Using OOF to Model Mechanical Behavior of Thermal Barrier Coatings

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- Scott Terry & Carlos Levi,
  Univ. of Calif. at Santa Barbara

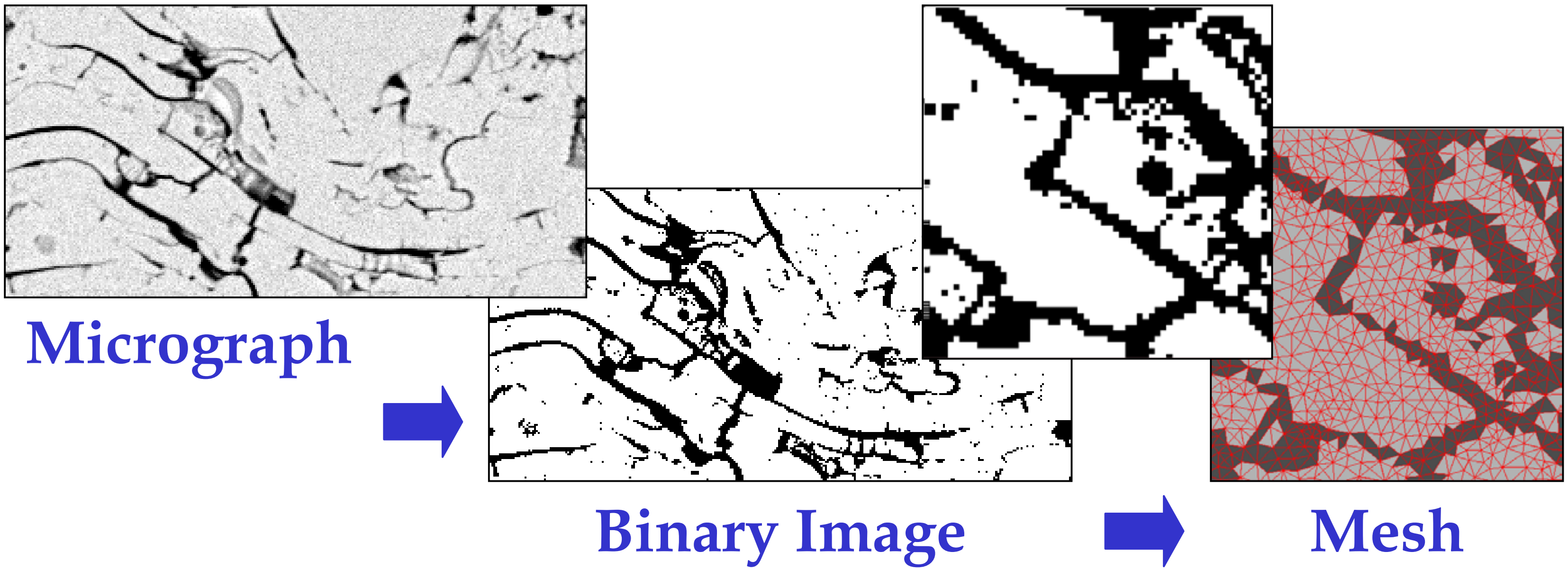
Technical Issues for TBC's

- Correlate properties with microstructure
  - to shorten materials development cycle
  - to improve materials & processing
  - to enable more reliable design
- Increase thermal protection
- Increase life
- Increase reliability,

  i.e., predict life, or coating spallation

APPROACH: Develop computational tools for elucidating influences of stochastic microstructural features (e.g., porosity) on physical properties; and provide insights into mechanisms that lead to TBC spallation via predictive micro-mechanical models of reliability.

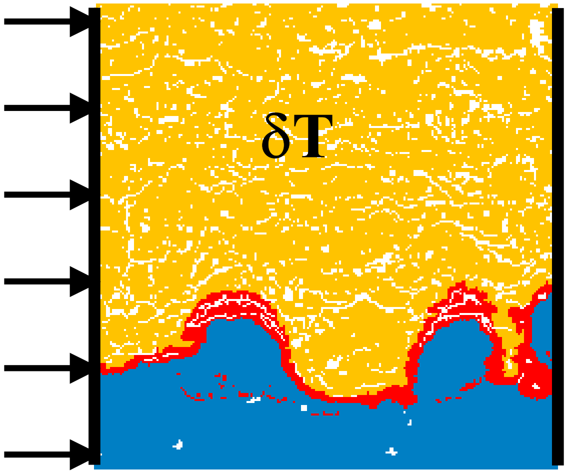
PPM2OOF Tool



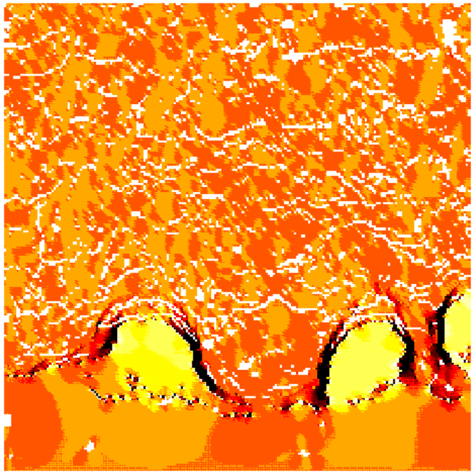
- Convert micrograph to ".ppm" (portable pixel map) file
- Select & identify phases to create binary image
- Assign constitutive physical properties to each phase
- Mesh in PPM2OOF via "Simple Mesh" or "Adaptive Mesh" – multiple algorithms that allow elements to adapt to the microstructure

