Predicting Thermal Properties From Microstructures

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

<edwin.fuller@nist.gov>

2002 MRS Fall Meeting
Symposium HH: High-Temperature Thermal Spray Coatings-Thermal Barrier Coatings
December 03, 2002

NIST
National Institute of Standards and Technology

Collaborators & Acknowledgments

- Stephen A. Langer, Information Tech. Lab, NIST
- Andrew C. E. Reid & Andrew R. Roosen, MSEL, NIST
- Marion Bartsch and Uwe Schulz, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Germany
- Jean Marc Dorvaux, Rémy Mevrel, and Odile Lavigne, ONERA, France
- Yougen Yang, Derek Hass, & Haydn N. G. Wadley, Univ. of Virginia
- James Ruud, N. S. Hari, James Grande, and Antonio Mogro-Campero, GE Corporate R & D Center

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.

Motivation: to predict thermal conductivity, k, of TBC's from microstructure

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
- Design of lower k TBC materials on computer
- Spray vendors qualify TBC's for thermal conductivity

Predicting Thermal Properties From Microstructures

TECHNICAL APPROACH: Develop computational tools for simulating properties and elucidating influences of stochastic, anisotropic microstructural features (e.g., porosity) on physical properties

CONTENTS:

- Microstructural simulation approach *(OOF)*
- Thermal Conductivity simulations
  - EB-PVD TBCs
  - EB-DVD TBCs
  - Thermal Spray TBCs

Building a Microstructural Model

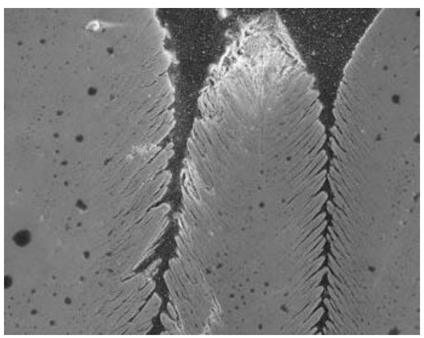
Experiments | Simulations

Microstructure Data (micrographs)

Fundamental Materials Data

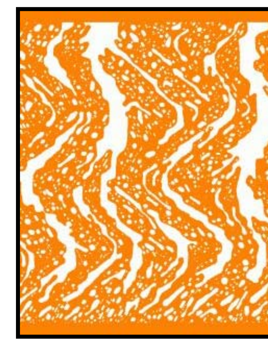
Materials Physics

easy-to-use Graphical User Interface (GUI) - ppm2oof



Object Structure Isomorphic to the Material

Finite Element Solver



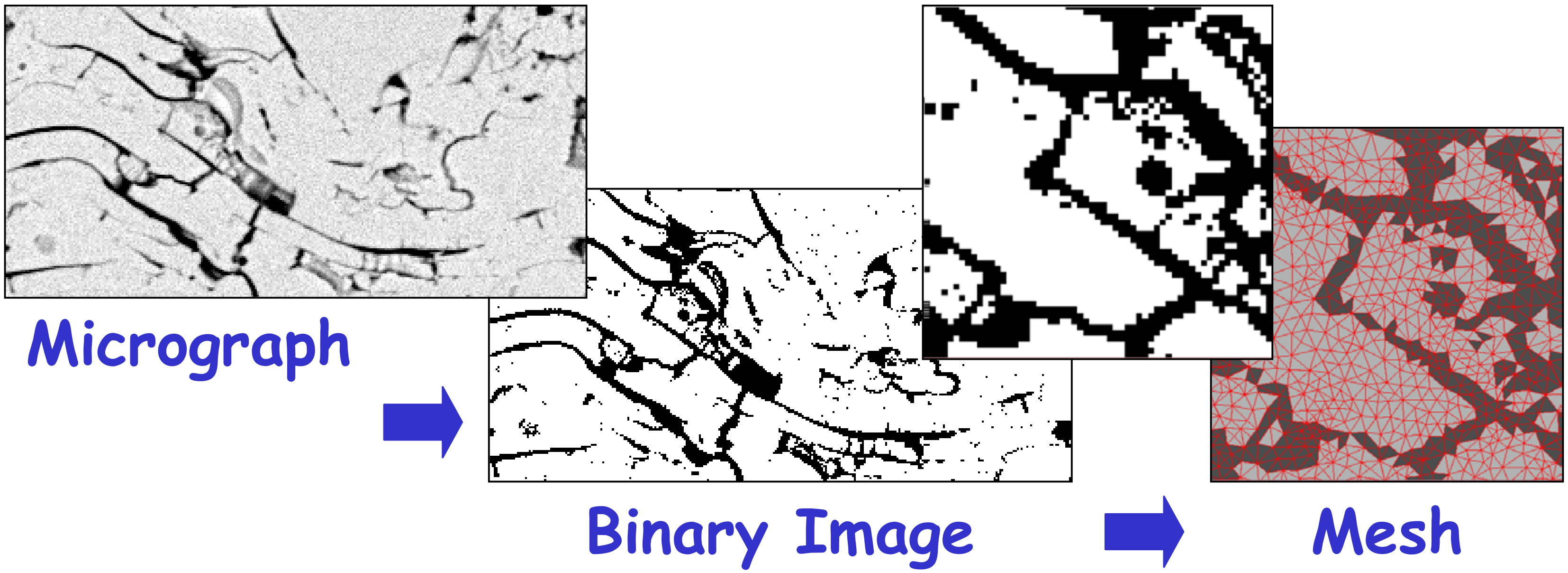
easy-to-use Graphical User Interface (GUI) - oof

Virtual Parametric Experiments

Visualization of Microstructural Physics

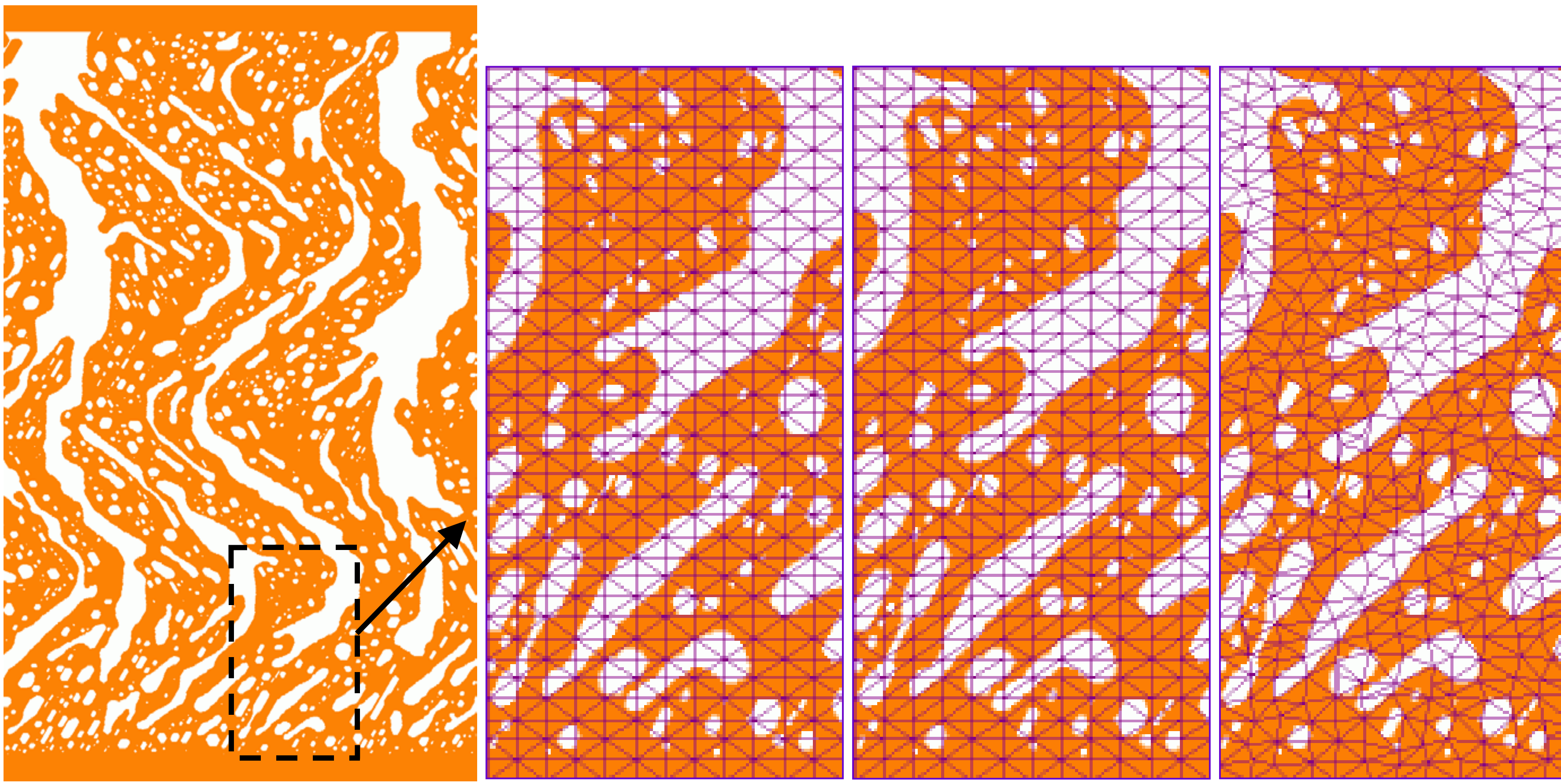
Effective Macroscopic Physical Properties

