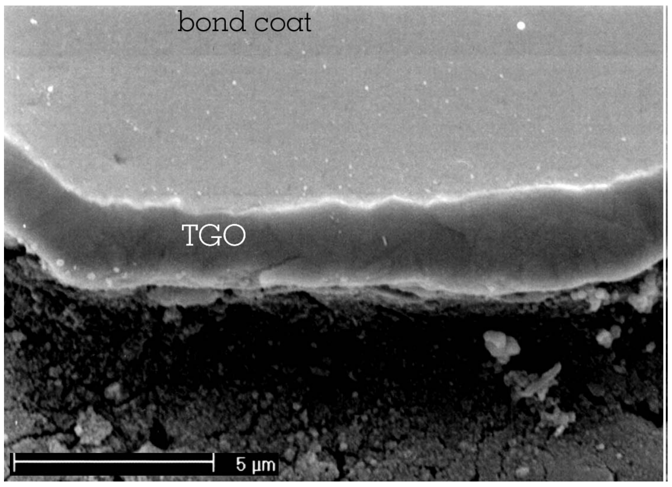
TEM brightfield micrograph showing fine grained zirconia at the TGO-TBC interface.

TBC influence on TGO Growth

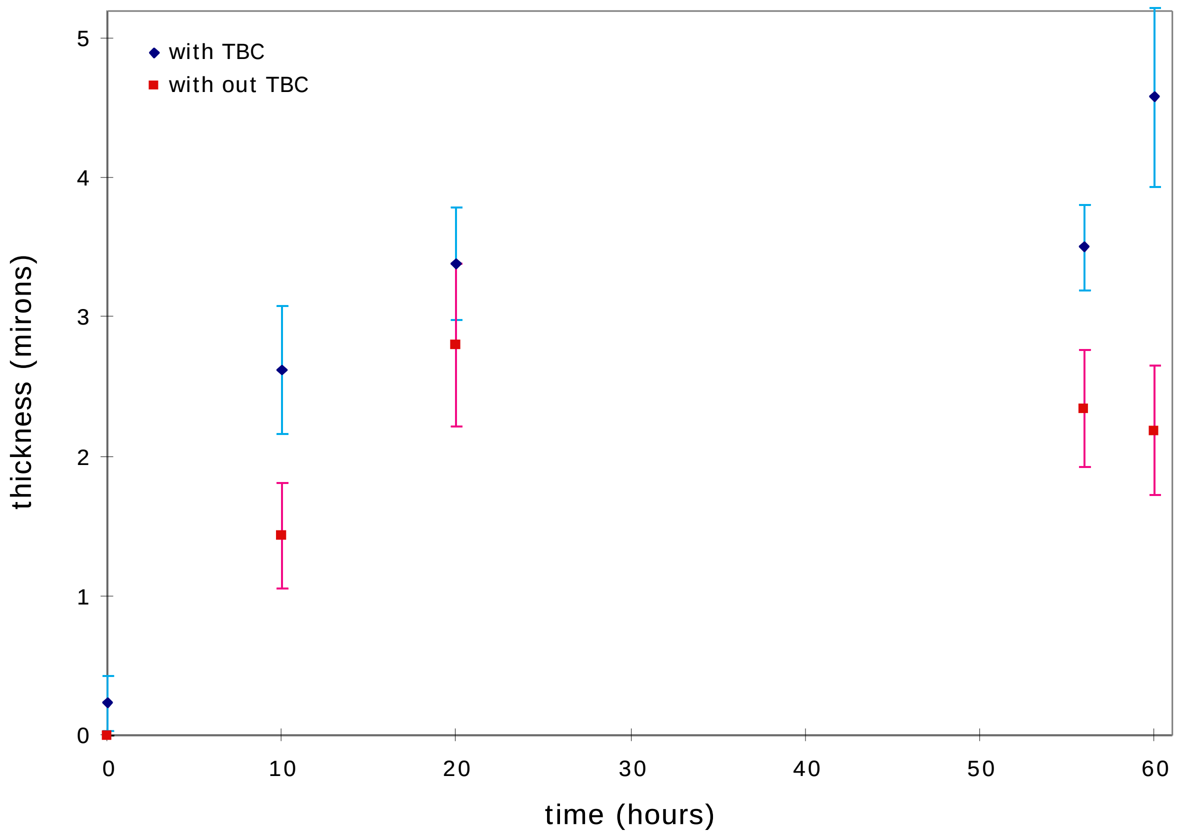
The as processed coating has a thin continuous alumina layer between the TBC and the bond coat, this alumina layer is much thinner on the same sample when not in contact with the TBC. With time at the oxidizing temperature, this difference increases as the TGO between the TBC and the bond coat grows at a faster rate. It appears that this is caused by the presence of the PSZ.



TGO under the TBC (60h at 1200˚C).



TGO on bare bond coat (60h at 1200˚C).