OOF Tool

Virtual Experiments:
constrained cooling



Visualize & Quantify:
normal residual stresses

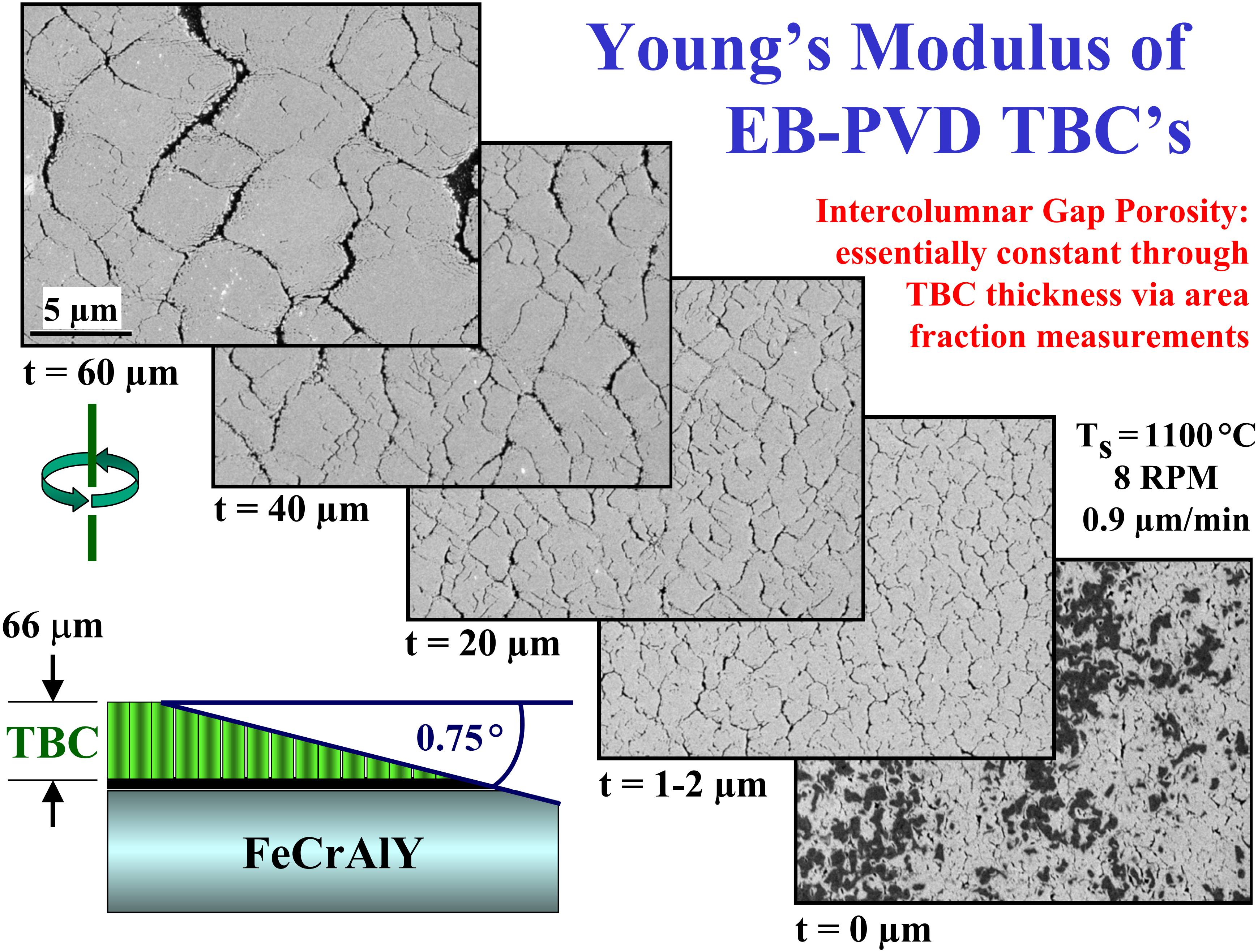


Perform virtual experiments on finite-element mesh:

- To determine effective macroscopic properties
- To elucidate parametric influences
- To visualize microstructural physics

Young's Modulus of EB-PVD TBC's

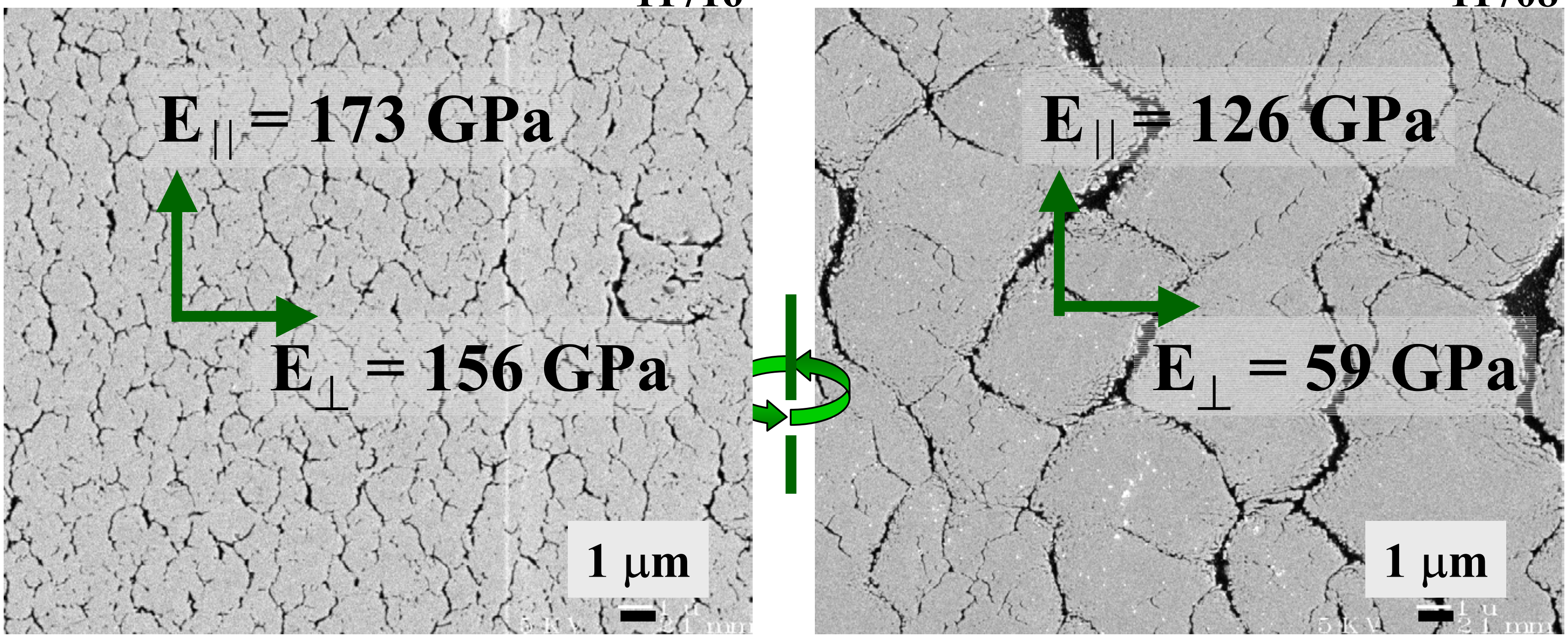
Intercolumnar Gap Porosity: essentially constant through TBC thickness via area fraction measurements



Courtesy of Scott Terry & Carlos Levi, University of California, Santa Barbara

EB-PVD TBC Cross Sections:

11716 11708



Near interface microstructure | **Surface microstructure**

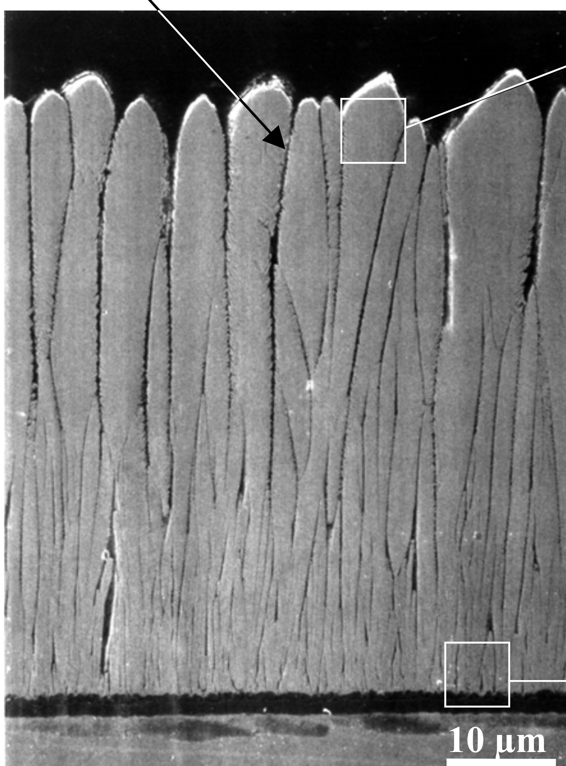
1.3 μ m from TGO/TBC interface | **60 μ m from TGO/TBC interface**

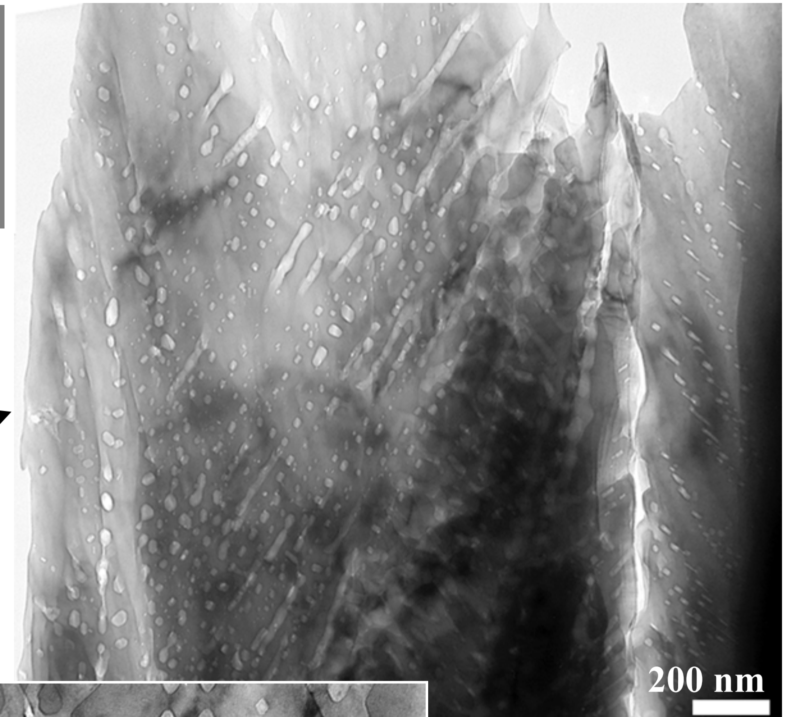
Courtesy of Scott Terry & Carlos Levi, University of California, Santa Barbara