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

Adaptive Meshing by Components: refine elements and move nodes via Monte Carlo *annealing* to reduce $\mathrm{E} = (1\text{-}\alpha)\mathrm{E}_{shape} + \alpha\, \mathrm{E}_{homogeneity}$



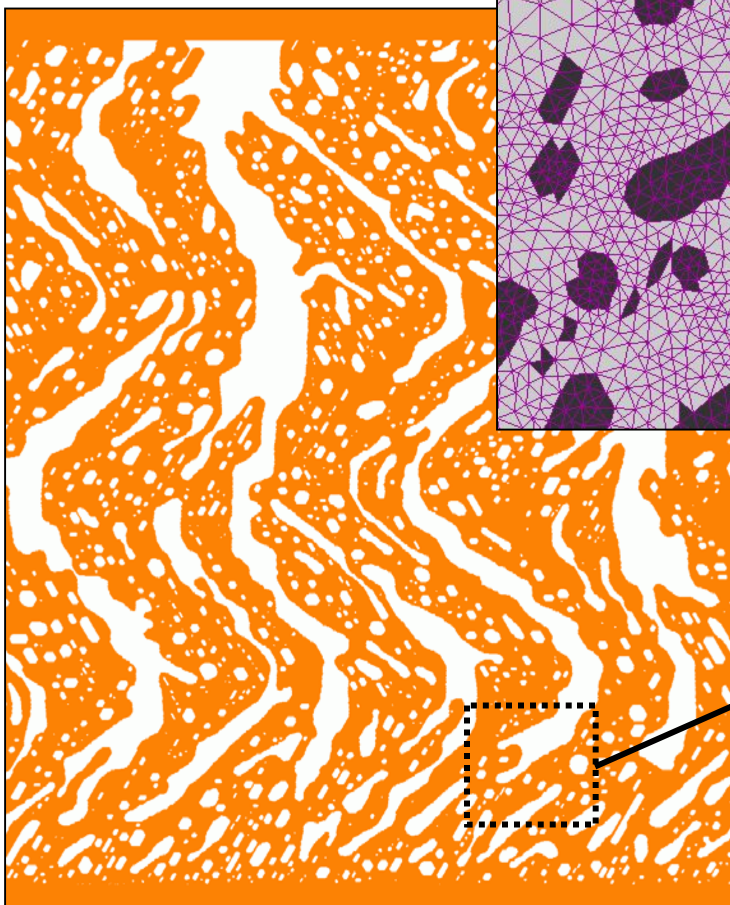
image

create mesh

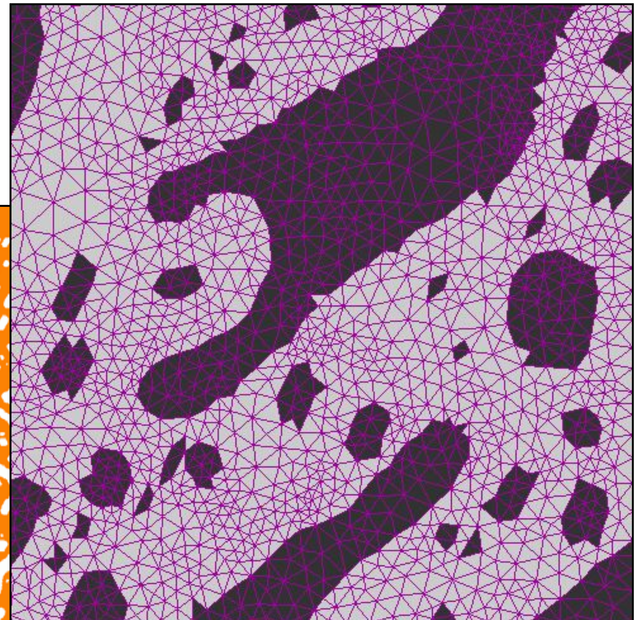
swap worst to reduce E

anneal to reduce E

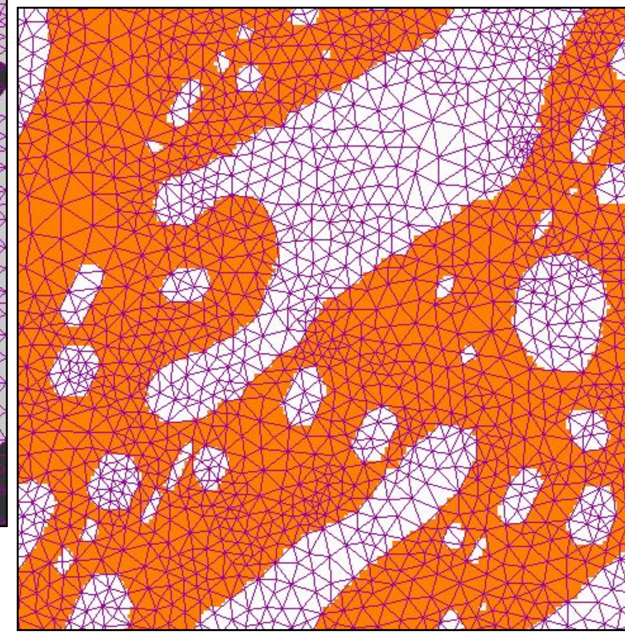
Adaptive Meshing by Components



pixel image



mesh



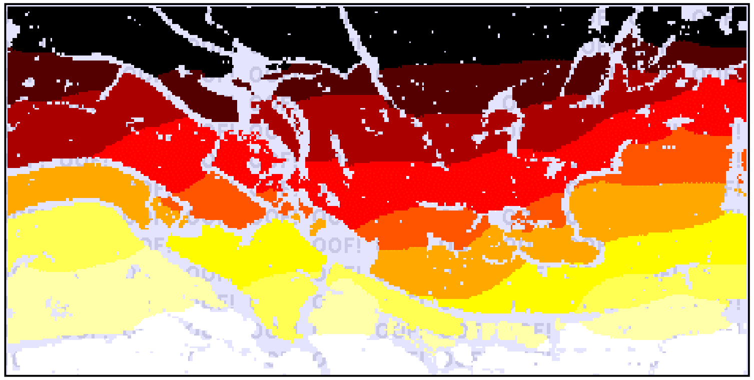
pixel image with mesh

Generate a finite-element mesh following the material boundaries

OOF Tool

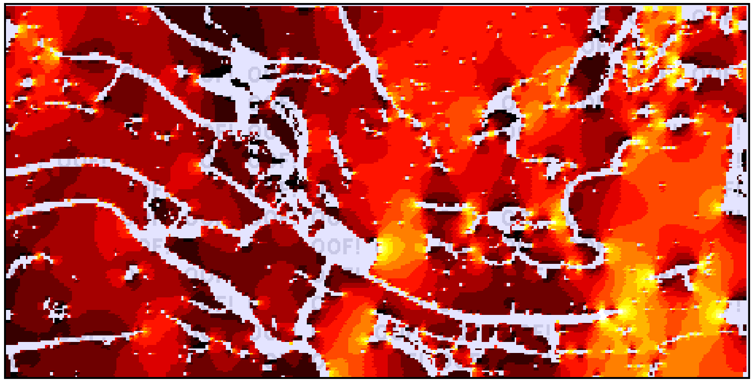
Virtual Experiments: Temperature Gradient

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

2.0 Current Development Effort

Stephen A. Langer & Andrew C. E. Reid

- Extensible and more flexible platform
- Enhanced image analysis tools
- Expanded element types
- Generalized constitutive relations (elasticity, piezoelectricity, etc.) w/coupling between fields

Equil. Eq.: $\nabla \bullet \Psi = f$	Constitutive Eq.: $\Psi = c \bullet \nabla \phi$