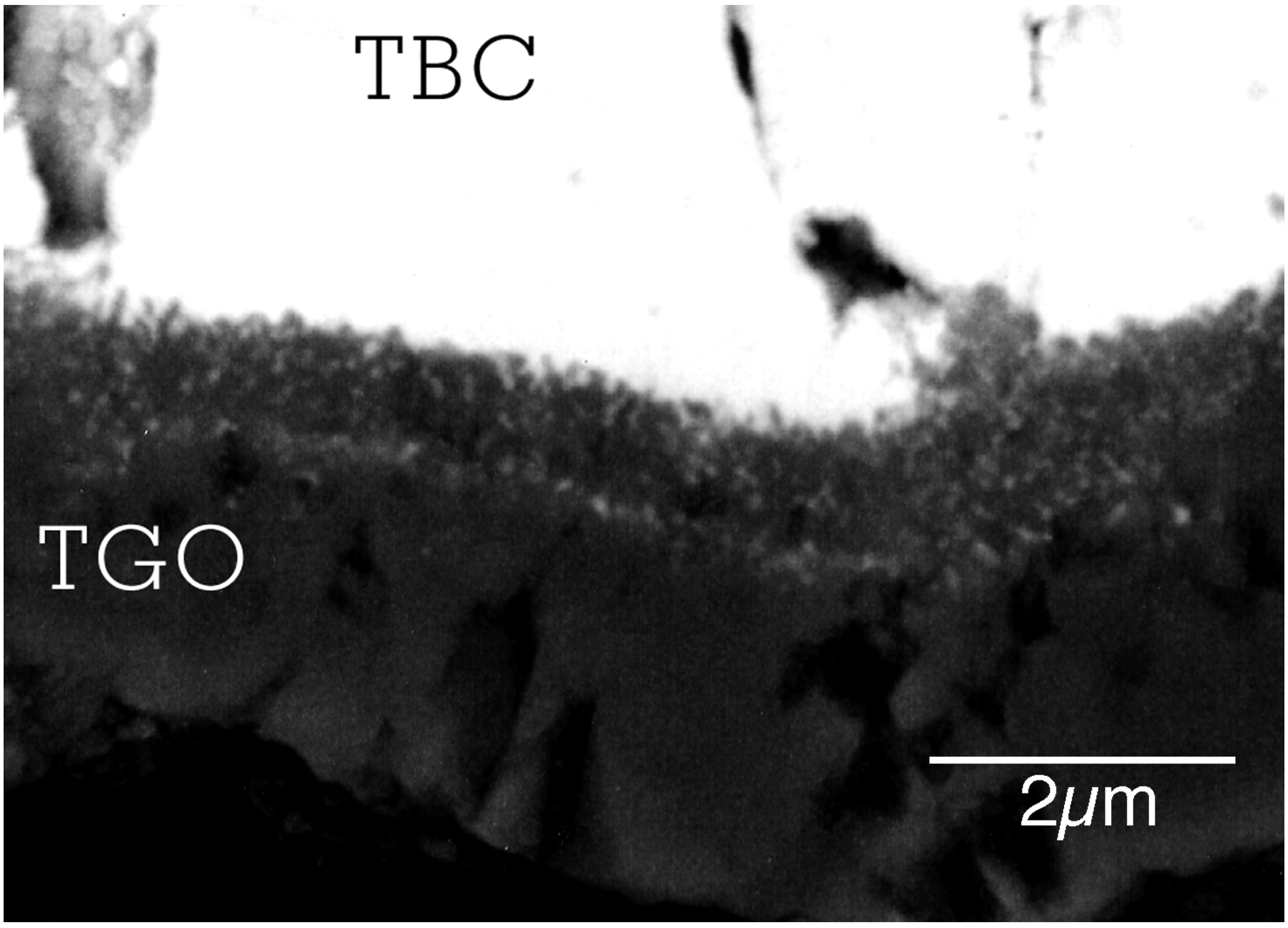


Incorporated PSZ in the TGO

◎**Zirconium and yttrium were detected in the TGO, and were segregated near the TGO-TBC interface.**

◎**An outward growth of the TGO may incorporate the fine grained PSZ behind the advancing TGO-TBC interface, and this two phase zone would not inhibit oxygen diffusion.**

◎**However, the development of this two phase zone and the more rapid growth of the TGO adjacent to the TBC is not fully understood**



Micrograph showing the intermixed region in the TGO adjacent to the TBC. Coating exposed for 20h at 1200˚C.

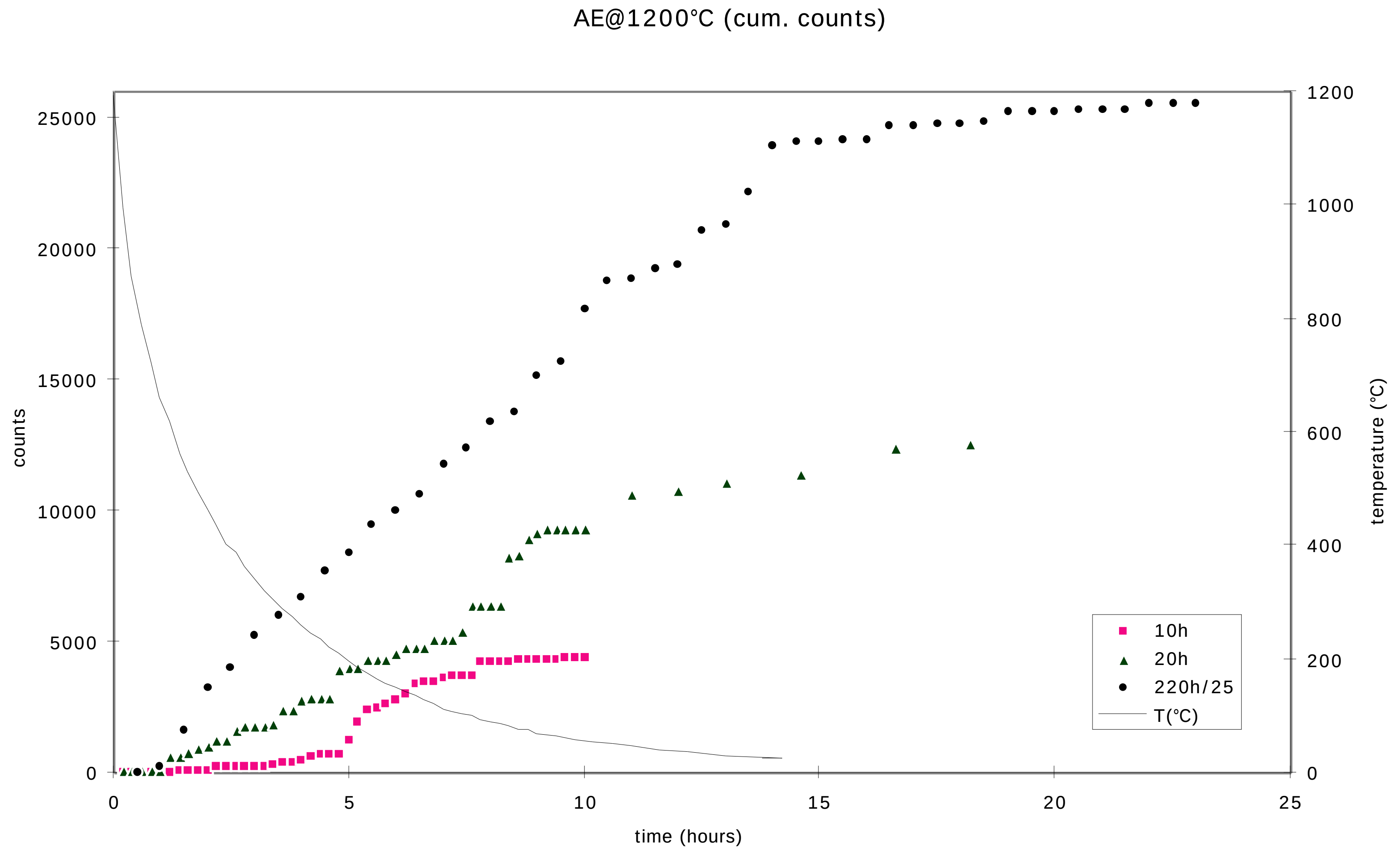
Acoustic Emission

Recorded Acoustic Emissions for Isothermal Oxidation Tests Showed:

-Acoustic Emissions only detected on cooling down

-Increase in Exposure Time Increases:
- **Total Number of Counts**
- **Rate of Emission**
- **Duration of Emission**

-Increase in Counts Correlates with Decrease in TBC Adhesion as Discovered from Indent Tests



Interfacial Toughness Testing; Measurements and Debonding Behavior

◎TBC's spontaneously spall after a 60h isothermal exposure at 1200°C.

◎The failure of these coatings was predominantly along the TGO-bond coat interface.

