Abstract

THERMAL PROPERTY PREDICTION VIA FINITE-ELEMENT SIMULATIONS

Edwin R. Fuller, Jr.,* National Institute of Standards and Technology,
Gaithersburg, Maryland 20899-8521, U.S.A.;
James Ruud, N. S. Hari, James C. Grande, Antonio Mogro-Campero,
GE Corporate Research and Development, Schenectady, NY 12301, U.S.A.

As thermal barrier coatings (TBC's) are used in more critical applications in advanced engines, extensive materials development effort in industry has been to produce more reliable and reproducible TBC's. Knowing basic physical properties of TBC's is essential for design and reliability assessment of components using these coatings. In particular, point-to-point knowledge of thermal conductivity is crucial in advanced turbine airfoil design to allow more precise part temperature and life assessment. As physical properties are difficult, costly, and time-consuming to measure directly, an alternate strategy is to develop finite-element schemes for calculating these properties directly from the complex material microstructure. Such a computational tool, called OOF for Object Oriented Finite element analysis, is used to simulate thermal conductivity of thermal-sprayed TBC's. Simulations are validated for a range of thermal-sprayed microstructures via thermal flash measurements of thermal diffusivity. This validation procedure has indicated many aspects of image analysis and the physics of thermal conductivity for fine microcracks that must be considered.

Thermal Property Prediction via Finite-Element Simulations

Edwin R. Fuller, Jr.,*
National Institute of Standards and Technology
Gaithersburg , MD 20899-8521, U.S.A.

James Ruud, N. S. Hari, James C. Grande, Antonio Mogro-Campero, GE Corporate Research and Development, Schenectady, NY 12301, U.S.A.

Symposium on Advanced Ceramic Coatings
Intl. Conf. on Advanced Ceramics & Composites
Cocoa Beach, FL - January 15, 2002

Collaborators & Acknowledgment

- Stephen A. Langer, Information Tech. Lab., NIST
- Edwin Garcia,MIT
- Mark R. Locatelli and Andrew C. E. Reid, Mater. Sci. & Engn. Lab., NIST

Support in part from the U.S. Department of Energy, Office of Industrial Technologies, Project Officer, Patricia Hoffman, Advanced Turbine Systems Program, is gratefully acknowledged.

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.

Motivation:
Predict Thermal Conductivity k of TBC's

Laser flash measurements are time consuming, expensive, and require special expertise. Accordingly, such measurements are:

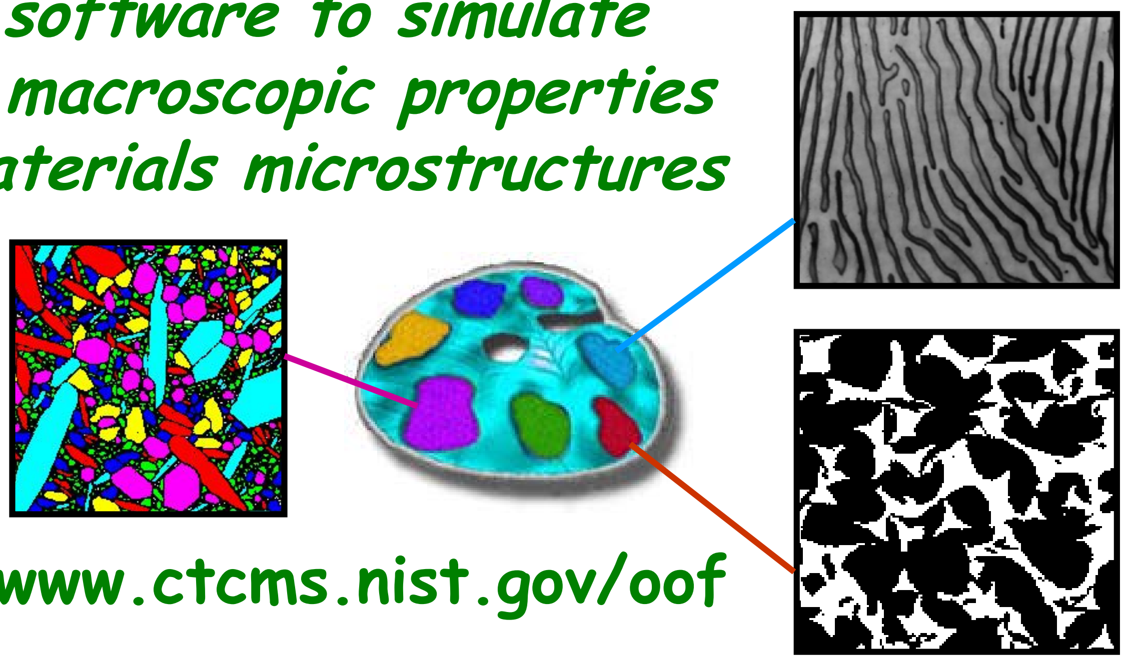
- *rarely made during materials development*
- *used sparingly by turbine part designers*
- *typically not included in production qualification & QC*

Benefits of inexpensive, widely available, rapid predictor

- More accurate cooling and lifing of gas turbine parts
- Optimization of k during TBC material development
- New lower k TBC materials designed on computer
- Spray vendors qualify TBC's for thermal conductivity
- Expansion to other properties after validation for k

Object Oriented Finite Element Analysis for Materials Science and Engineering

Public domain software to simulate and elucidate macroscopic properties of complex materials microstructures