- Linear and nonlinear solvers
  with automatic mesh refinement

Planned Additions

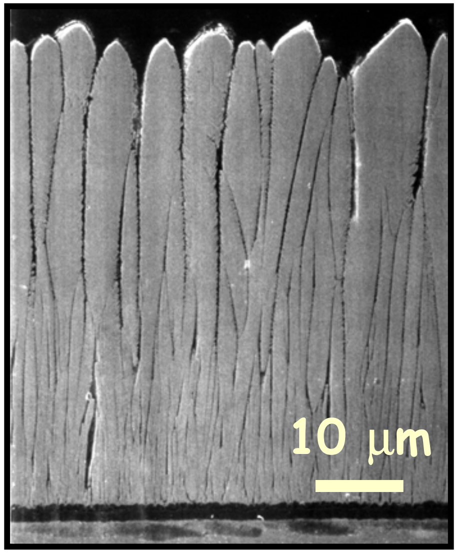
- 3-dimensional finite element solver
- Time-dependent solver
- Plasticity

Predicting Thermal Properties From Microstructures

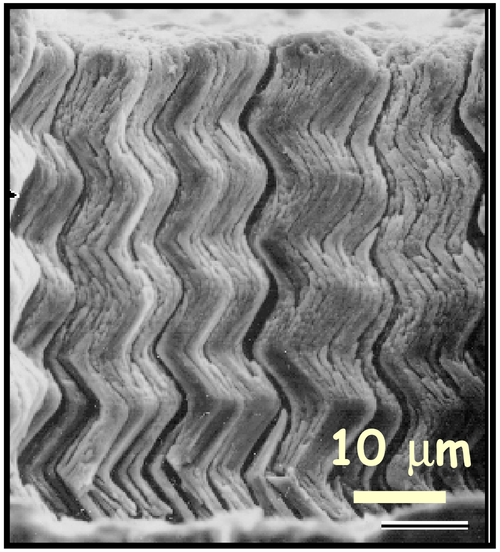
CONTENTS:

- Microstructural simulation approach *(OOF)*
- Thermal Conductivity simulations
  - EB-PVD TBCs
  - EB-DVD TBCs
  - Thermal Spray TBCs

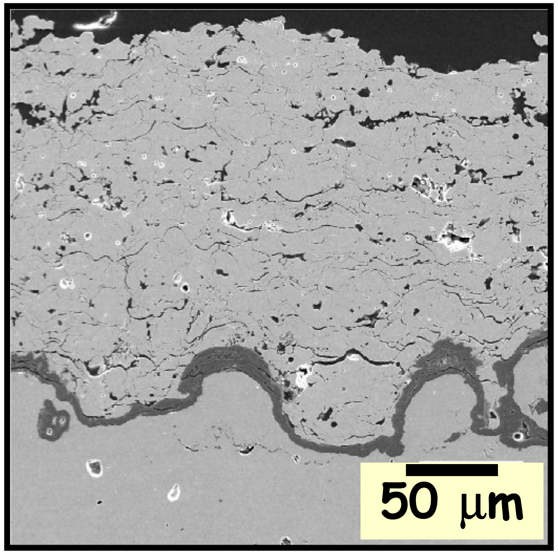
Types of Thermal Barrier Coatings and Deposition Processes



EB-PVD TBC's



EB-DVD TBC's

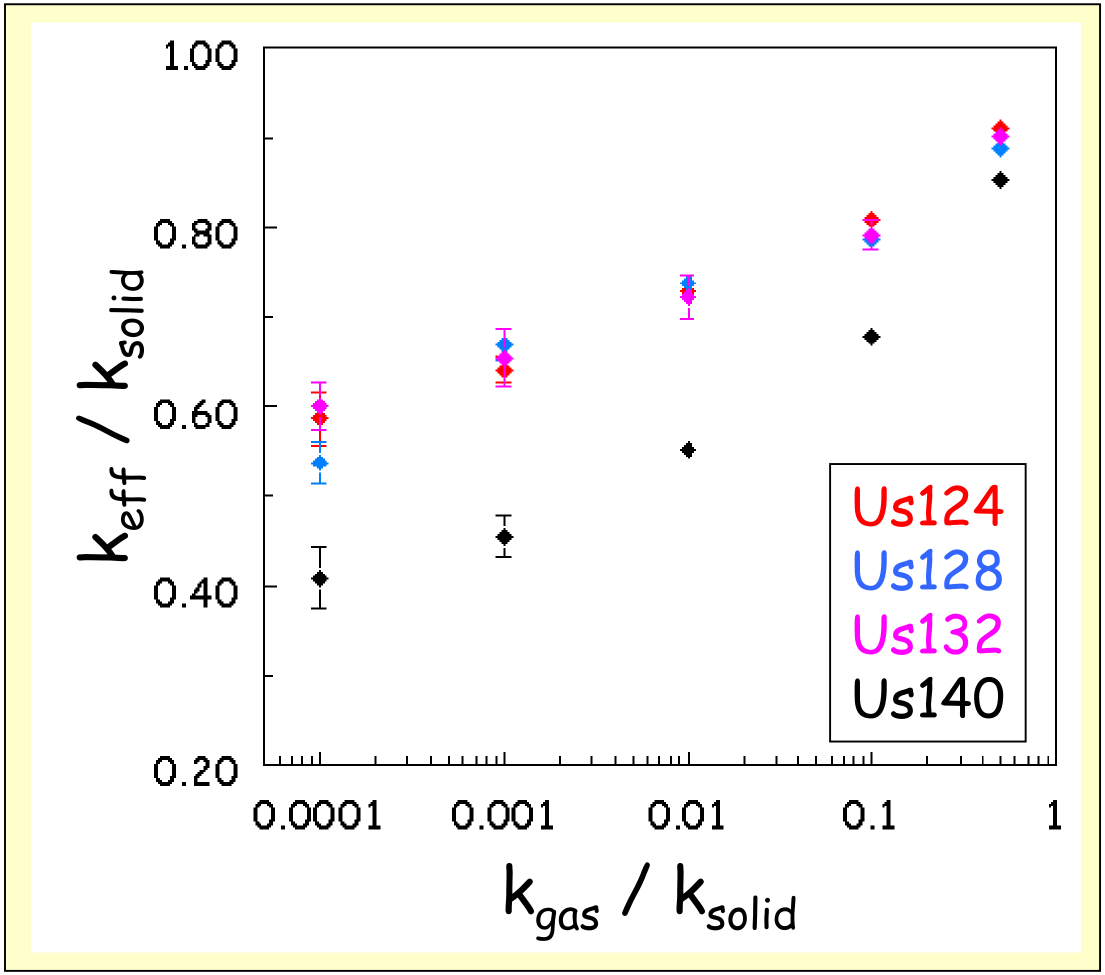


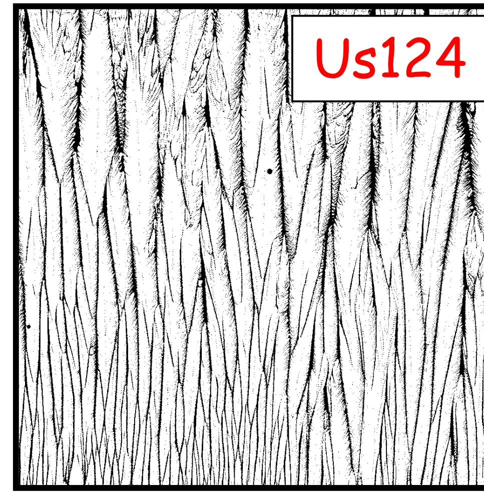
APS TBC's

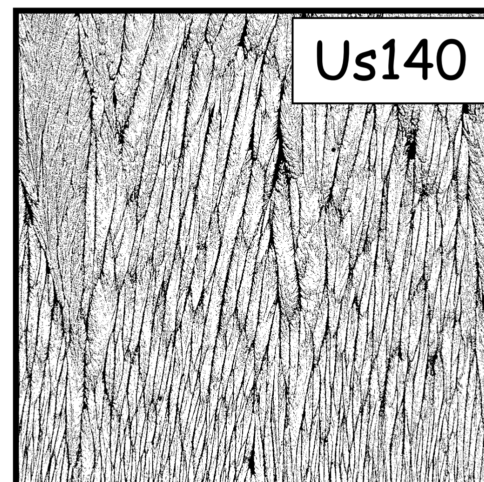
Selected Deposition Processes
for the yttria stabilized zirconia (YSZ) ceramic top coat

- electron-beam physical vapor deposition (EB-PVD)
- electron-beam directed vapor deposition (EB-DVD)
- thermal spray (TS) or air plasma spray (APS)