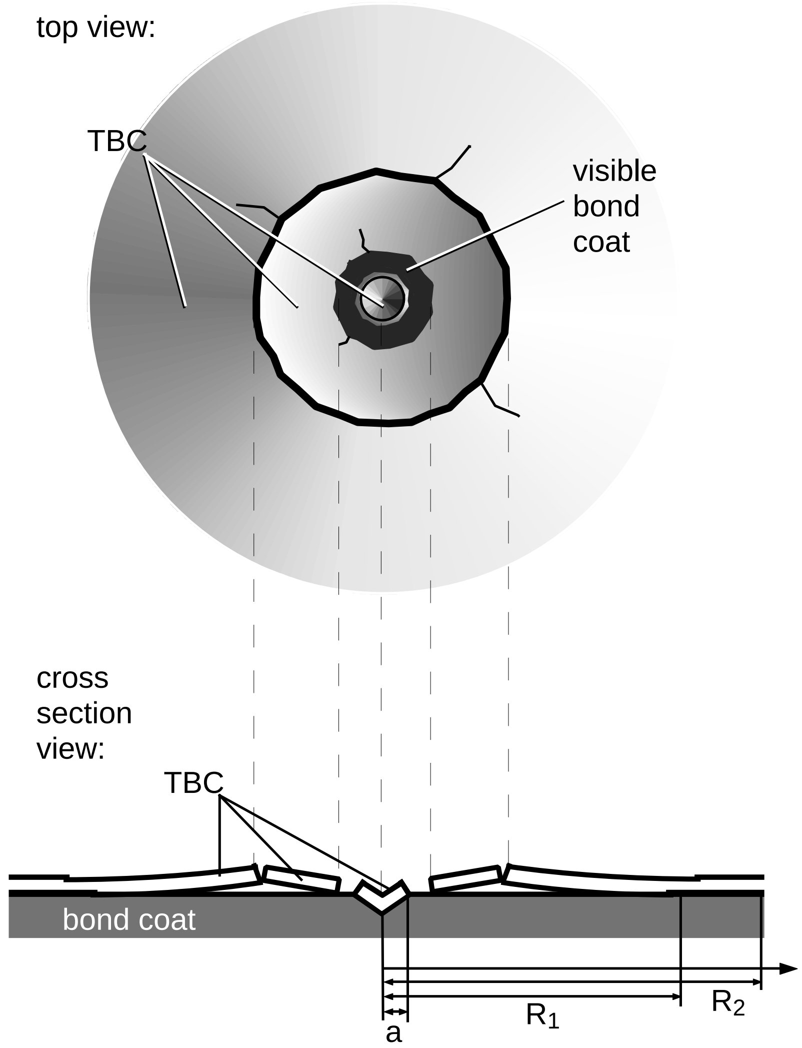
◎To show the degradation of this interface prior to spallation, an indent test was used to induce TBC debonding.

◎Measurement of the extent of debonding can be used to estimate the fracture toughness of the interface.

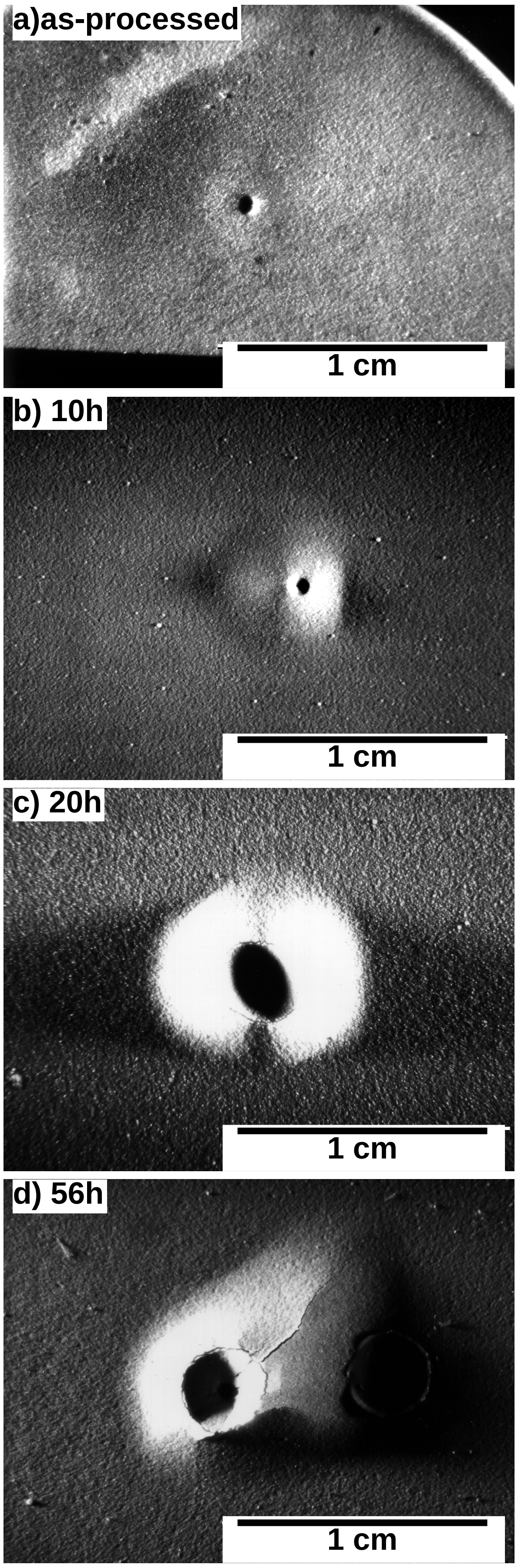
◎Schematic of Induced Debonding from the Indent Test:

•R1 is the debond radius apparent immediately after the indent test as the size of the buckle.

•R2 is the radius of debond when the TBC was pulled from the sample after the indent test.



◎ Indent Test Micrographs

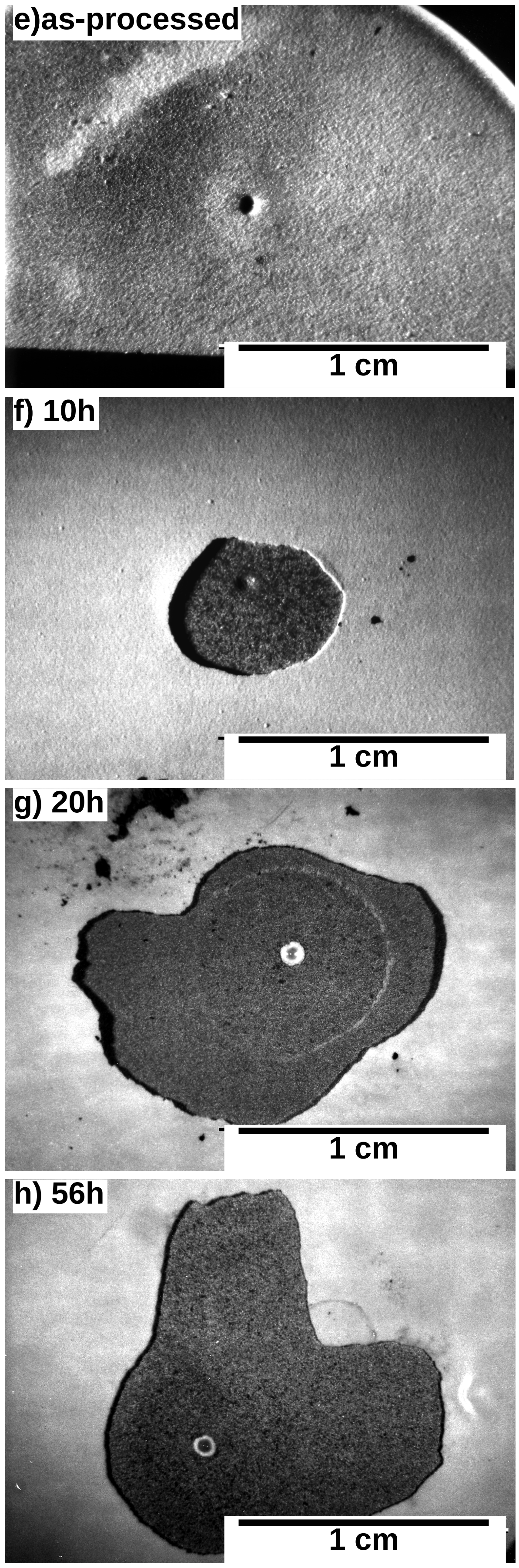


Micrographs showing the TBCs immediately after indenting.