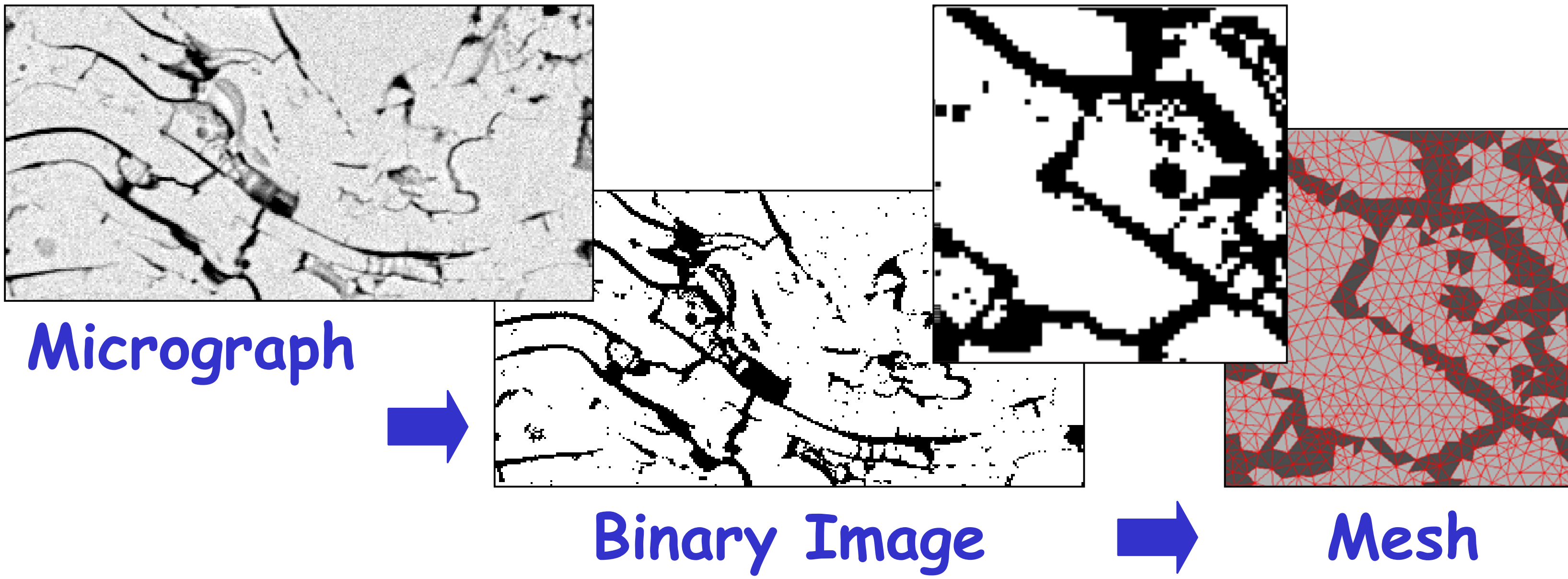


http://www.ctcms.nist.gov/oof

INDUSTRY WEEK

1999 Technologies of the Year Award

PPM2OOF Tool

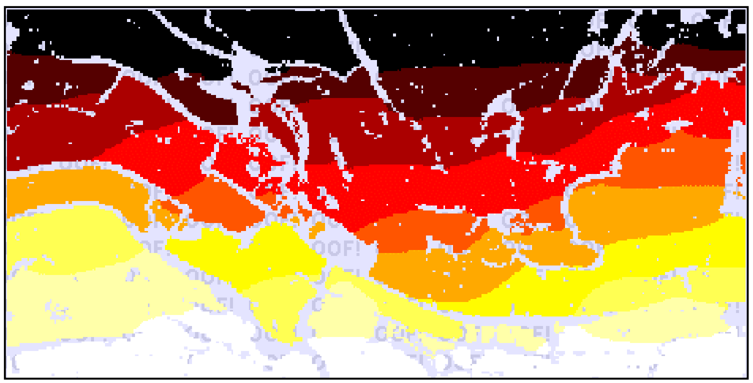


- Convert micrograph to ".ppm" (portable pixel map) file
- Select & identify phases to create binary image
- Assign constitutive physical properties to each phase
- Mesh in PPM2OOF via "Simple Mesh" or "Adaptive Mesh" – multiple algorithms that allow elements to adapt to the microstructure

OOF Tool

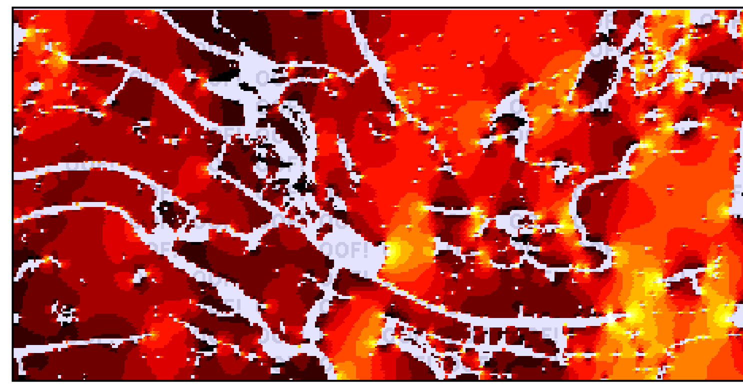
Virtual Experiments: Temperature Gradient

To + δT



To - δT

Visualize & Quantify: Heat Flux Distribution



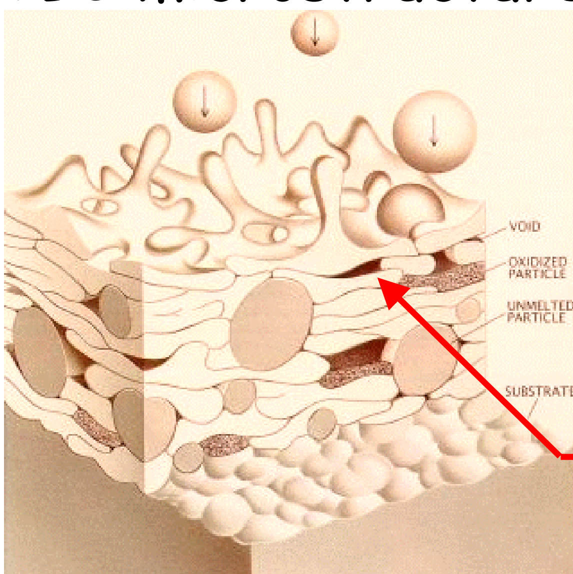
Perform virtual experiments on finite-element mesh:

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

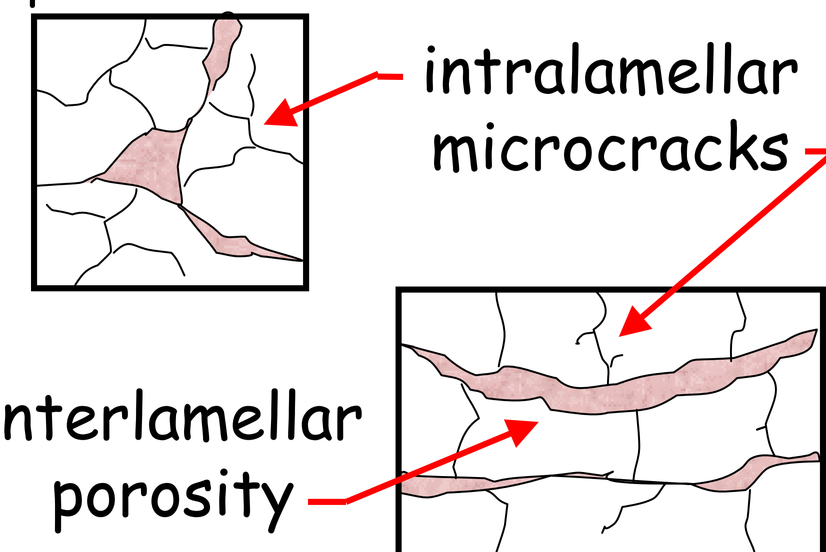
Anisotropic Thermal & Elastic Properties

With *OOF* systematically elucidate the influence of porosity (pores and microcracks & their spatial and size distribution) on thermal and elastic behavior

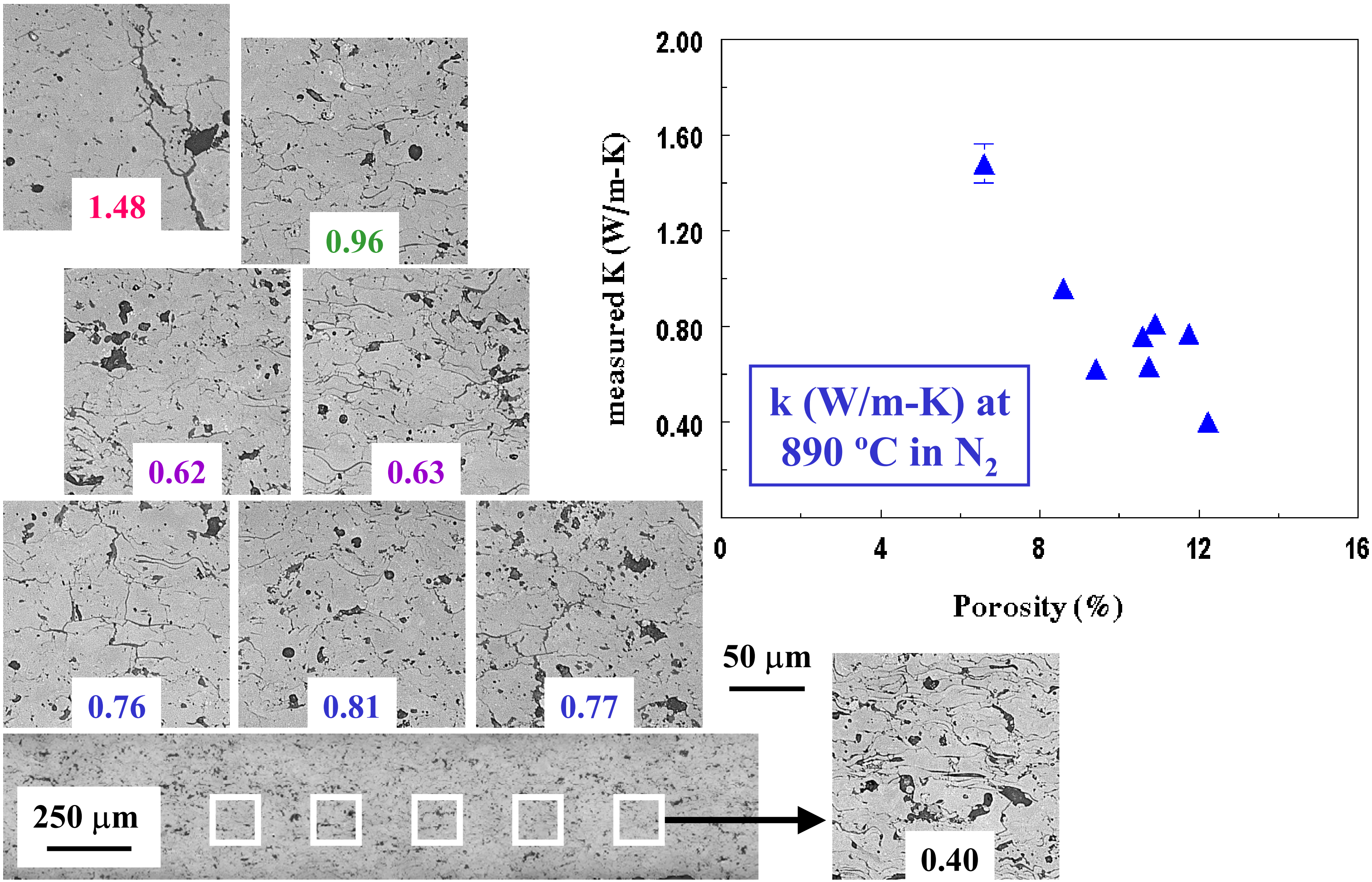
TBC microstructure



Herbert Herman, *Sci. Amer.*, **259** [3], 112-117 (Sept 1988).