Thermal Conductivity of EB-PVD TBC's

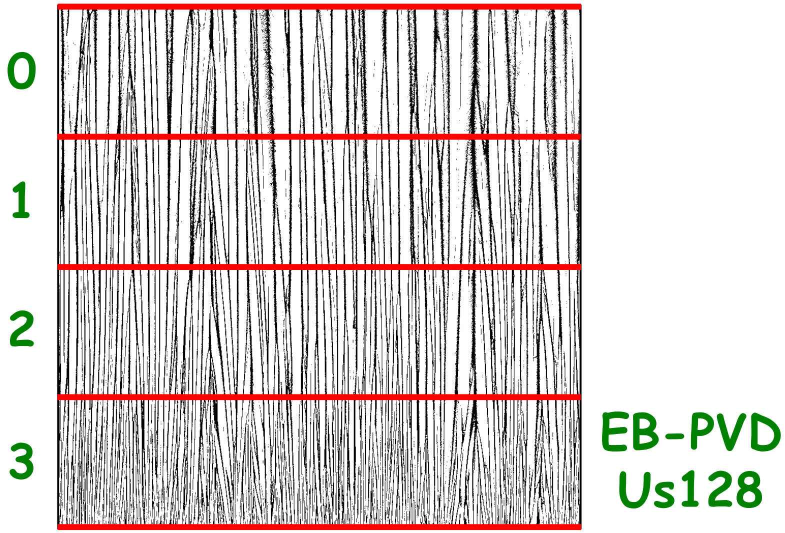


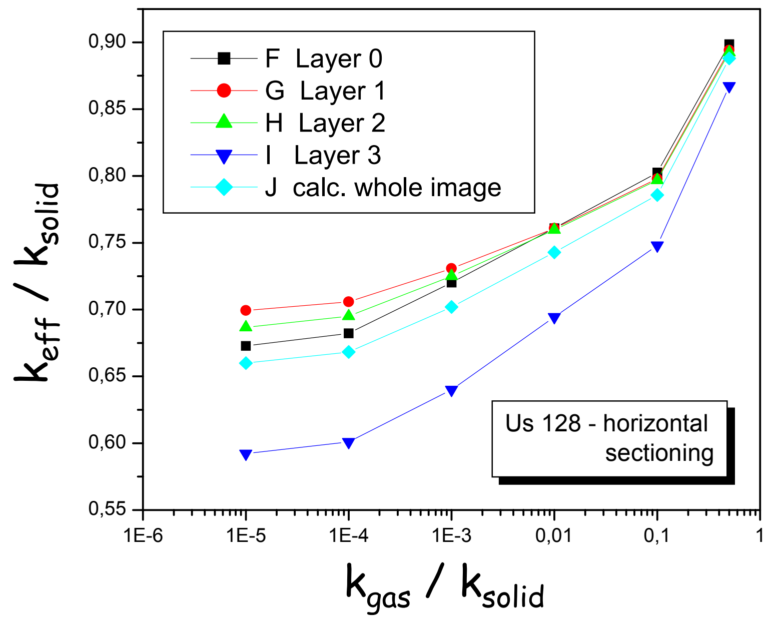


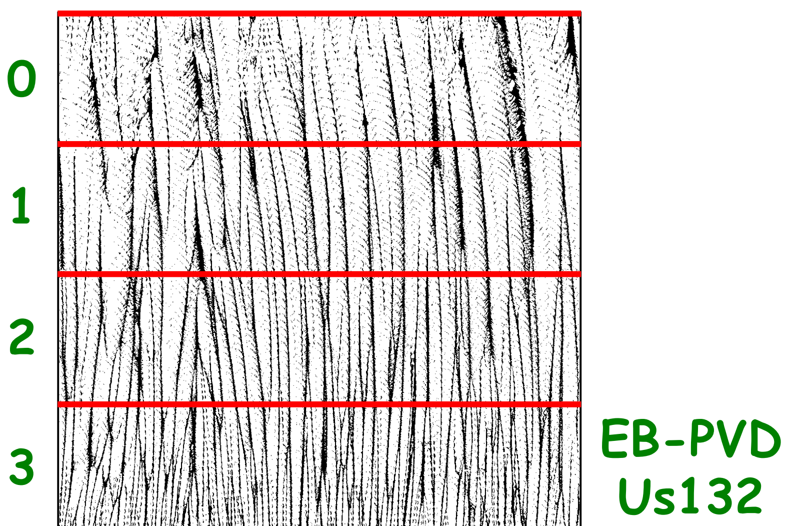


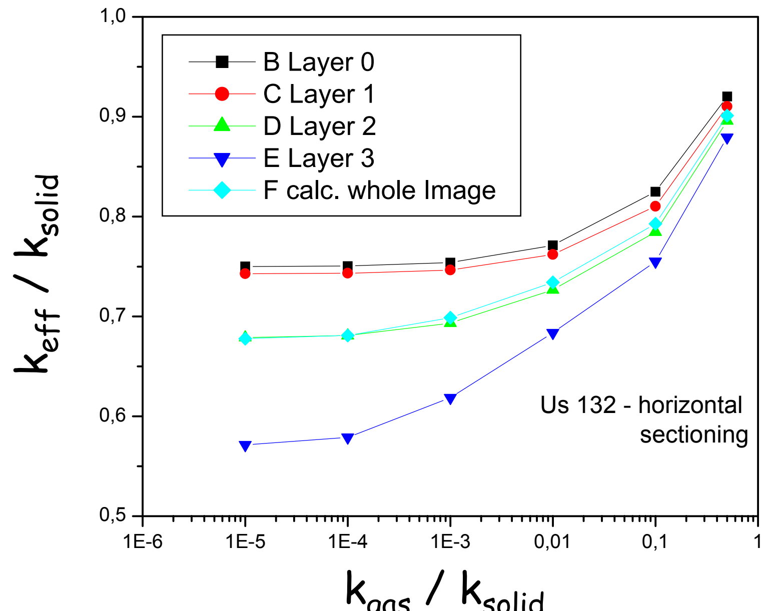
Marion Bartsch & Uwe Schulz, DLR, Germany;
Jean Marc Dorvaux, Rémy Mevrel, & Odile Lavigne, ONERA, France