1a) shows only the indenter mark

1b) shows only the buckle

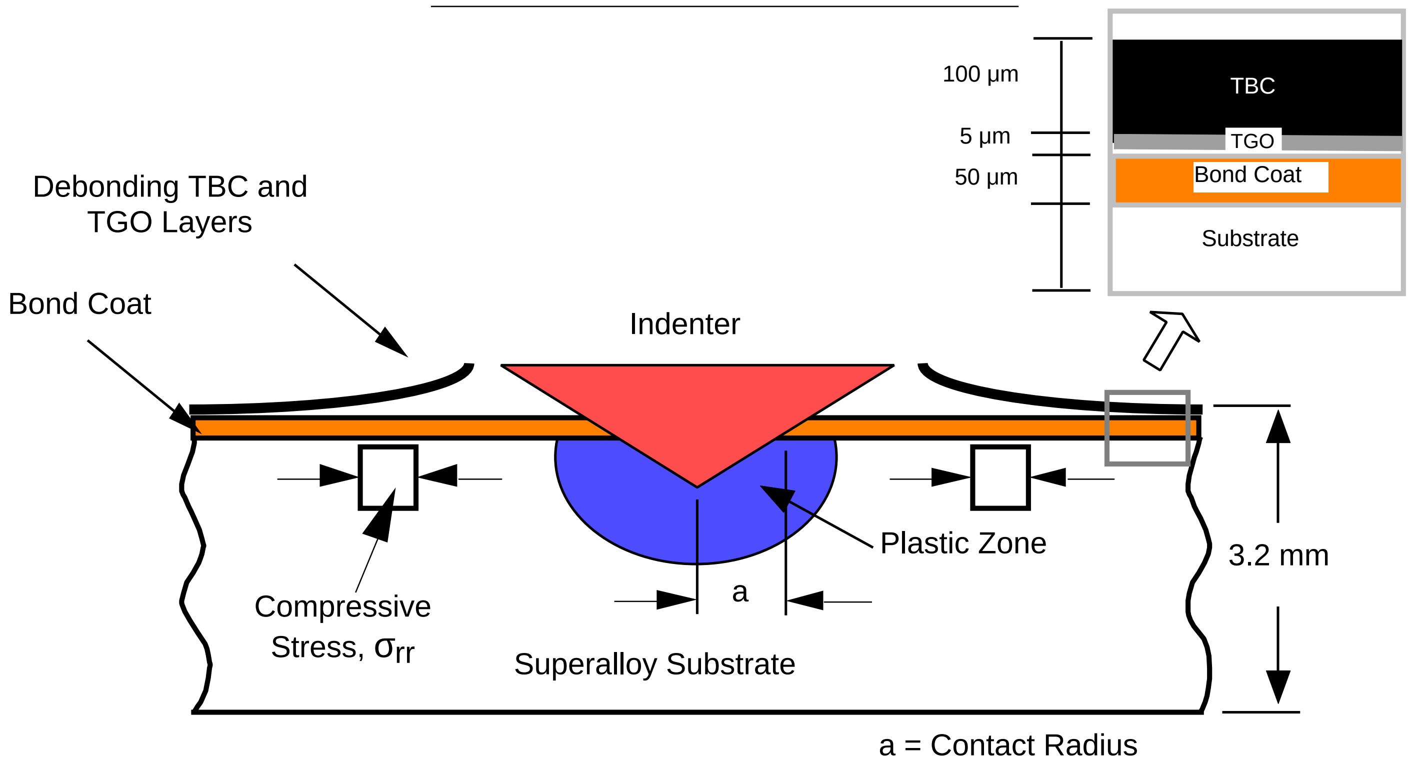
1c&d) shows crater and buckling



Micrographs showing the samples with TBC removed after indent tests; e, f, g, and h.

FRACTURE MECHANICS

Interfacial Toughness Testing; Determining the Toughness from Measured Debond Radii



- ◎ **Indentation Test Using Rockwell Hardness Tester with Brale C Indenter**
- ◎ **TBC/Oxide Layers Penetrated**
- ◎ **Plastic Deformation Induced in Bond Coat/Superalloy Substrate**
- ◎ **Compressive Radial Stress from Indent Drives Axisymmetric Delamination**
- ◎ **Radius of Debonding is Determined by the Interfacial Toughness**
- ◎ **Use Measured Debond Radii to Quantify Toughness Changes with High Temperature Exposures**

Existing Work

◎ **Indentation of Diamond Coatings on Titanium Alloy Substrates**
M.D. Drory and J.W. Hutchinson, Proc. R. Soc. Lond. A (1996)

◎ **Modeling Assumptions**

- **A Single Coating and a Single Substrate Material**
- **Substrate is Infinitely Large**
- **Sharp Wedge Indenter Assumed**
- **The Biaxial Residual Stress in the Coating is Known**

◎ **Limitations**

- **Results are Presented Only for Specific Substrate Stress vs. Strain Behaviors**
- **Results Given are Strictly Valid Only for:** $2 < R/a < 5$

Experimental Results and Preliminary Toughness Estimates

◎ **Use Existing Work and Approximations to Obtain Preliminary Estimates of Toughness Values**

◎ **Steps to Estimate Interface Toughnesses from Experiments:**

- **Specify the Residual Strain in TBC/Oxide Layers**
- **Approximate Applied Strains Due to Indentation Using Available Results in Drory & Hutchinson**
- **Calculate the Total Strain (Residual Plus Applied)**
- **Calculate Stress Intensity Factor as a Function of R/a**
- **Use Measured R and a Values to Estimate Kc**

◎ Experimental Measurements

- Debond Radii of Sample Specimens from Indentation Test, Measured Before Coating Pull-Off, at 90° Intervals

Time (hrs)	Debond Radii (cm)				
	i	ii	iii	iv	Average
56	0.31	0.42	0.32	0.65	0.35*
20	0.32	0.32	0.34	0.34	0.33
10	0.15	0.24	0.19	0.18	0.19
0	0.0	0.0	0.0	0.0	0.0

*This average excludes the radius at location iv, which was affected by cracking of the TBC in the radial direction.

◎ Interfacial Toughness Estimates

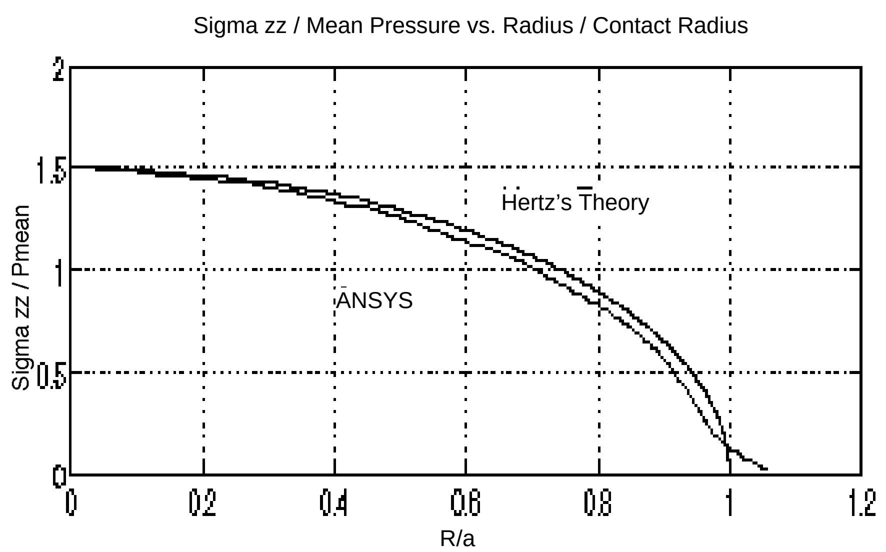
- Kc Estimated Using Two Sets of Substrate Constitutive Behaviors Which Bracket Nickel Superalloy Behavior
- Average Debond Radii Before Coating Pull-Of Used
- Single Coating Thickness of 105μm Used
- Assume average Residual Stress in Coating