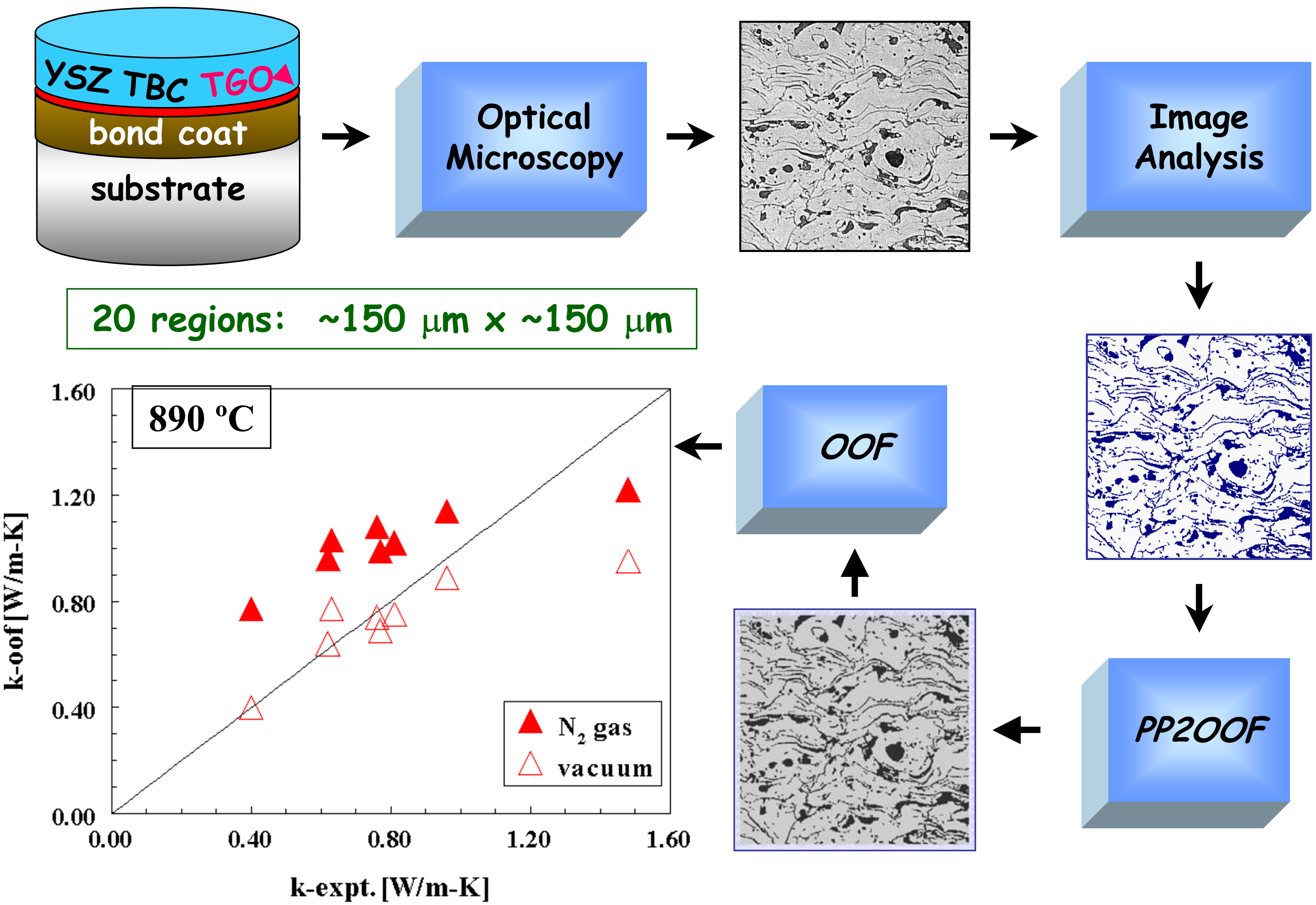


TBC Thermal Conductivity Measurements



James Ruud, N. S. Hari, James Grande, & A. Mogro-Campero, GE Corp. R&D

Thermal Conductivity via OOF Simulations



Influences of Image Resolution

Calculated K_{bulk}:

Heat Flux Distribution

1.076 W/m·K

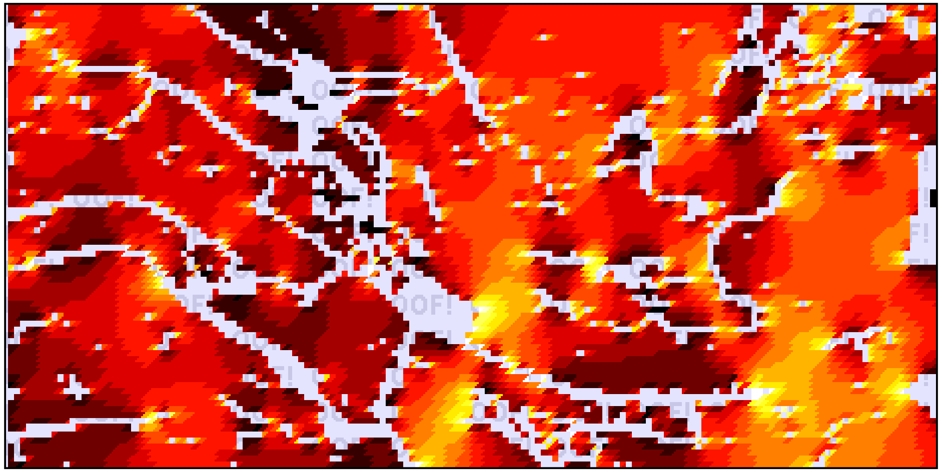
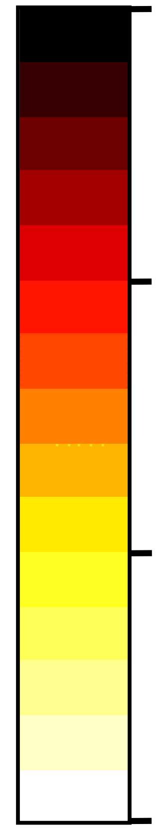