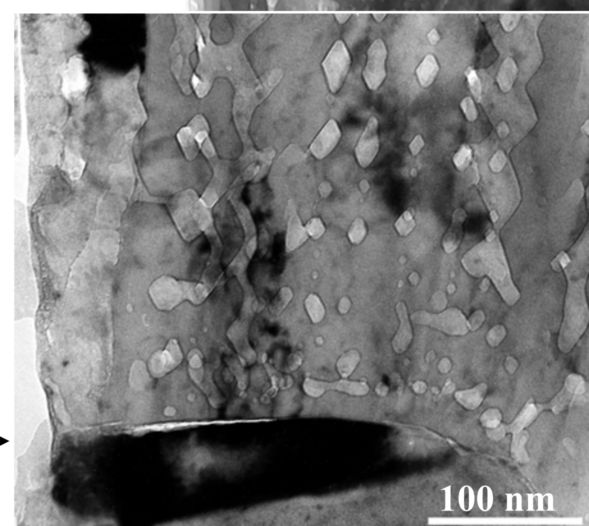
Porosity: key to TBC Performance

Intercolumnar
➪ Compliance

Intracolumnar
➪ Insulation







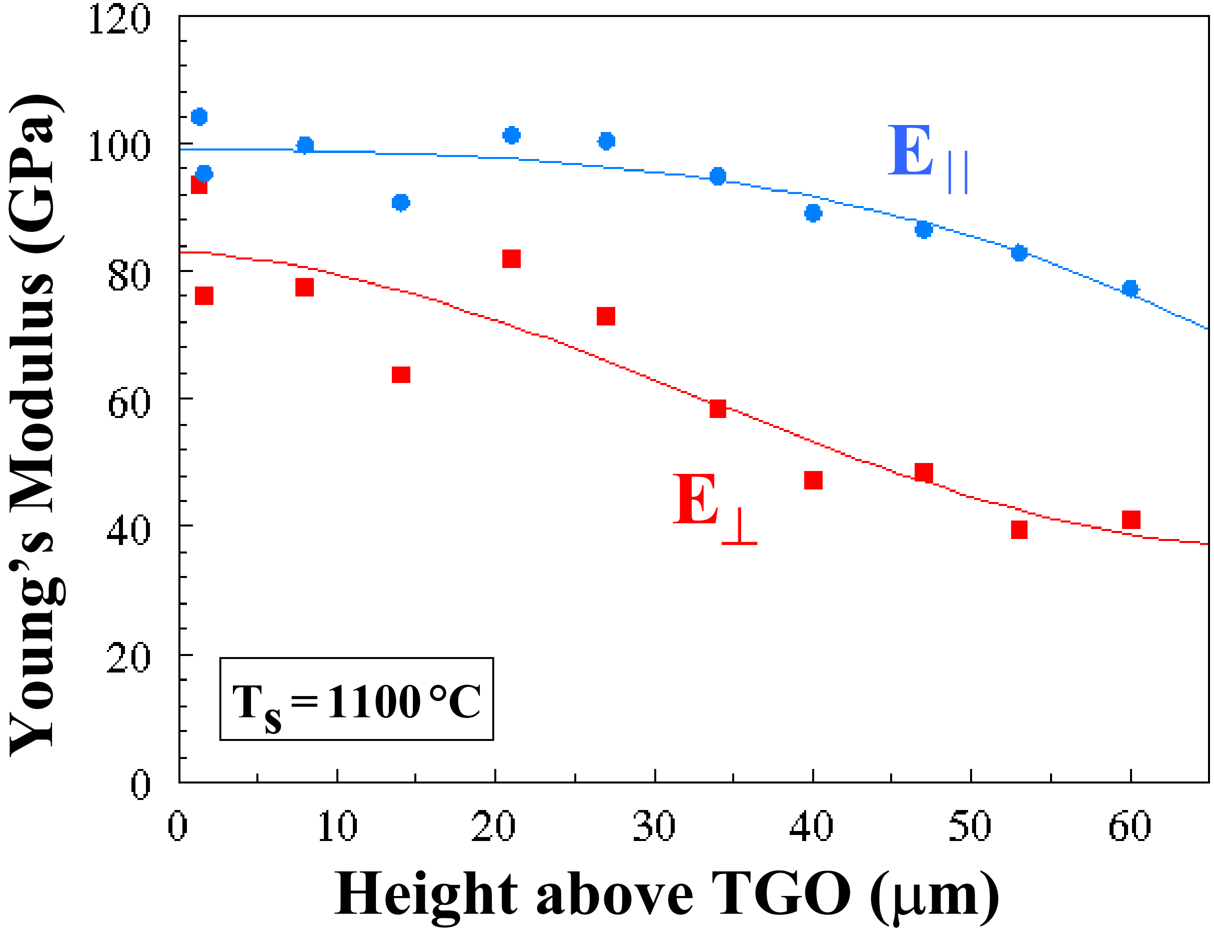
Different scales of shadowing

TEM courtesy of E. Sommer and M. Rühle MPI-Stuttgart

Courtesy of Scott Terry & Carlos Levi, University of California, Santa Barbara

Young’s Modulus of EB-PVD TBC’s

Modulus is anisotropic and position dependent

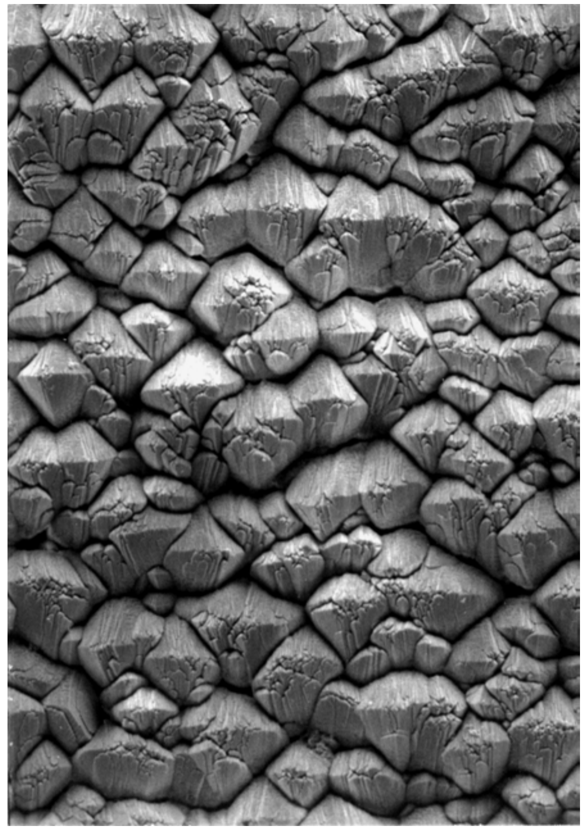


<60% modulus reduction due to intracolumnar porosity>

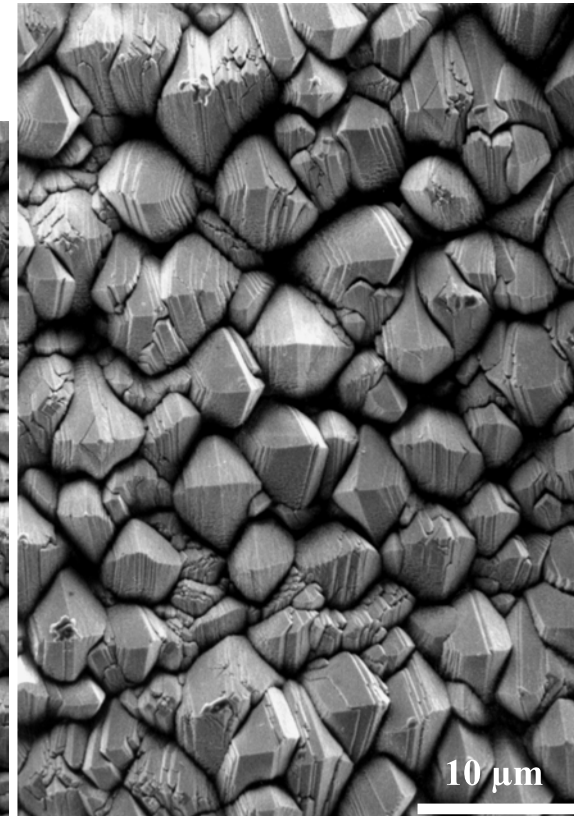
Effect of Temperature on Surface Morphology and Texture