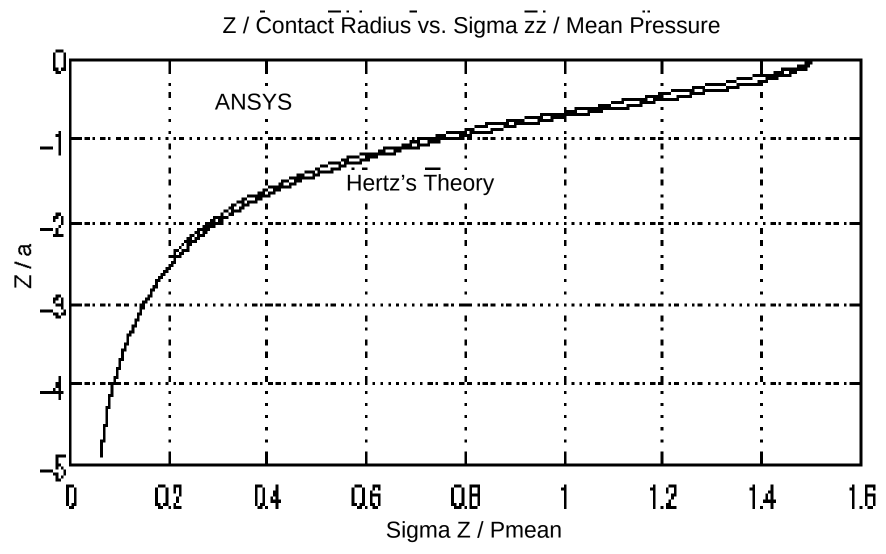
Hrs	Kc (ksi in$^{(1/2)}$)	
	$(\sigma_y/E_s, N)=(0.005,0.01)$	$(\sigma_y/E_s, N)=(0.0025,0.1)$
56	0.0183	0.0183
20	0.0206	0.0206
10	0.1328	0.0821

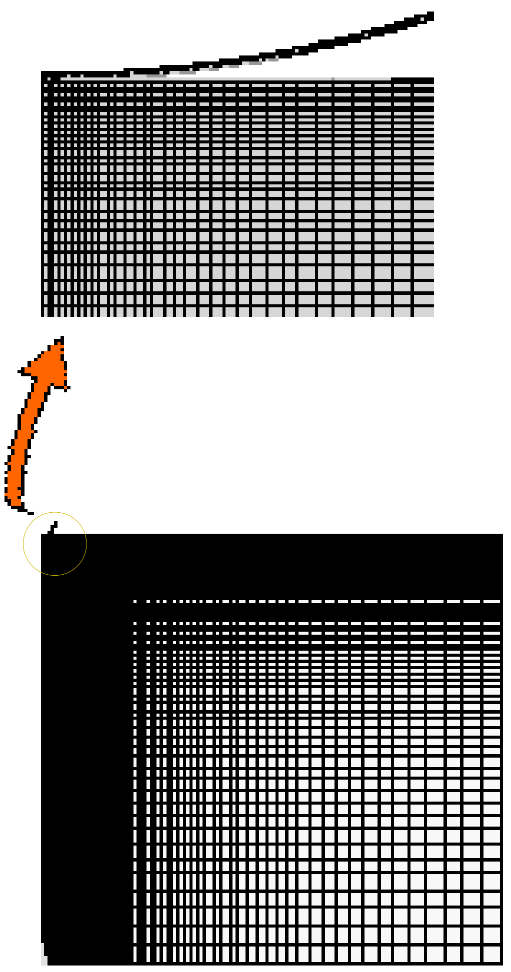
- First Reported Interfacial Toughness Values for These TBC Systems
- Debond Radii are Large, so Results are Insensitive to Constitutive Behavior Used in Indent Models
- If Residual Stresses Are the Same in Each Specimen, the *Percent Reduction* in Toughness is Independent of Assumed Residual Stress Magnitudes
- Significant Toughness Reductions Seen with Exposure
- Indents of The Back Side (TGO and Bond Coat Only) Show no Debonding (Likely a Thickness Effect)

Current Modeling Effort

- Use Finite Element Models of the Indent Test to Methodically Eliminate Assumptions of Drory & Hutchinson
- Immediate Goal: Results for any Radius of Debonding and any Indenter Shape for a Single Coating and Substrate
- Verification: Results from Model of Elastic Sphere Indentation Agree with Hertz Theory