Variation with Deposition *Layer*

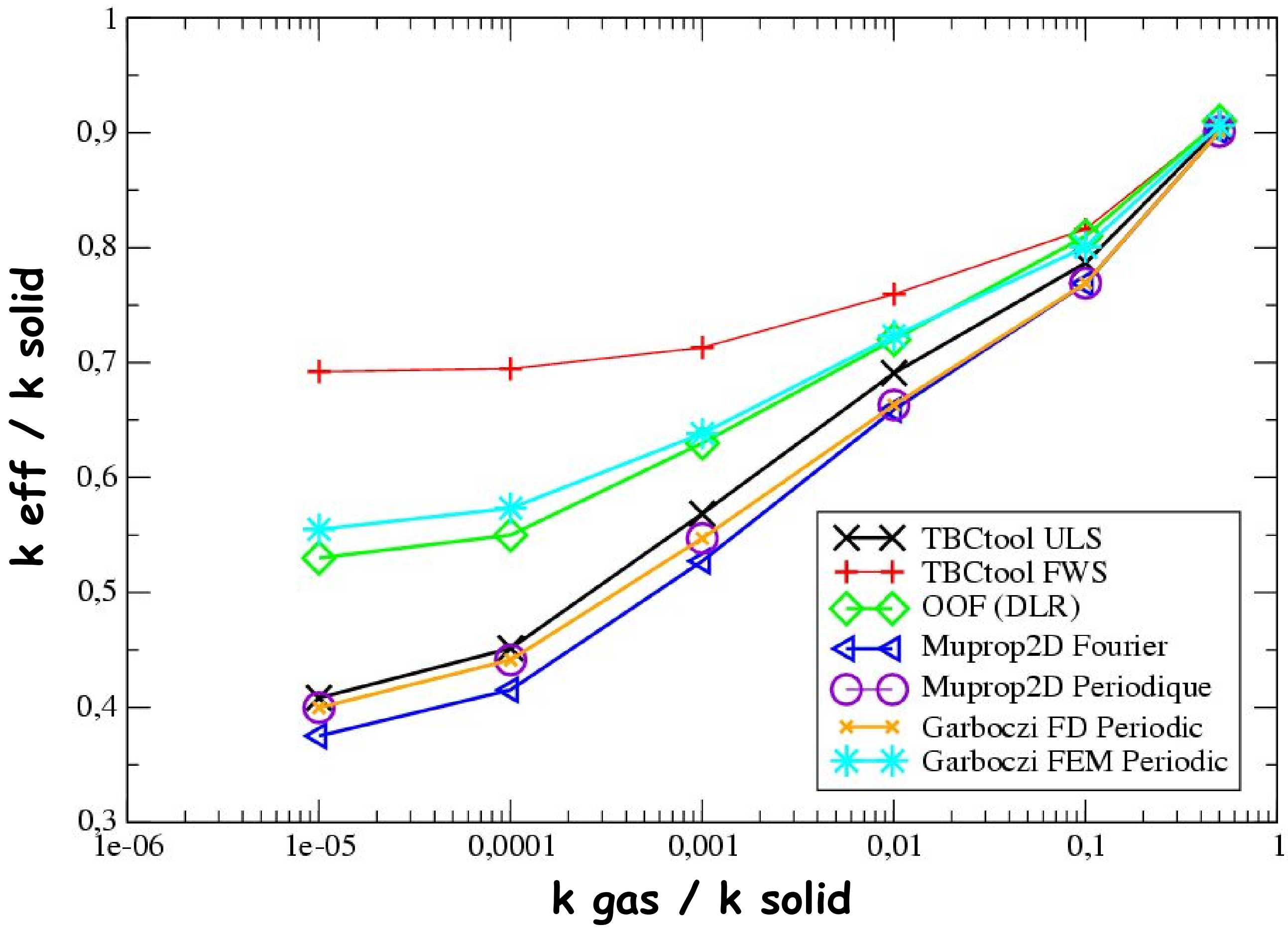


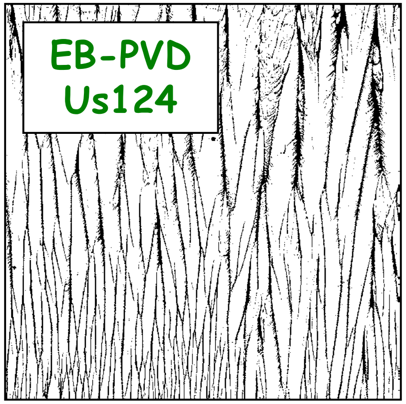


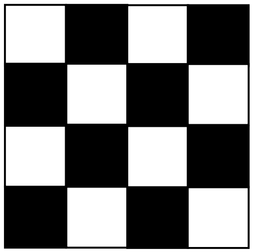




Comparison of Computational Tools and Simulation Boundary Conditions



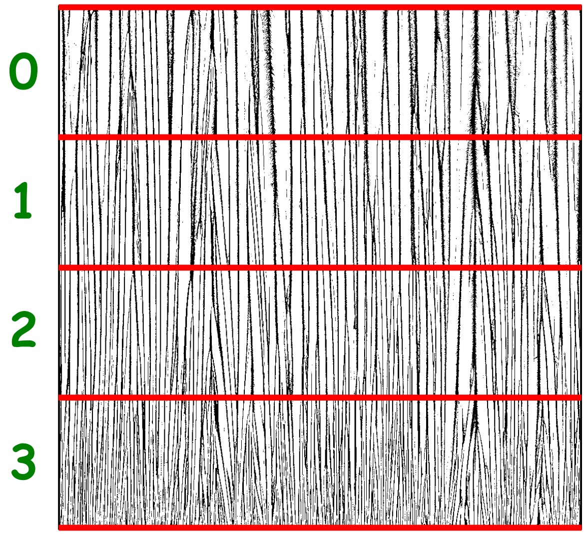




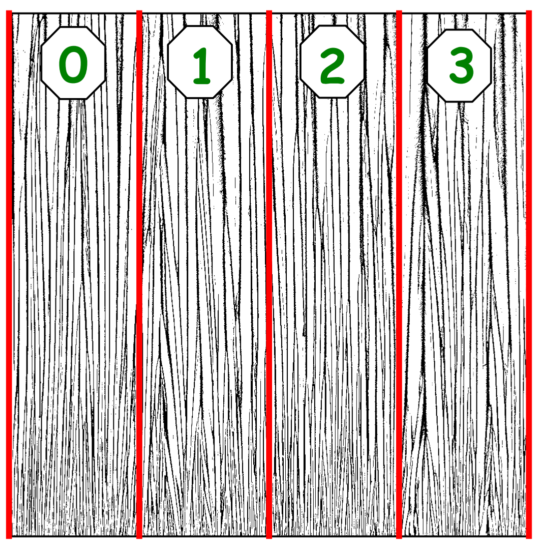
Jean Marc Dorvaux & Rémy Mevrel, ONERA, France

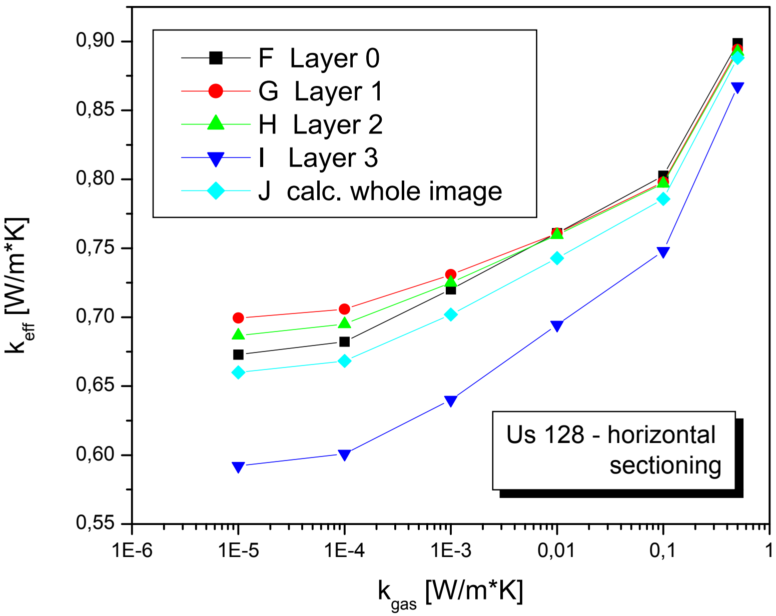
Marion Bartsch & Uwe Schulz, DLR, Germany

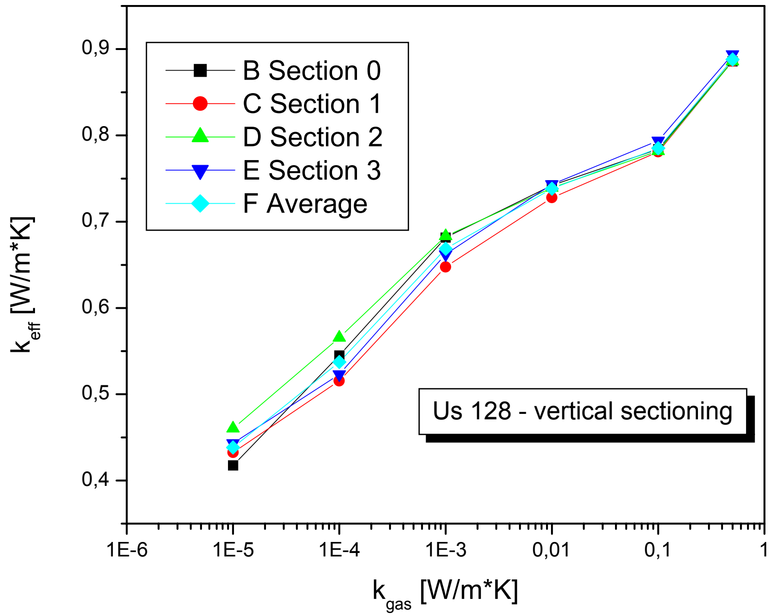
Percolation Influence on Properties



EB-PVD - Us128







Optimization of Low Conductivity EB-DVD Microstructures

Electron-Beam Directed Vapor Deposition coating microstructure via kinetic Monte Carlo simulation