Rotating Substrates

T_s = 900 °C



T_s = 1000 °C



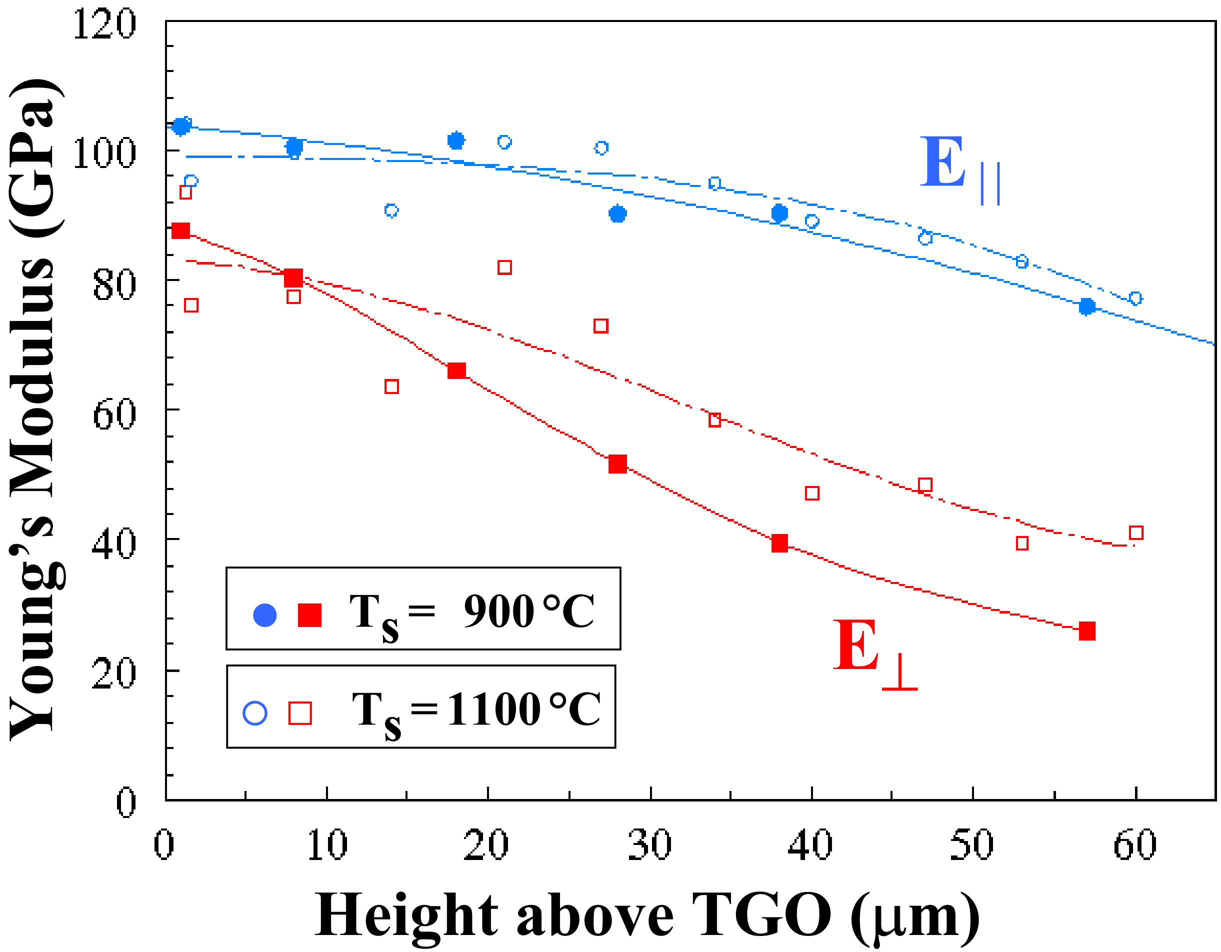
T_s = 1100 °C

8 RPM, ~0.9 μm/min
(Flux ~ 3.2 μm/min)

Courtesy of Scott Terry & Carlos Levi, University of California, Santa Barbara

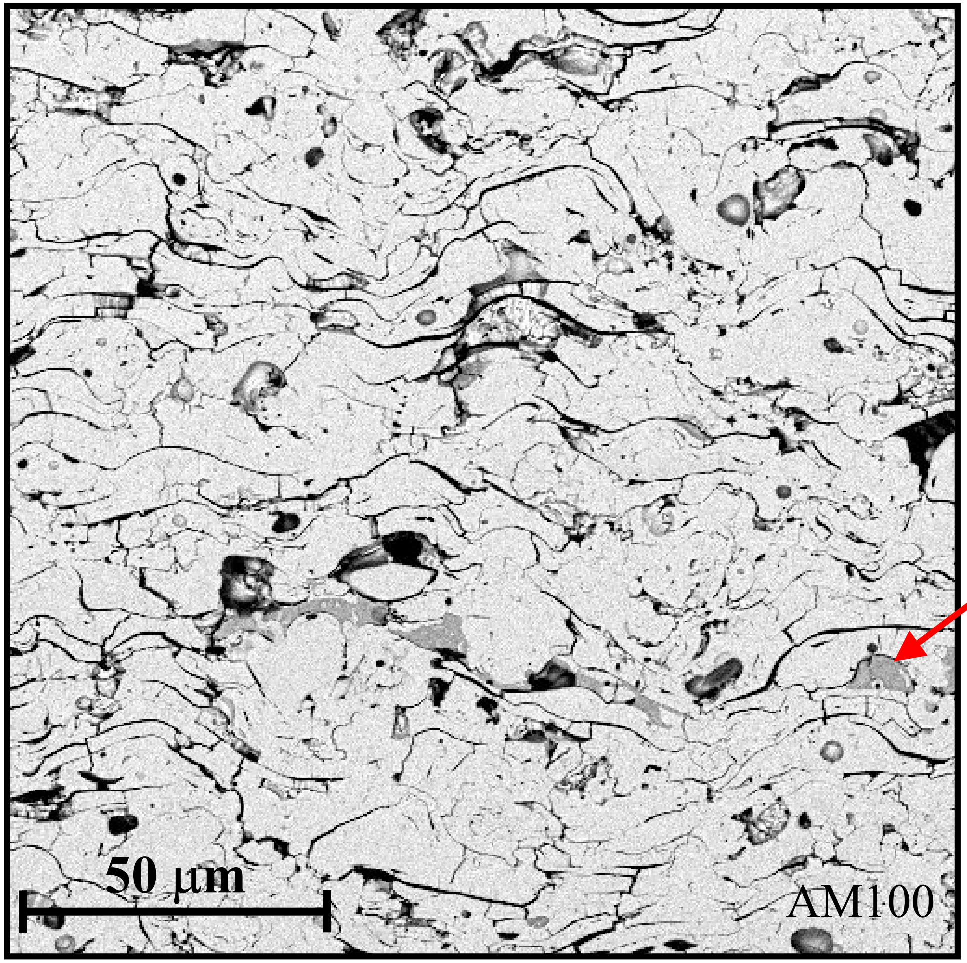
Young's Modulus of EB-PVD TBC's

Modulus is anisotropic and position dependent