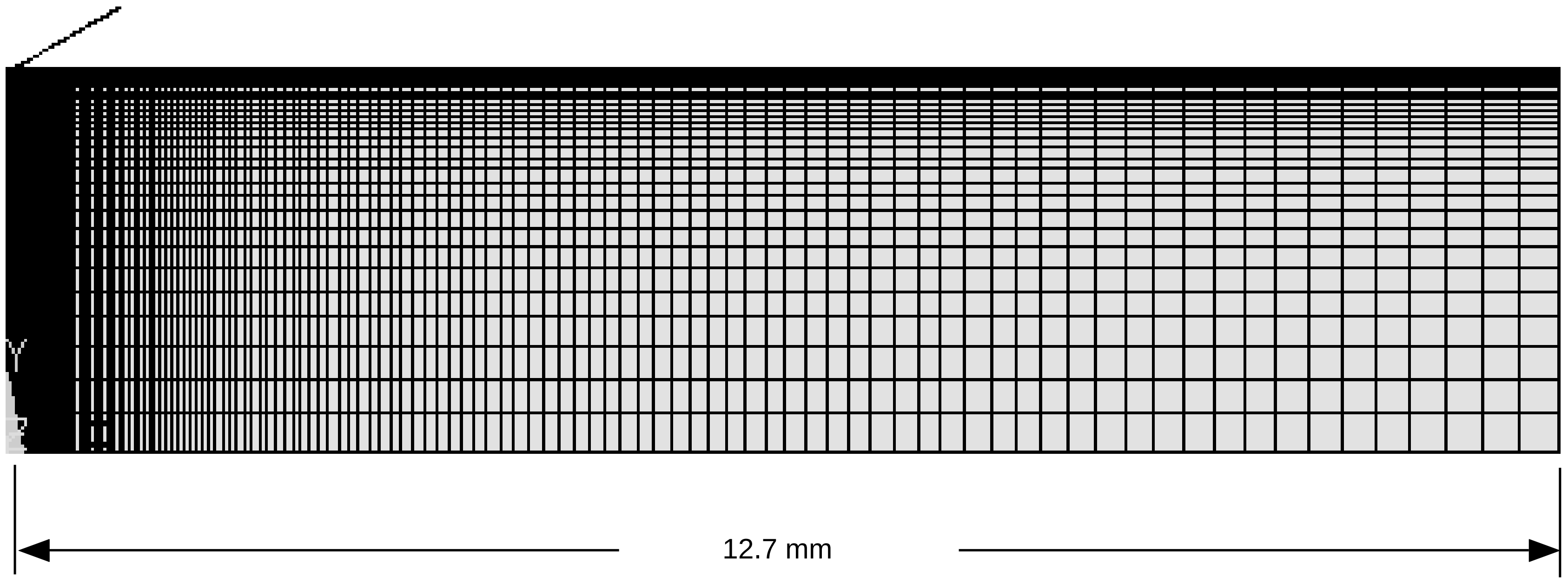




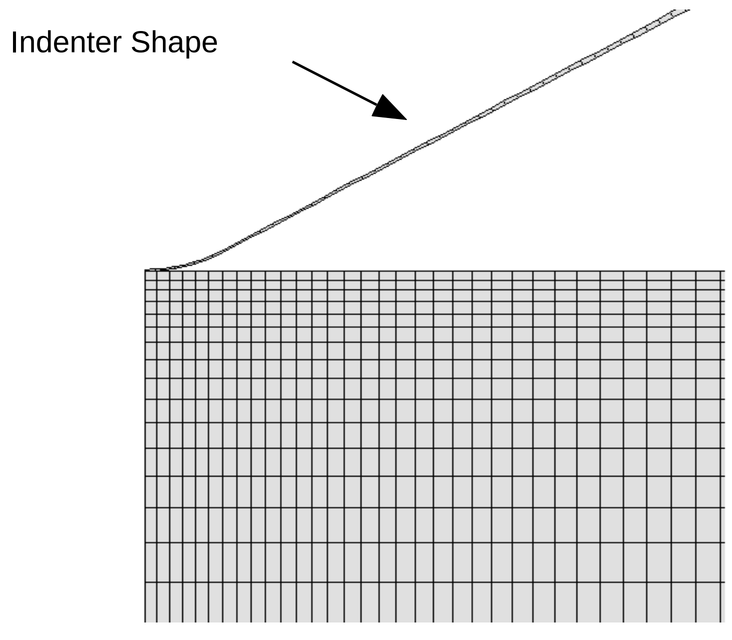


ANSYS Model Using Axisymmetric Contact Element

◎ Current Models of Elastic-Plastic Indentation Using a Brale C Indenter

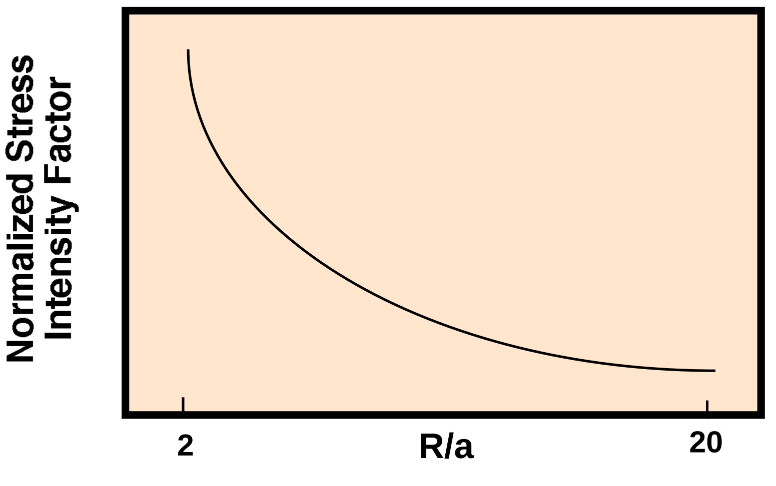


Full Model



Indent Region

Long-Term Modeling Goal:
K vs. R Plots for
Use with TBC Systems



-Given K versus R plots, Indent Tests can Routinely be Used for Evaluating TBC System Interfacial Toughnesses.

FEM MODELING

Wavy Interface Effect On Thermal Residual Stress State and Spallation by Finite Element Models

Numerical Models:

- **◎ Elastic-Plastic FEM numerical models based on microscope image profiles of Pt-Al/EB- PVD specimens with wavy interfaces, a hump, a valley and an idealized half circle geometry, were developed.**

- **◎ 2-D axisymmetric FEM models with the central axis and bottom side fixed, using triangle elements, the high density element meshes are generated across BC and oxide interface, especially for wavy interfaces.**

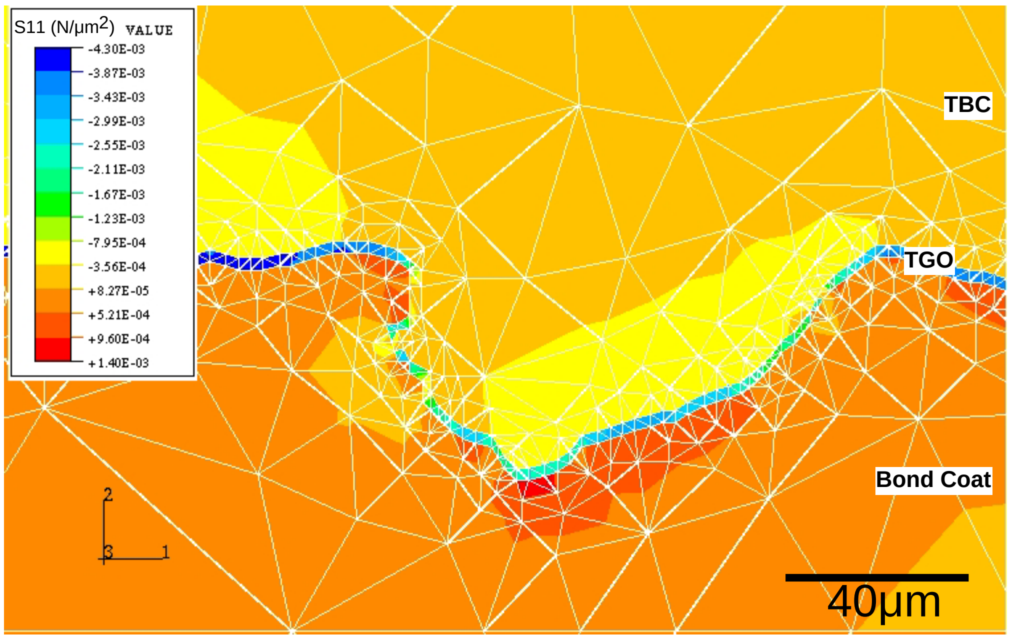
Thermal Loading:

- **◎ TBC Systems are stress free at high temperature, 1100˚C, and are cooled down to room temperature, 20˚C, in multiple steps.**

Material Properties:

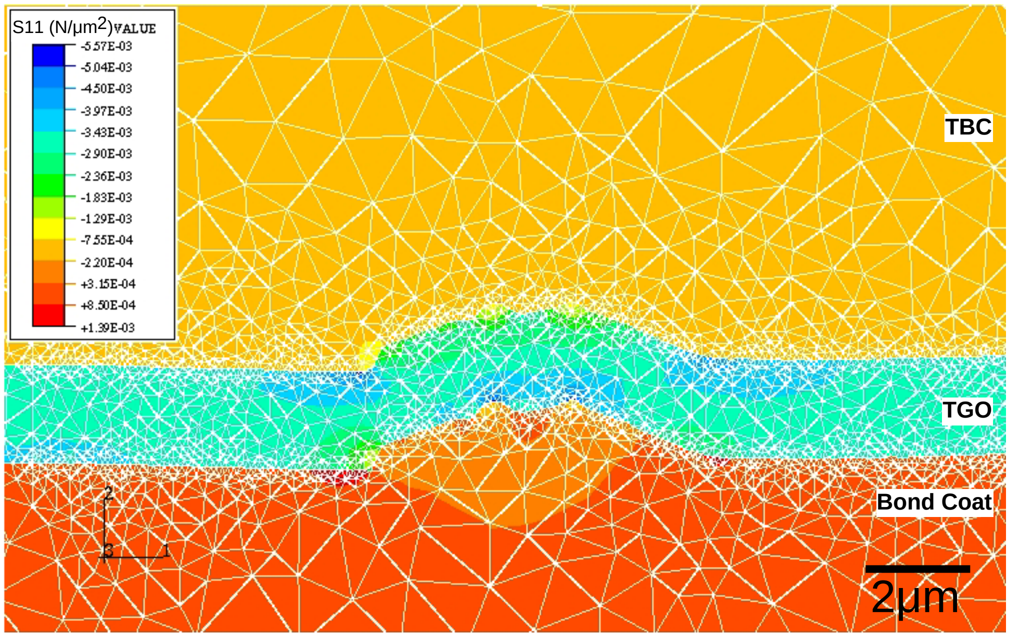
- **◎Temperature-dependent Elastic-Plastic properties and thermal expansion coefficients from available literature are used for calculations.**

Horizontal Elastic Stress Component, Pt-Al/EB-PVD with a Valley



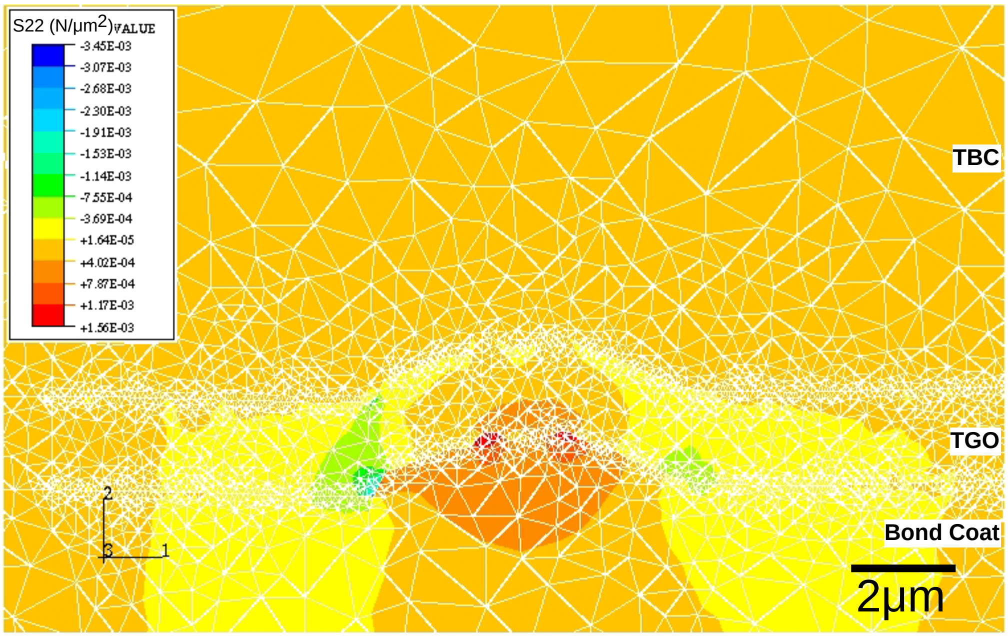
Compressive Stress in TGO and Stress Concentration due to the Valley

Horizontal Elastic Stress Component, Pt-Al/EB-PVD with a Hump



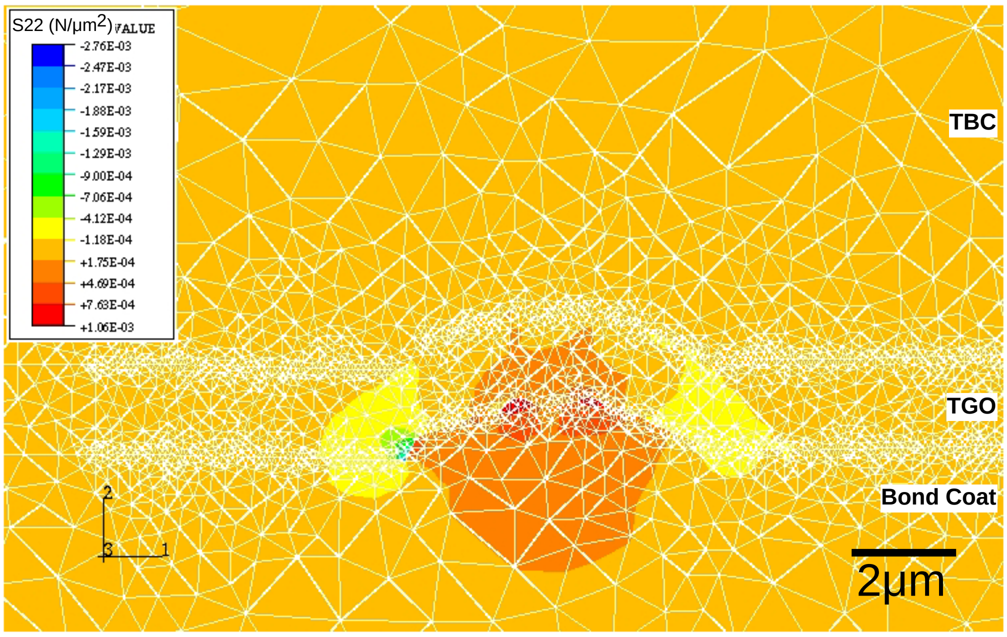
Compressive Stress in TGO and Stress Concentration due to the Hump

Vertical Elastic Stress Component, Pt-Al/EB-PVD with a Hump



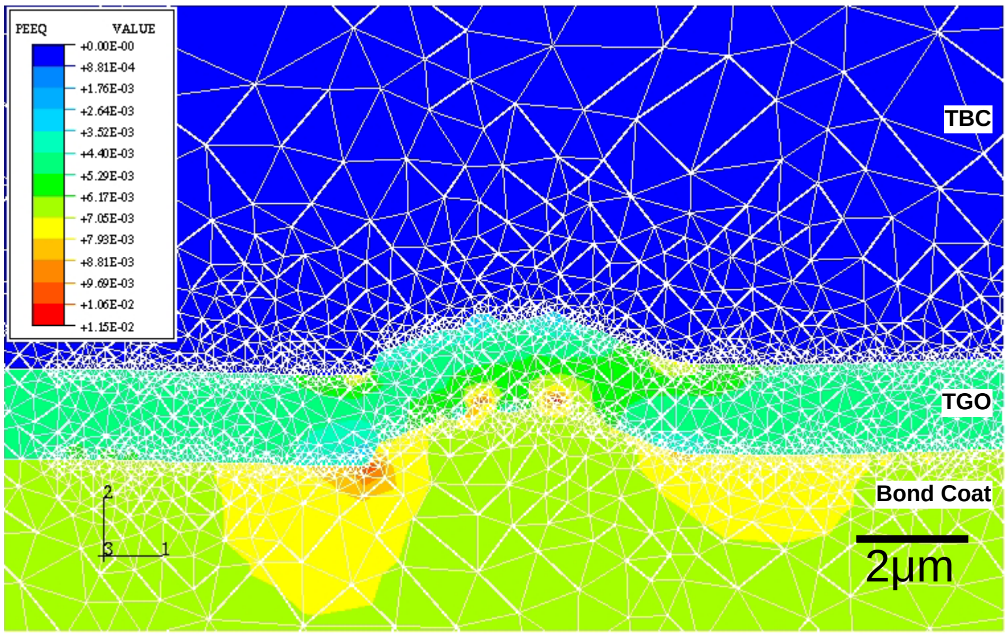
Tensile Stress at the Hump Peak can cause Fracture Parallel to the TGO-Bond Coat Interface