- Deposition at

  $T/T_m = 0.23$

- Annealed at

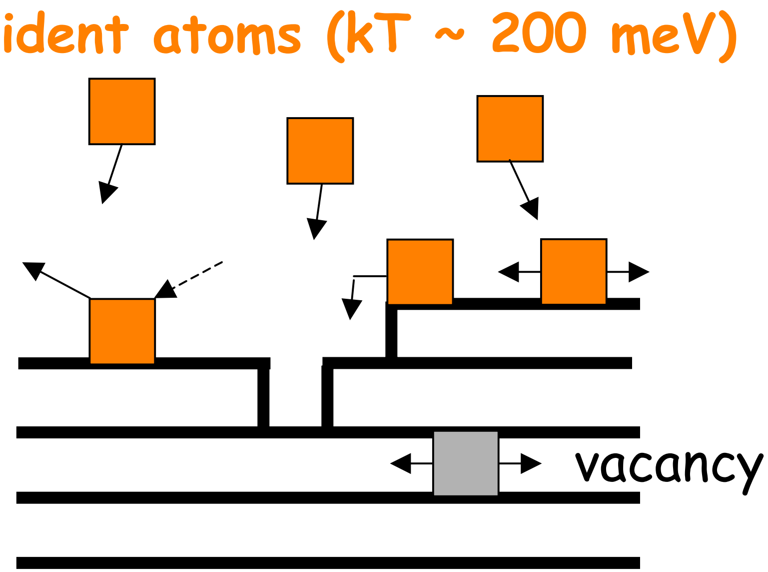
  $T/T_m = 0.43$

substrate was periodically inclined to the vapor flux

Yougen Yang, Derek D. Hass, & Haydn N. G. Wadley, Univ. of Virginia

Kinetic Monte Carlo Simulation of Atomic Condensation

Physical Vapor Deposition

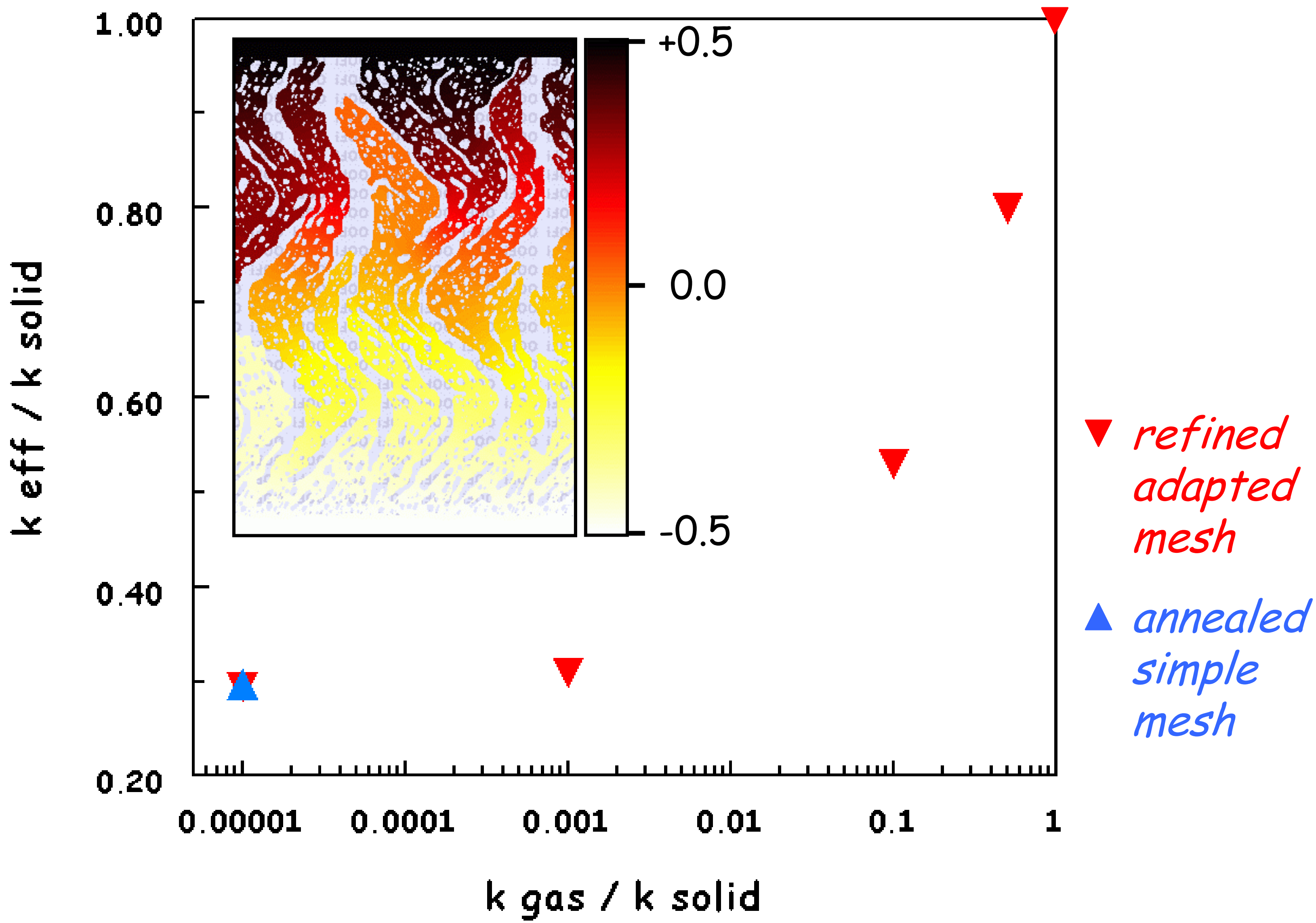


Assembly Process:

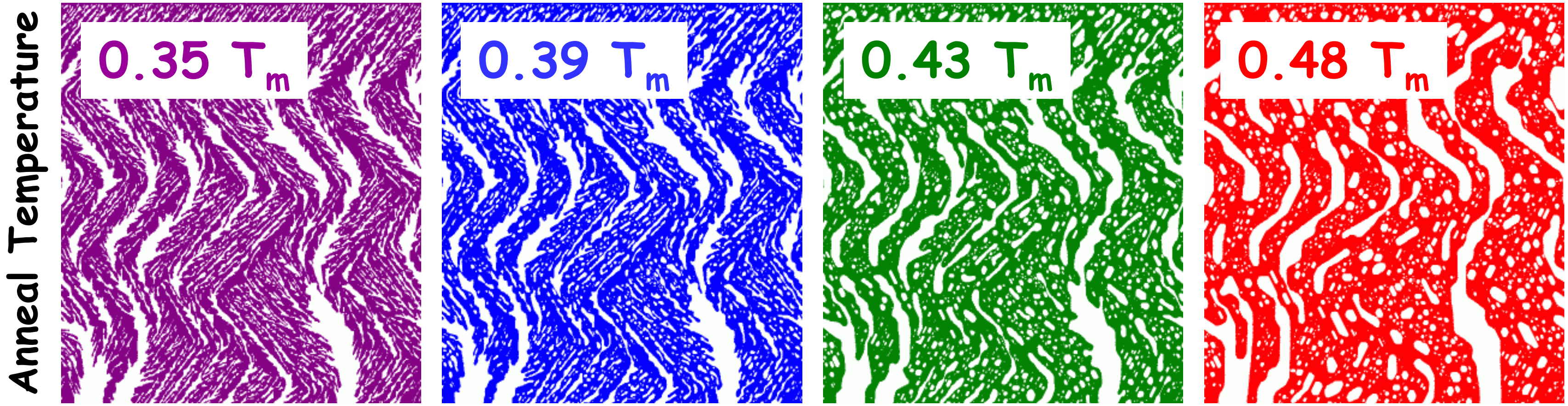
- Condensation
- Thermal diffusion (surface, bulk)
- Incident atom-growing surface interactions, including reflection, resputtering, etc.

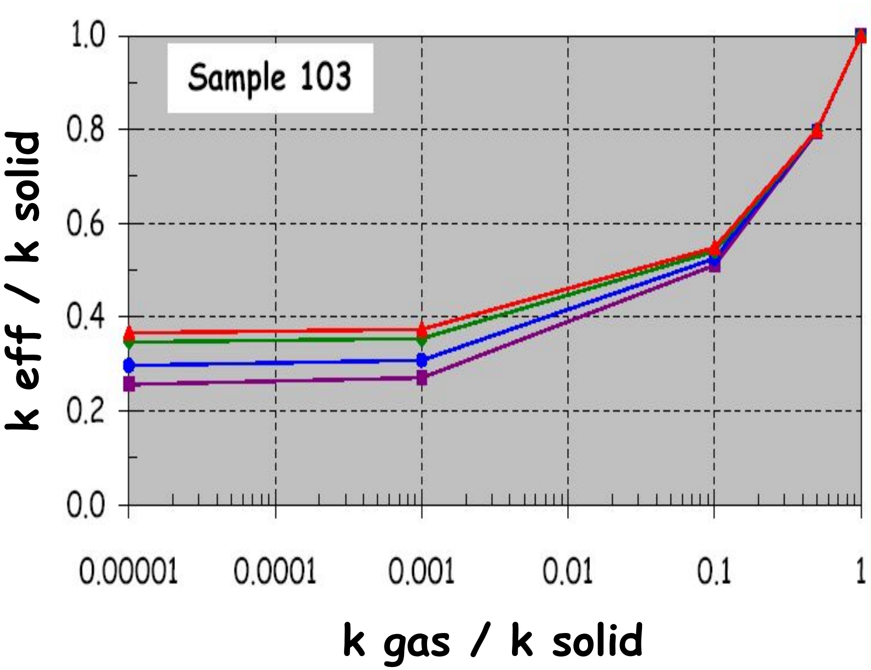
kinetic Monte Carlo (kMC) for diffusion
Molecular Dynamics (MD) for effects of energy