<60% modulus reduction due to intracolumnar porosity>

Section View of a ZrO_2 – 8 wt% Y_2O_3 Plasma Sprayed Thermal Barrier Coating

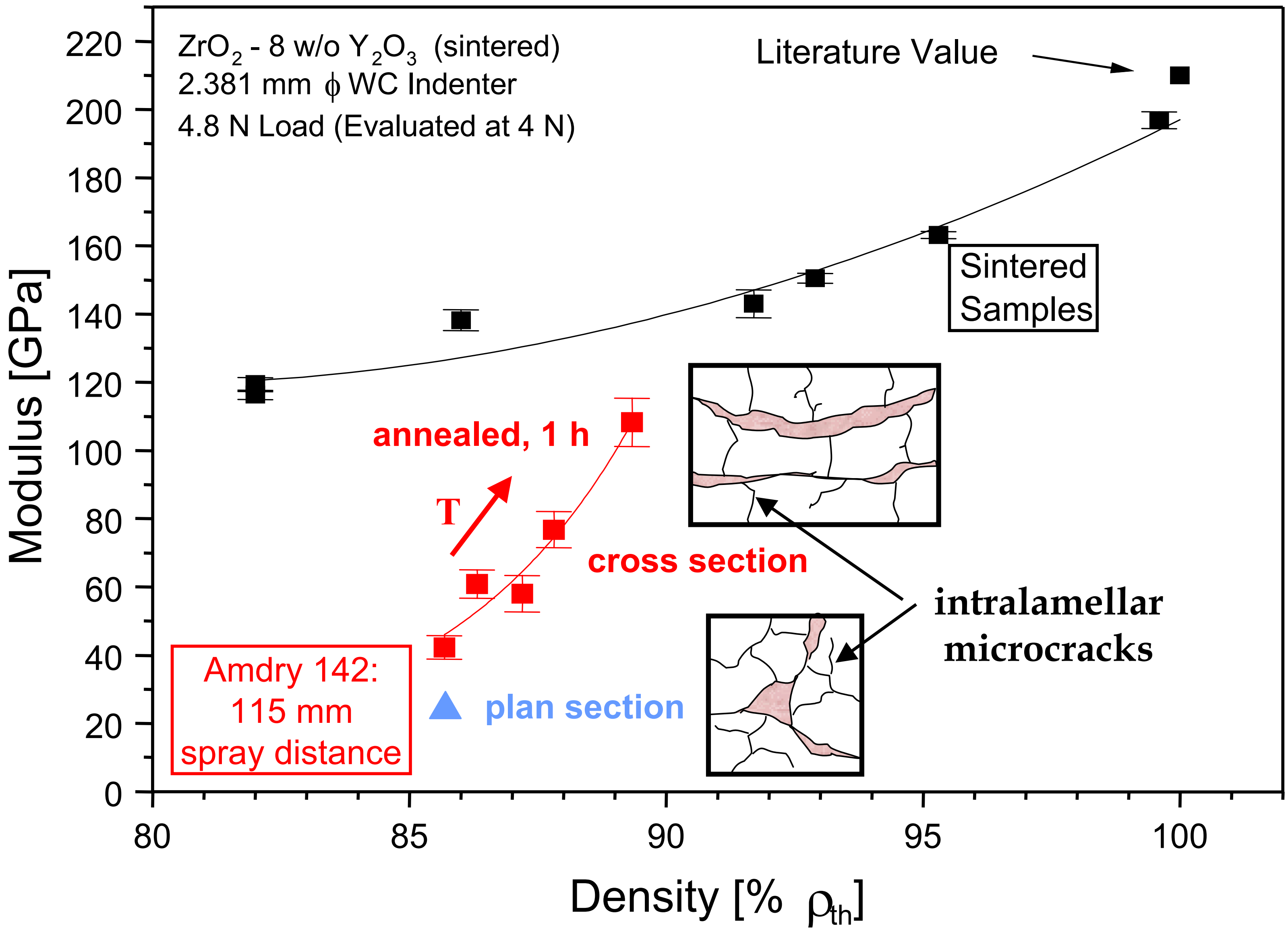


Free Standing Monolith

more than 50 plasma spray parameters!

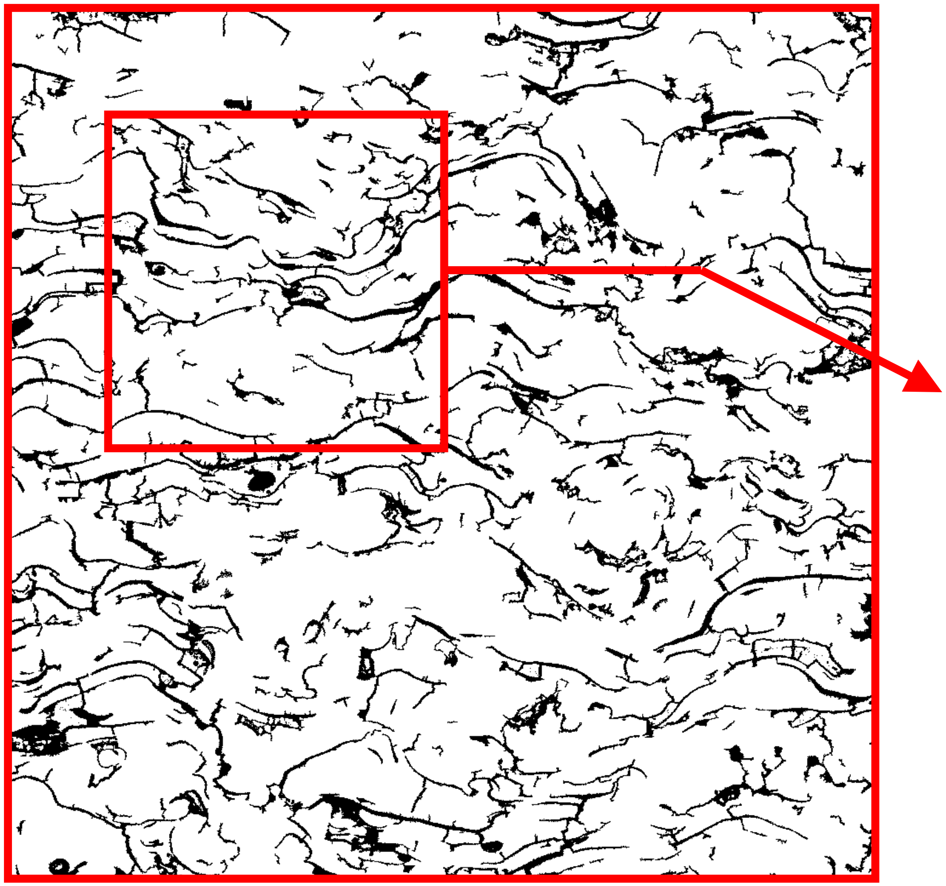
Fabricated at Thermal Spray Laboratory, SUNY, Stony Brook (Jan Ilavsky)