Image Resolution: 0.428 μm/pixel



0.940 W/m·K

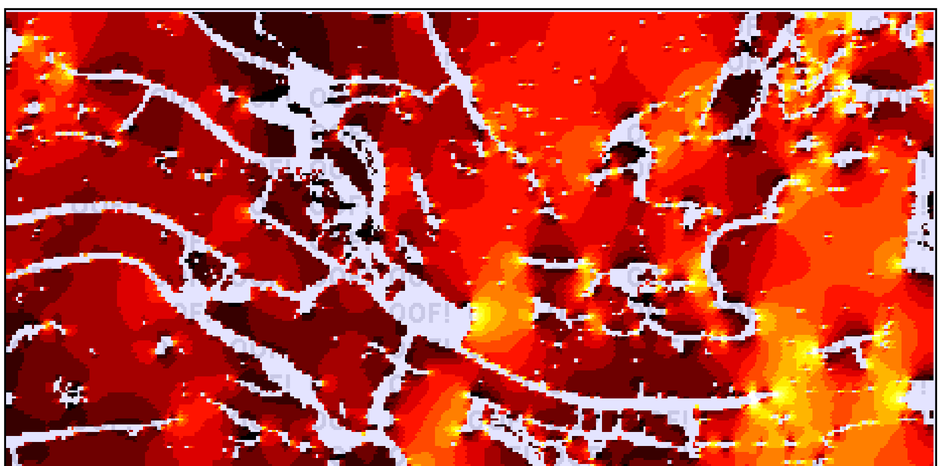
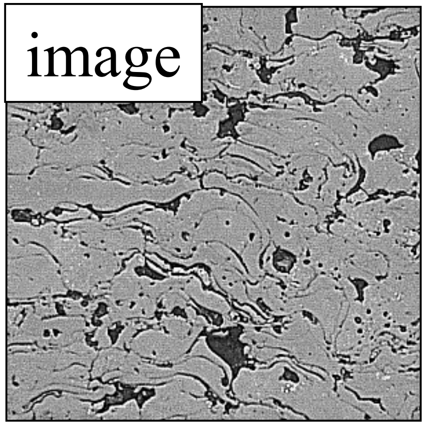
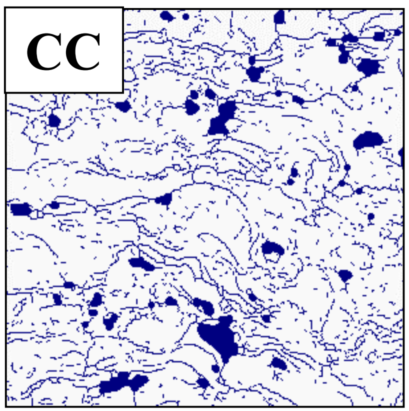