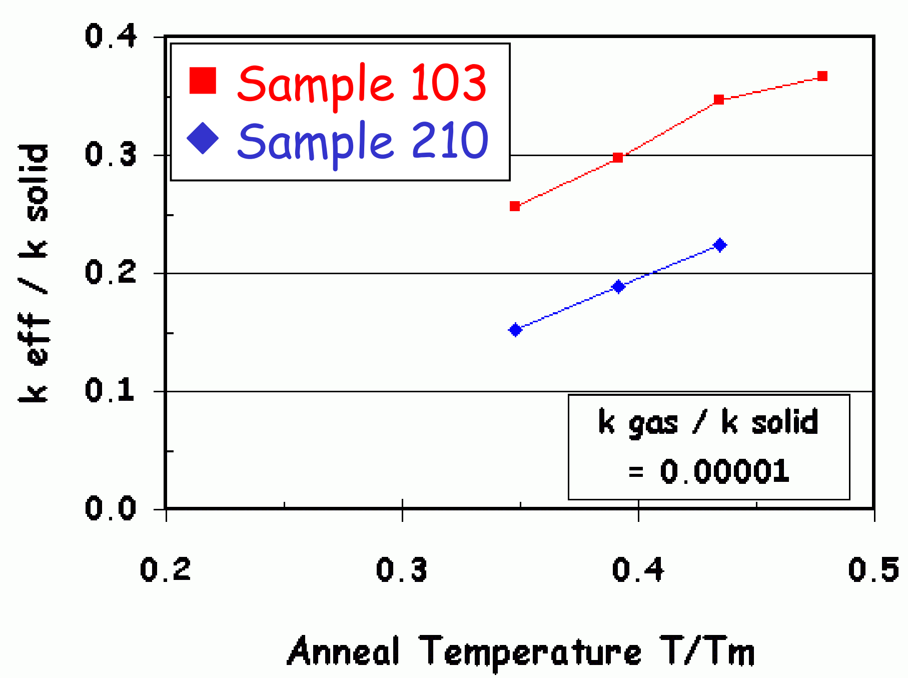
Effective Thermal Conductivity



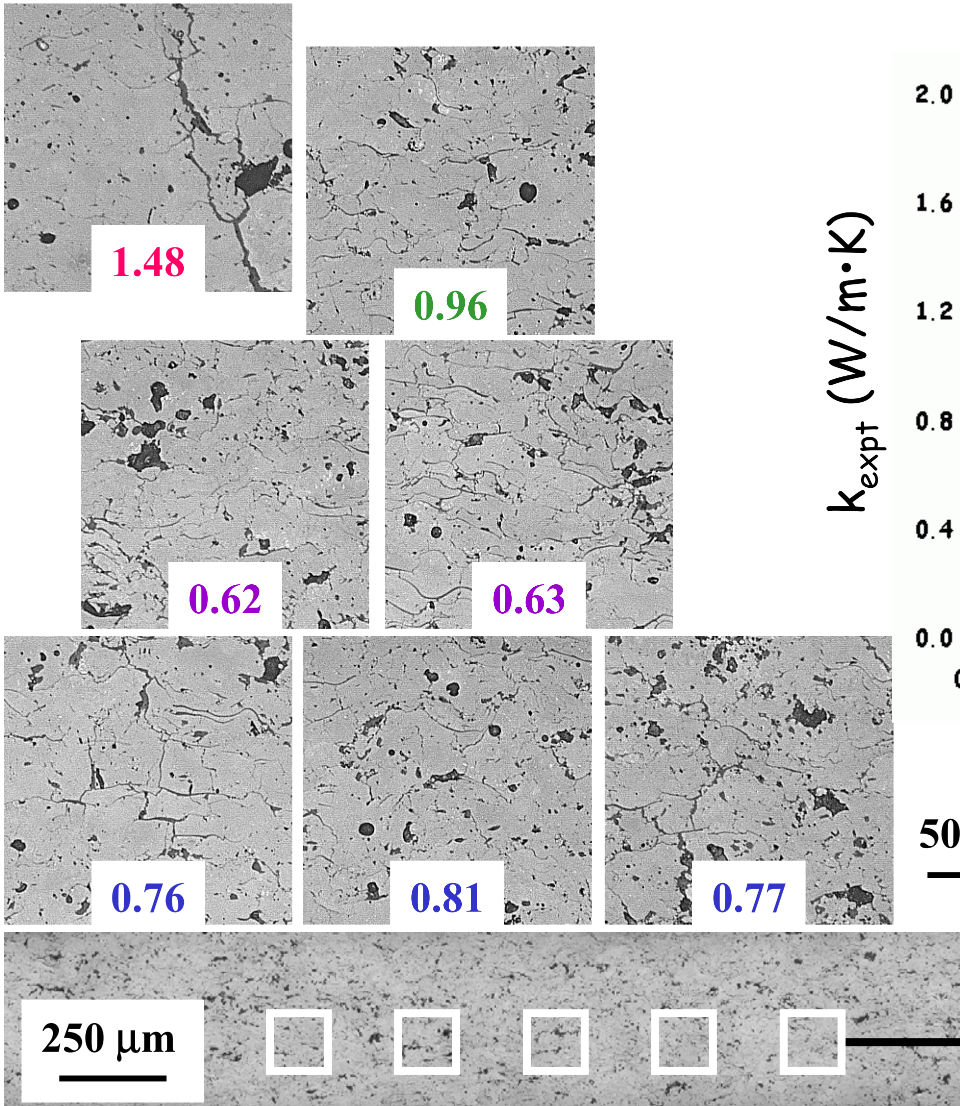
Thermal Conductivity Simulations

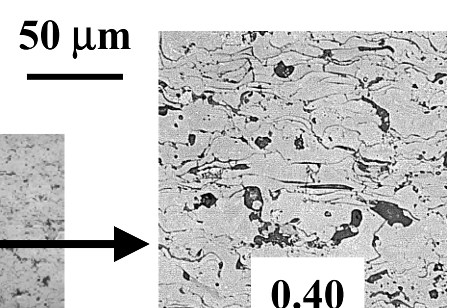


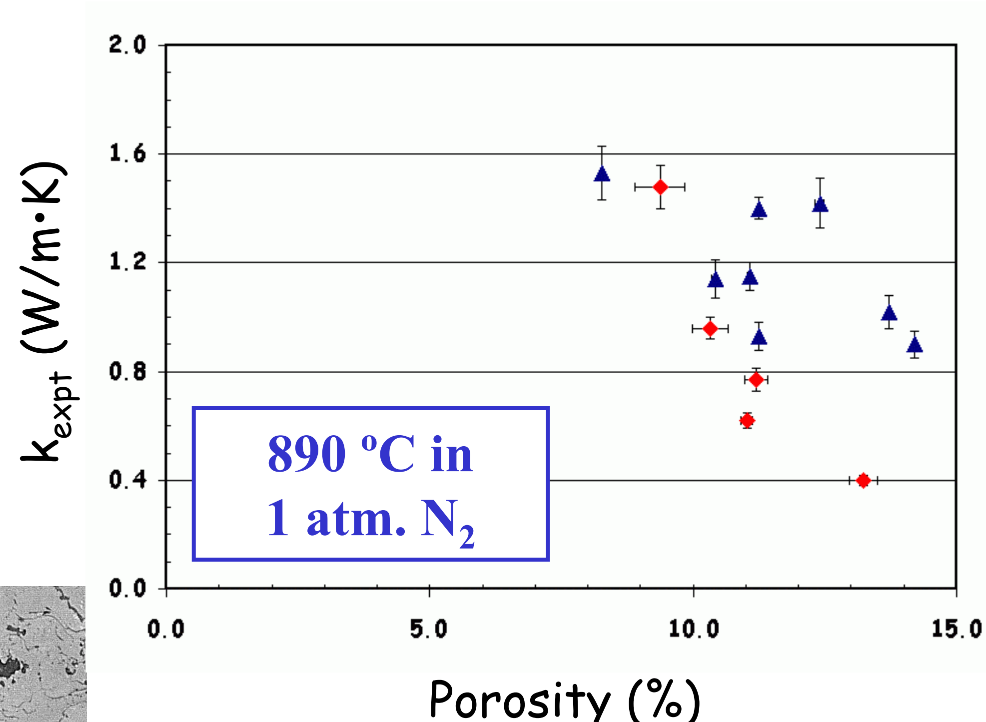


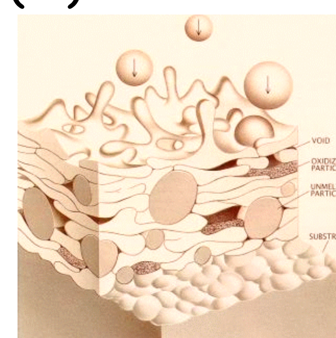


TBC Thermal Conductivity Measurements



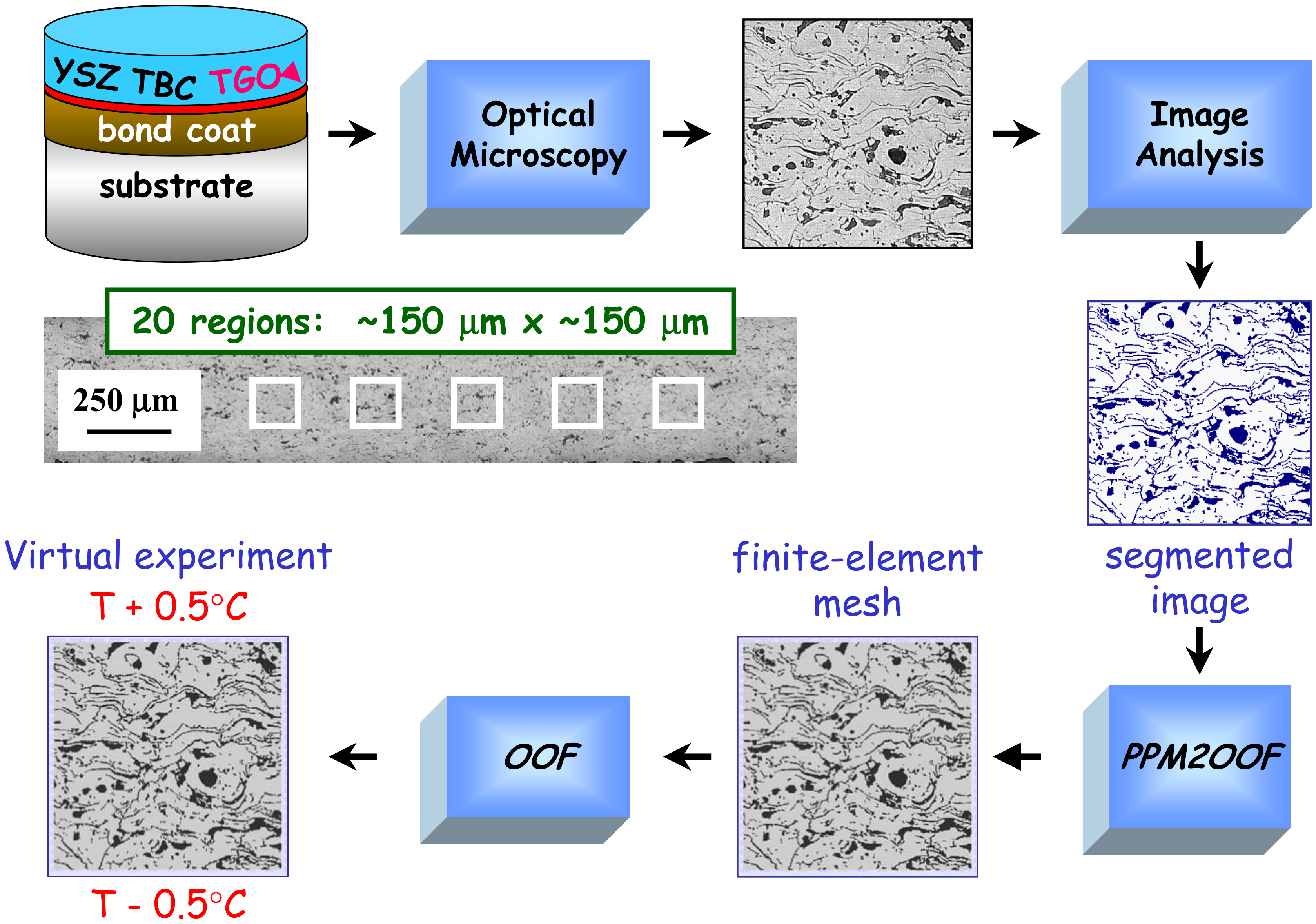