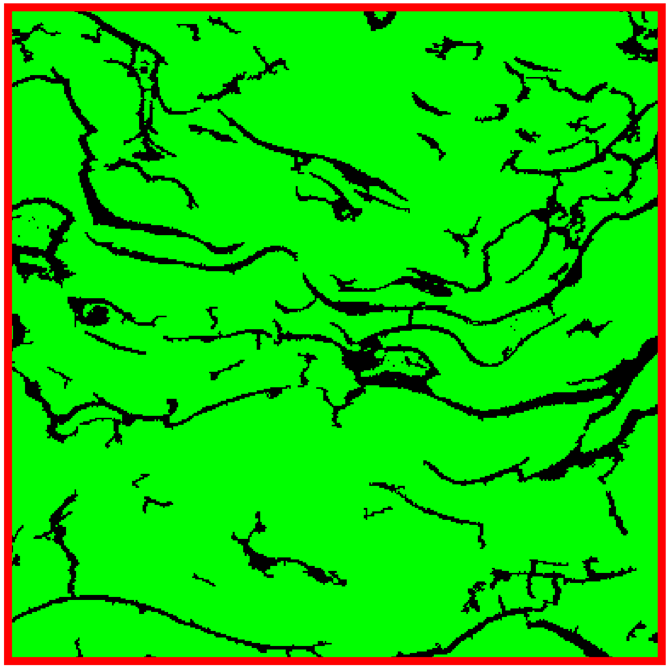
Young's Modulus versus Porosity



J. S. Wallace and J. Ilavsky, J. of Thermal Spray Tech., 7, [4], 521-526 (1998).

Calculating Average Elastic Properties of a Representative Region

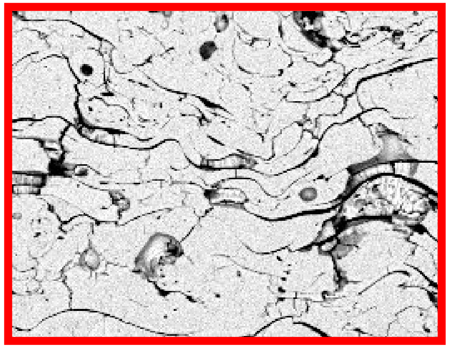


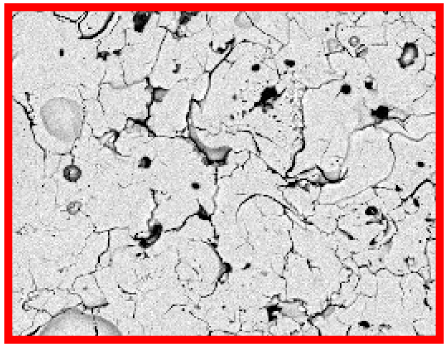


85 μm

Effective Elastic Young's Modulus Calculated From Microstructural Finite Elements

	Porosity (%)	Section Moduli (GPa)		Porosity (%)	Plan Moduli (GPa)	
		E_x	E_y		E_x	E_y
Calc.:	12 ± 1	39 ± 10	13 ± 7	6	83	90
Expt.:	11	28		11	19	

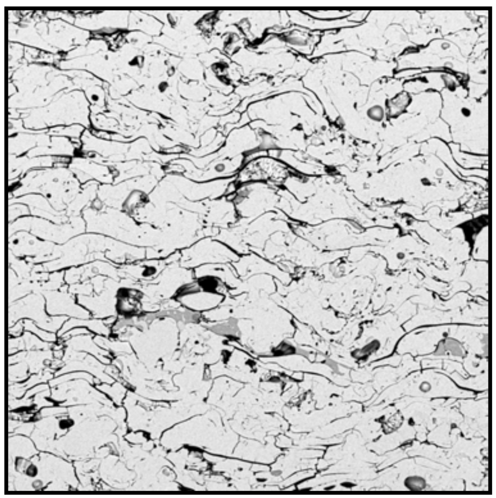


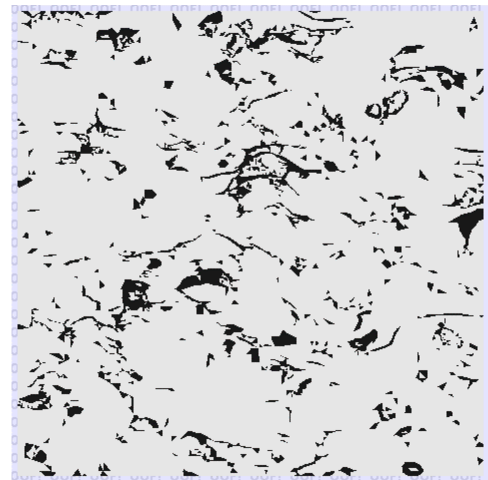


ZrO_2 – 8 wt% Y_2O_3: E = 214 GPa ν = 0.310

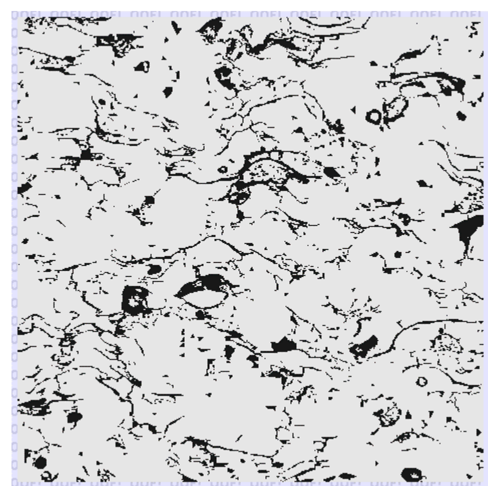
How to Generate Effective Meshes?