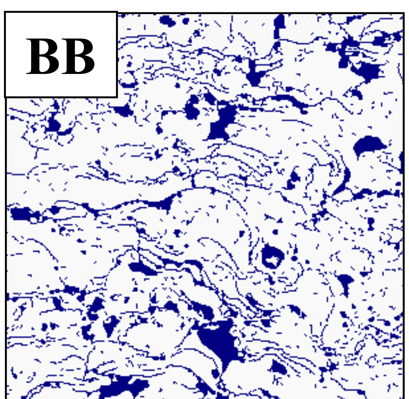
Image Resolution: 0.214 μm/pixel

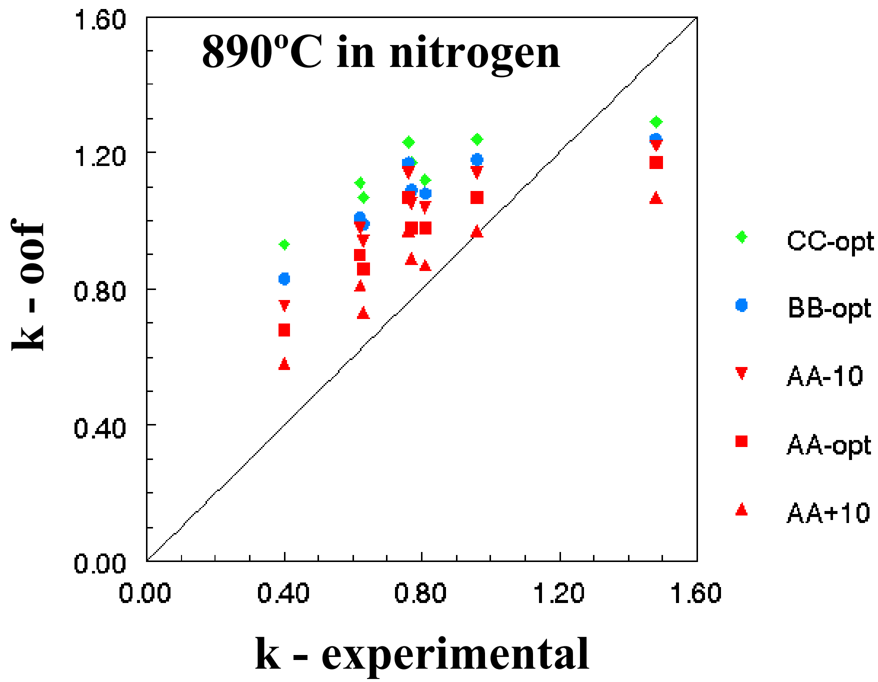
64.2 μm x 32.1 μm

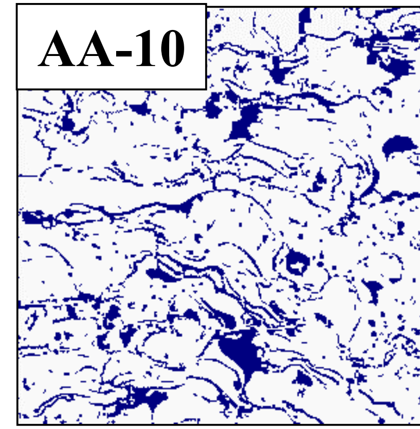
Variation in image analysis protocol

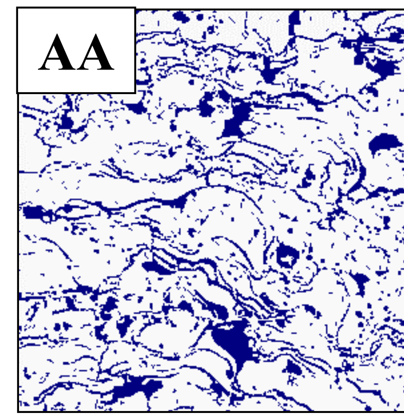


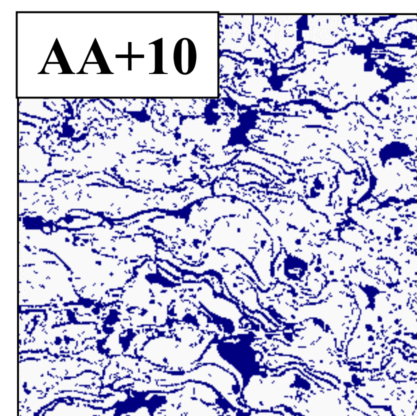








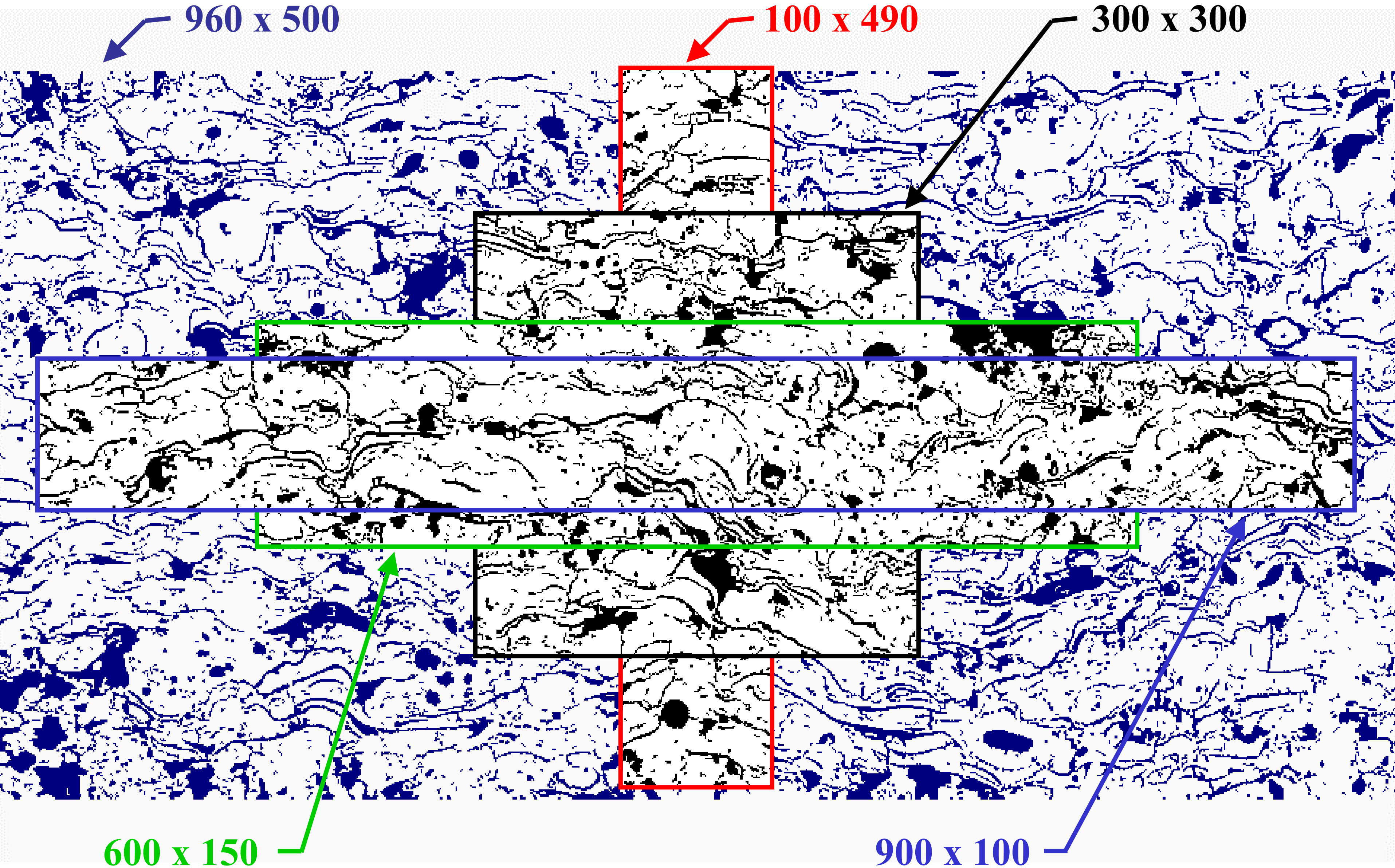




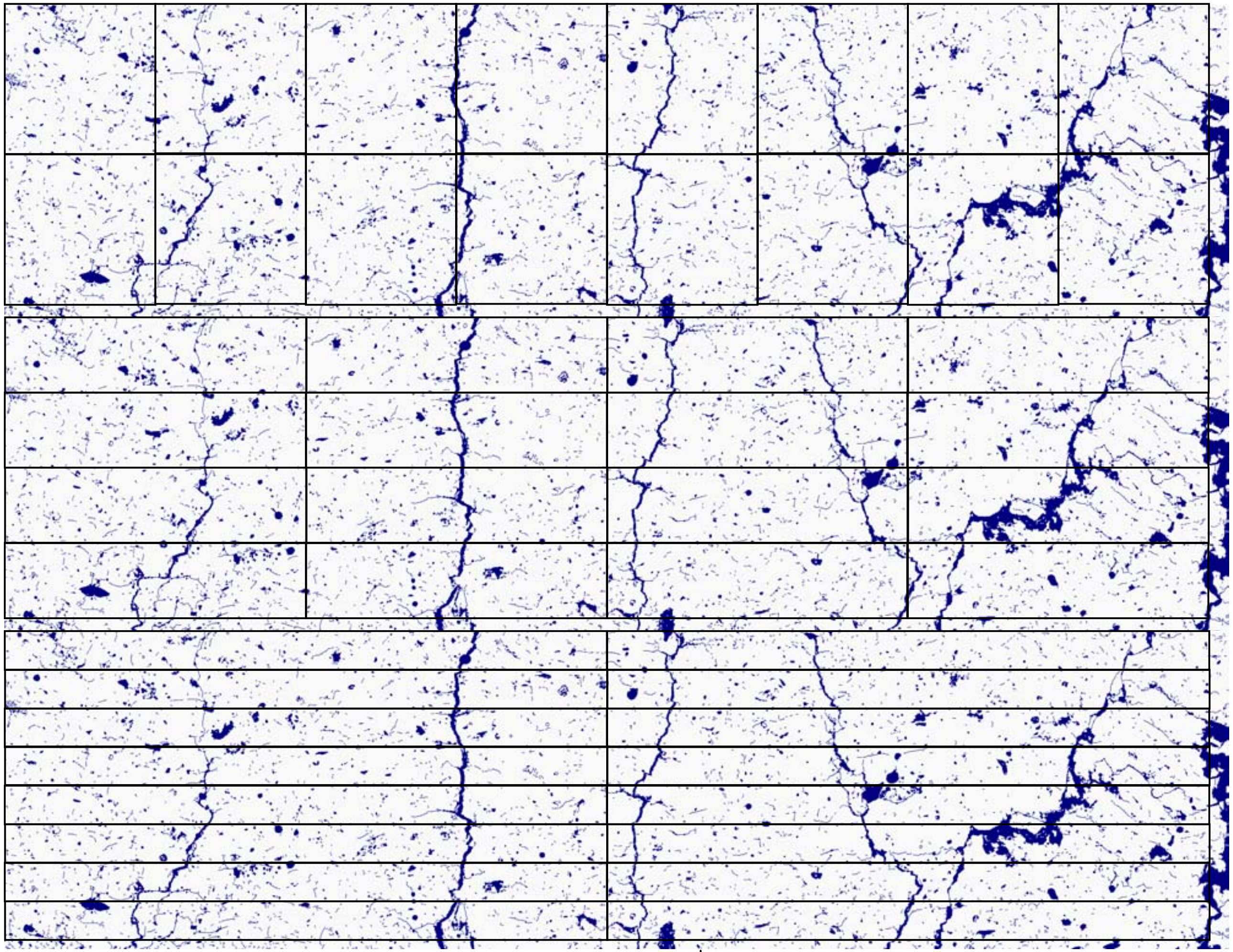
Variation from *CC* to *AA+10*

- Increased porosity