Vertical Stress Component (Elastic-Plastic Case), Pt-Al/EB-PVD with a Hump

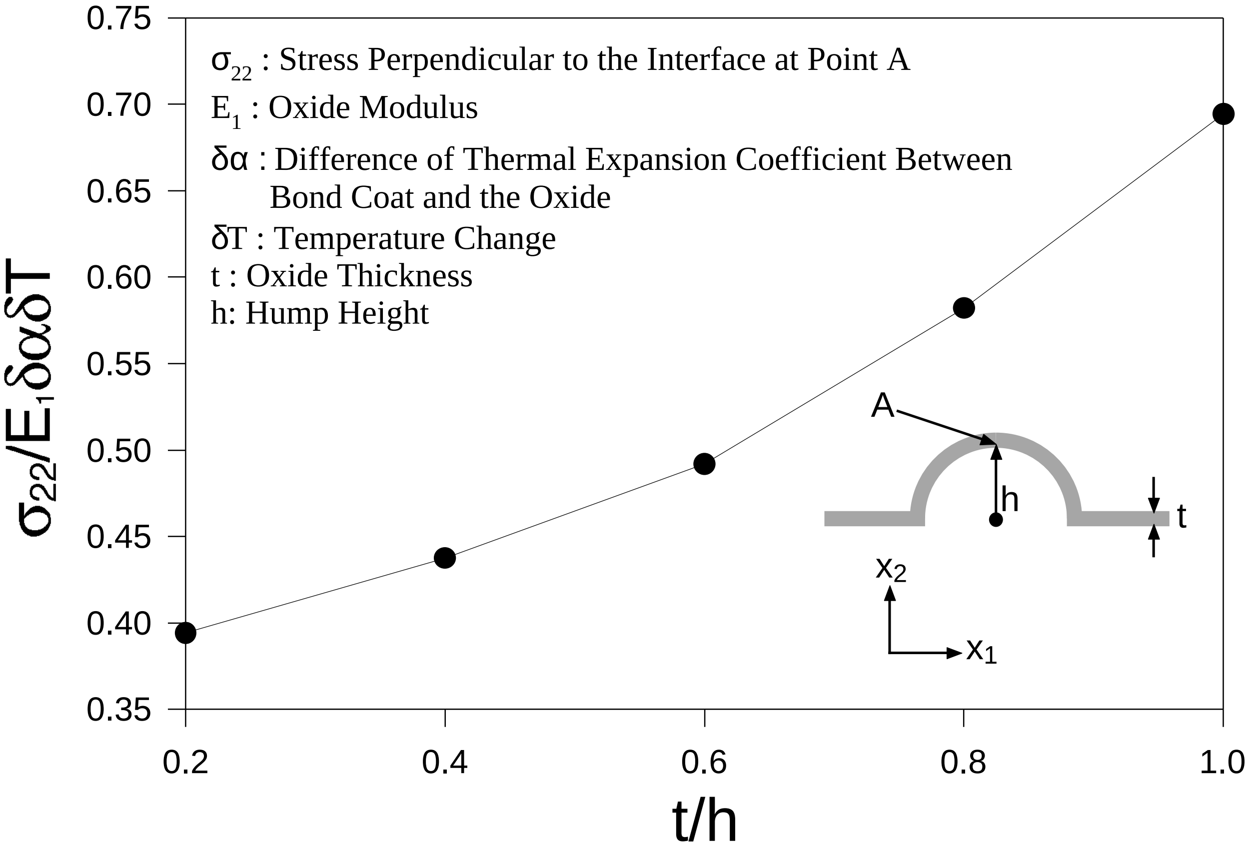


- **Interface Tensile Stress Reduced 50% due to Plastic Deformation in the Bond Coat**
- **Stress Still Large Enough to cause Fracture Parallel to TGO-Bond Coat Interface**

Equivalent Plastic Strain, Pt-Al/EB-PVD with a Hump



Plastic Strain Zone Around a Hump, Largest Values at the Hump Peak and the Transition Zone of the TGO-Bond Coat Interface



Conclusions

TBC Characterization

- ◎A thin continuous alumina layer exists between the TBC and bond coat. Near the TBC-TGO layer, the TBC has a very fine grain structure.
- ◎Debonding of the coating is predominantly along the TGO-bond coat interface.
- ◎Qualitative results from the indent test show a decrease in fracture toughness of the interfaces with time at temperature
- ◎Exposed coatings show an intermixed region of PSZ and alumina at the TBC-TGO interface.
- ◎The oxide grows thicker under the TBC than on the bare bond coat. It appears that the intermixed PSZ could provide a short circuit path for oxygen.

Fracture Mechanics

- ◎ Indent Test Gives Good Qualitative and Quantitative Feedback on Changes in Adhesion with Exposure
- ◎Quantitative Estimates from Indent Tests Show Substantial Decreases in Interfacial Fracture Toughness with Time and Temperature.
- ◎Goal is to Also Measure Toughnesses via Indents of The Back Side (TGO and Bond Coat Only). Thus Far no Debonding is Observed (Likely a Thickness Effect).
- ◎Refined Models of Indent Tests are Under Development
- ◎Long-Term Goal is to Use Models to Present K vs. R/a Results Valid for Typical TBC Systems for Straightforward Use of this Test by Coatings Engineers

FEM Modeling

◎ Stress Concentration Due to Wavy Interfaces

-Stress Parallel to the Interface

This component of stress in oxide is compressive and increases for wavy interfaces.

-Stress Normal to the Interface at Humps and Valleys

- Large tensile stresses found across the oxide thickness at the hump peaks and flat to valley transition areas.
- Plastic deformation of bond coat leads to a reduction of these stresses, but the tension is still larger than the known strength of the oxide.

◎ Possible Implications to Interface Failure

-Bond coat humps and valleys give tensile stress greater than the known oxide tensile strength even for the case of plastic strain in the bond coat. This may compromise the oxide as a diffusion barrier and lead to locally accelerated oxidation.

-Increased oxide thickness leads to higher cross oxide tensile stresses. It has also been shown in the fracture literature to lead to higher strain energy release rate for oxide separation, increase in thickness is detrimental.

Future Work

◎Consider the Effects of 1100˚C Exposures on Microstructural Development on the EB-PVD and also Plasma Sprayed Coatings

◎Continuation of Failure Mode Determination

◎Consideration of the Effect of Substrate Size in Indent Modeling

◎Consideration of Interaction Effects in Indent Tests: How Many Indents are Possible on a Single Sample

◎Modeling of the Actual Indent Specimen Which has 4 Layers (TBC, TGO, Bond Coat and Substrate)

◎Use Enhanced Model Results to More Accurately Extract Toughnesses from Experiments

◎Extend FEM Modeling to Indent Test