Original Image



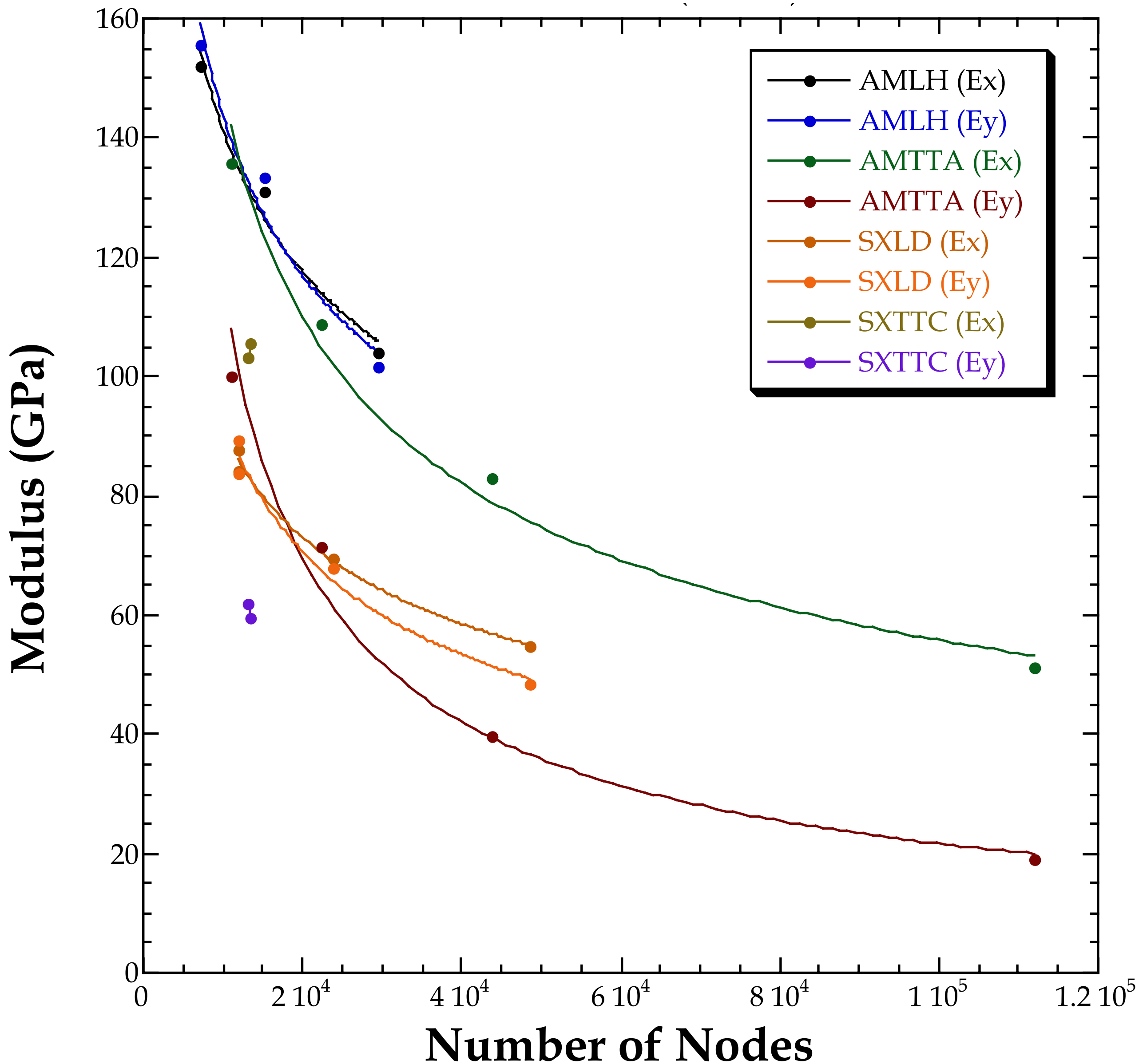


Low Res. Mesh
E_x = 136 GPa
E_y = 100 GPa
Nodes = 10,894



High Res. Mesh
E_x = 83 GPa
E_y = 40 GPa
Nodes = 43,887

Modulus versus Mesh Resolution

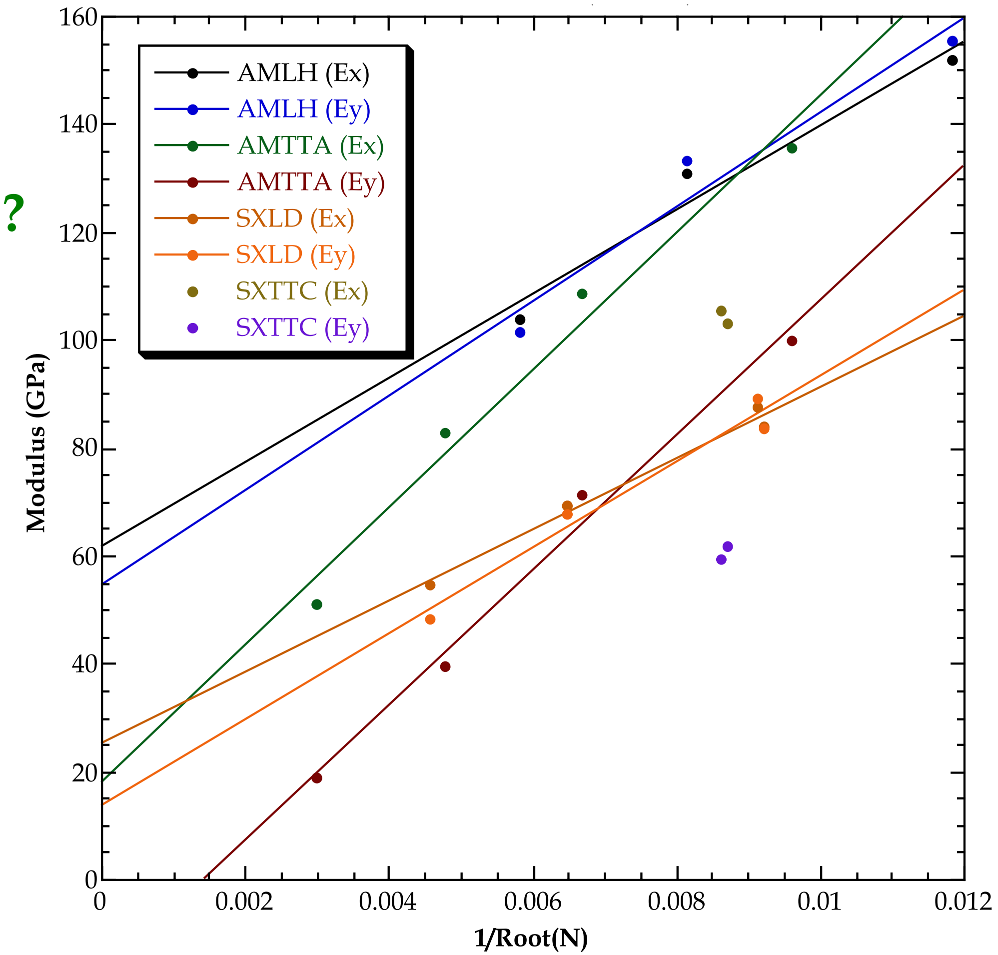


Modulus versus Mesh Resolution

How accurate should mesh be?

If the structure is truly random, then errors in simulation might vary with the spacing between nodes:

$$E \propto \frac{1}{\sqrt{N}} \quad ????$$



Critical Issues

- Does the mesh resolution capture the essential features that affect behavior?

  E.g., Does the mesh capture the essence of the fine cracks?

- If the mesh resolution is changed, does the simulated behavior also change?
- This there asymptotic behavior?
- Can these techniques be validated in a general manner?

Modeling Mechanical Behavior of TBC's

SUMMARY:

- **Microstructure-based, finite-element simulations provide a new paradigm for property measurements of complex materials, such as, TBC's.**
- **Sample preparation & image analysis are critical for obtaining accurate, quantitative measures of behavior.**
- **Mesh resolution can have significant influences on determined properties.**
- **Finite-element simulations help to elucidate the influences of stochastic microstructural features (e.g., porosity) on the elastic behavior of complex TBC microstructures.**