- Thicker crack widths
- Better connected cracks
- Nonetheless, still missed some low-contrast, thin cracks

Average of 20 regions produced nearly correct ordering of k_{OOF}



960 x 500
100 x 490
300 x 300
600 x 150
900 x 100



300 x 300

600 x 150

1200 x 75

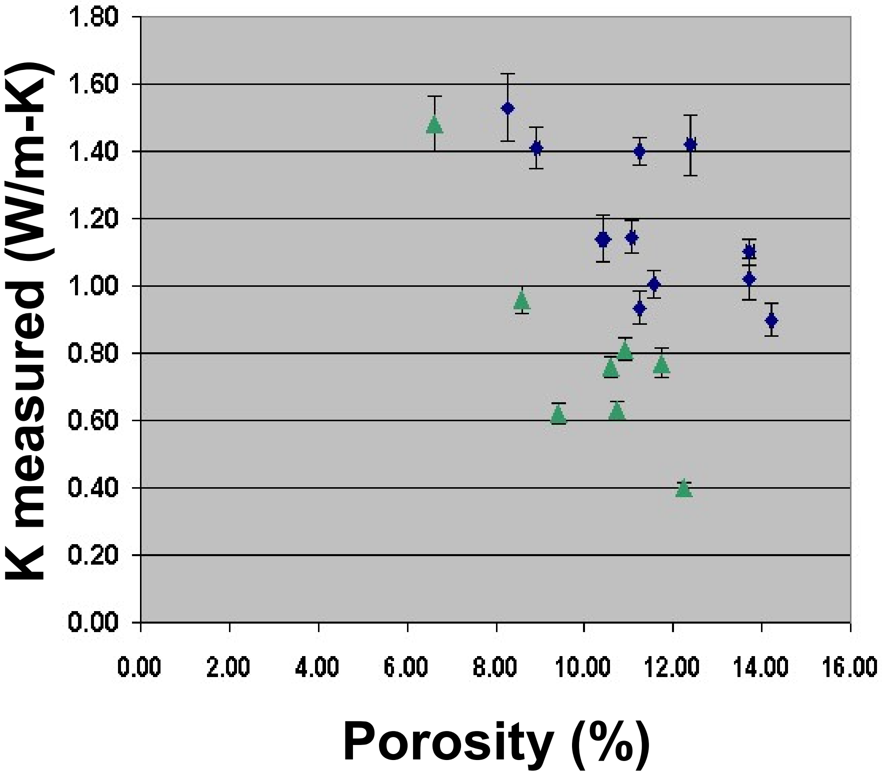
Size	890°C in N_2	890°C in vacuum
	k_{OOF}	k_{OOF}
300 x 300	1.33 ± 8.7%	1.22 ± 15.6%
600 x 150	1.35 ± 8.3%	1.27 ± 12.2%
1200 x 75	1.37 ± 4.6%	1.31 ± 6.1%

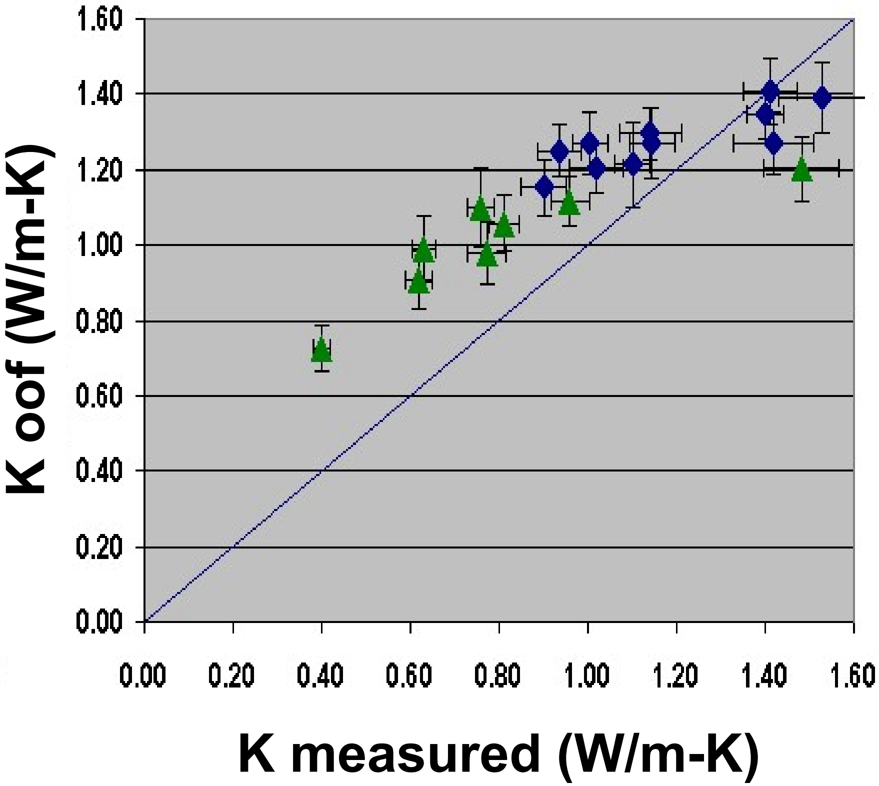
average of 16 adjacent sections in one image

Expt. Value in W/m-K at 890 °C In 1 atm N_2:

K_{expt} = 1.48 ± 5.7%

Comparison of Two Specimen Sets at 890 °C in N_2

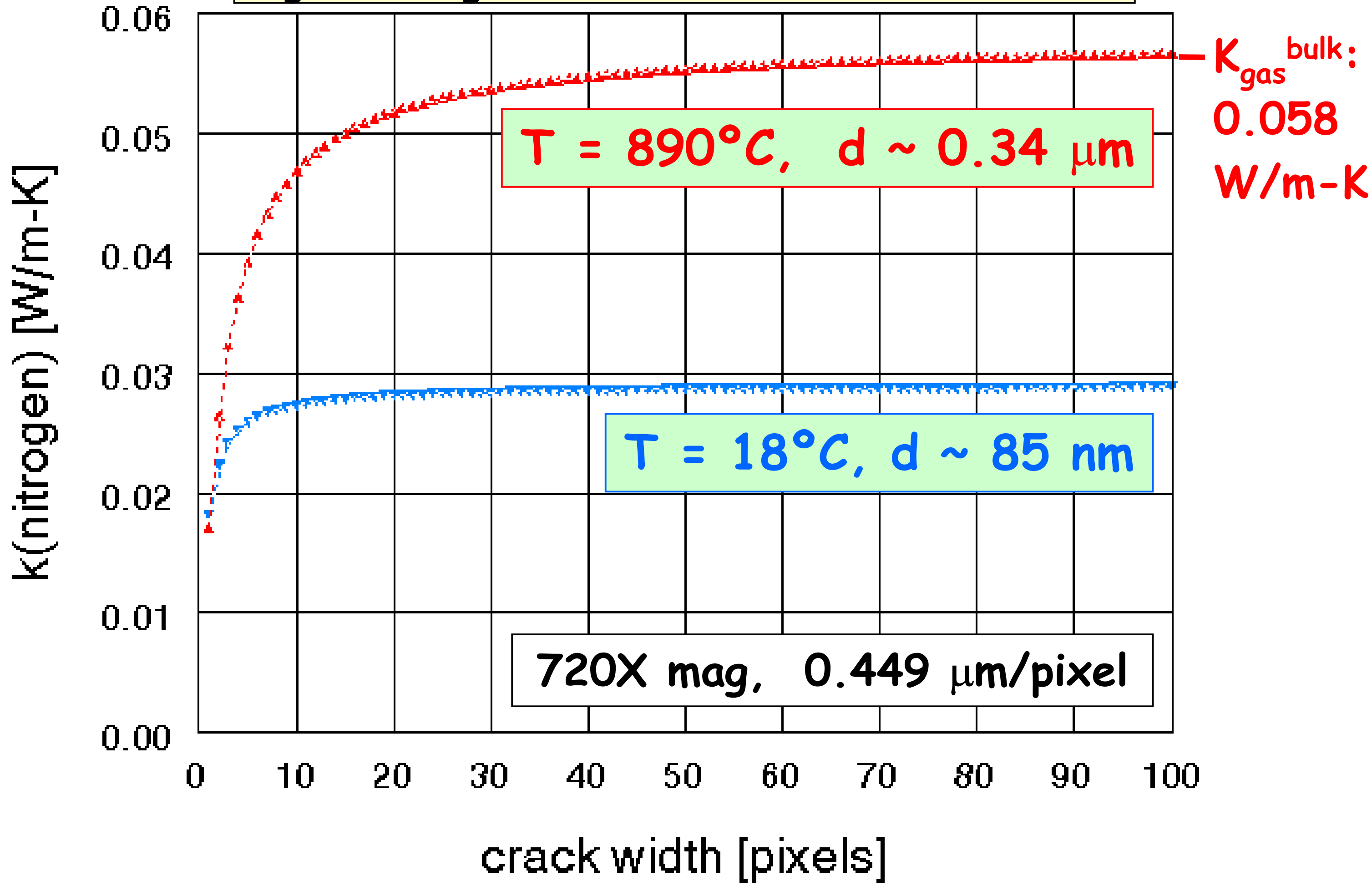




- *Consistent correlation for wide range of microstructures*
- *Data below ~1 W/m-K, slope of ≈1, but high absolute value*
- *Data above ~1 W/m-K, slope of <1; (vertically cracked)*

Influences of Feature Size

$$k_{gas} = k_{gas}^{bulk} / [1 + 3.17(d/x)]$$



A. Mogro-Campero, C. A. Johnson, P. J. Bednarczyk, R. B. Dinwiddie, H. Wang, Surf. & Coat. Tech., **94-95**, 102-105 (1997).

Thermal Property Prediction via Finite-Element Simulations

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.
- Dimensions of microstructural feature can have significant influences on determined properties.
- Finite-element simulations help to elucidate the influences of stochastic microstructural features (e.g., porosity) on the thermal conductivity of complex TBC microstructures.