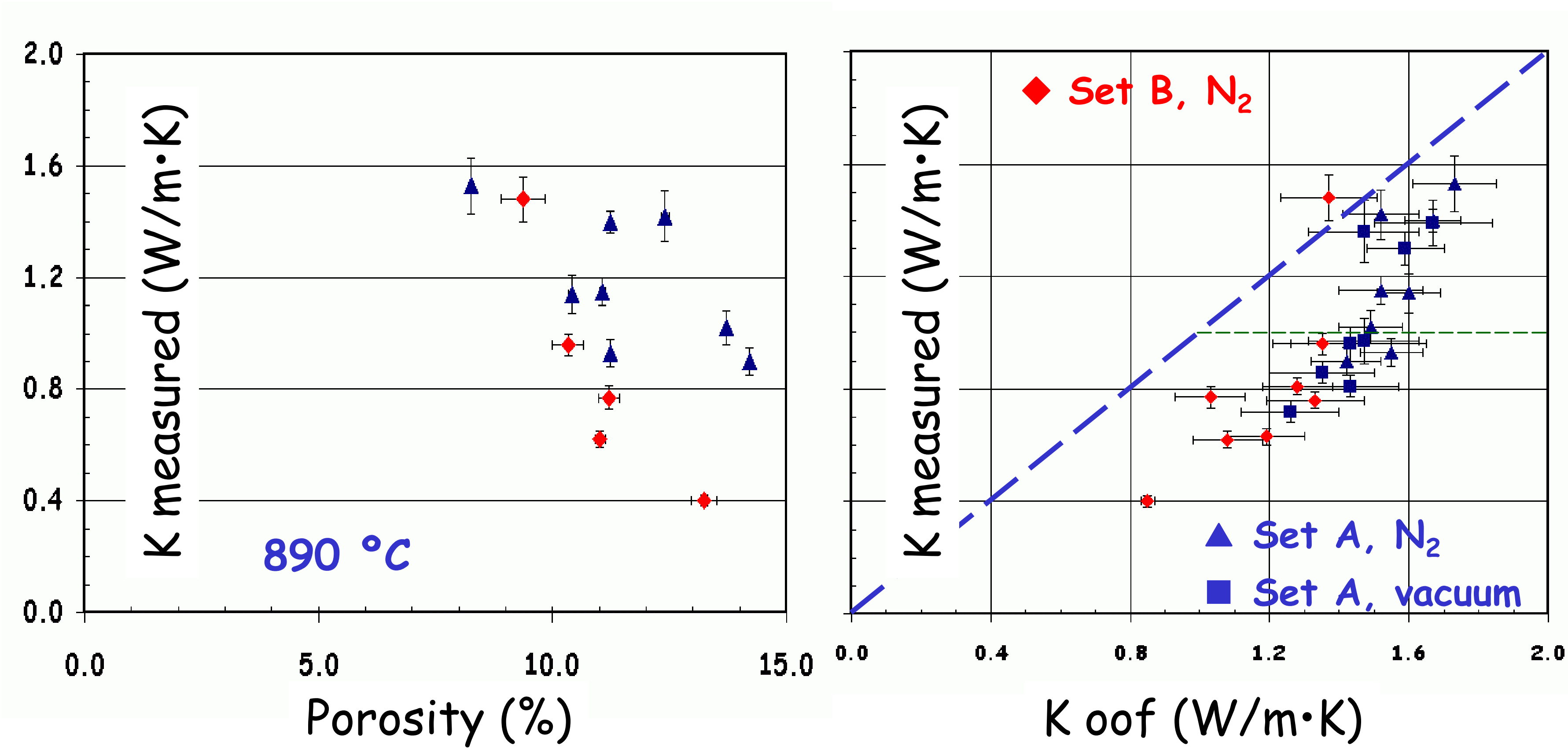


James Ruud, N. S. Hari, James Grande, & A. Mogro-Campero, GE Corp. R&D

Thermal Conductivity via OOF Simulations



Results for Two Sets of TBC Microstructures



- *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 Image Resolution

Calculated K_{bulk}:

Heat Flux Distribution

1.076 W/m·K

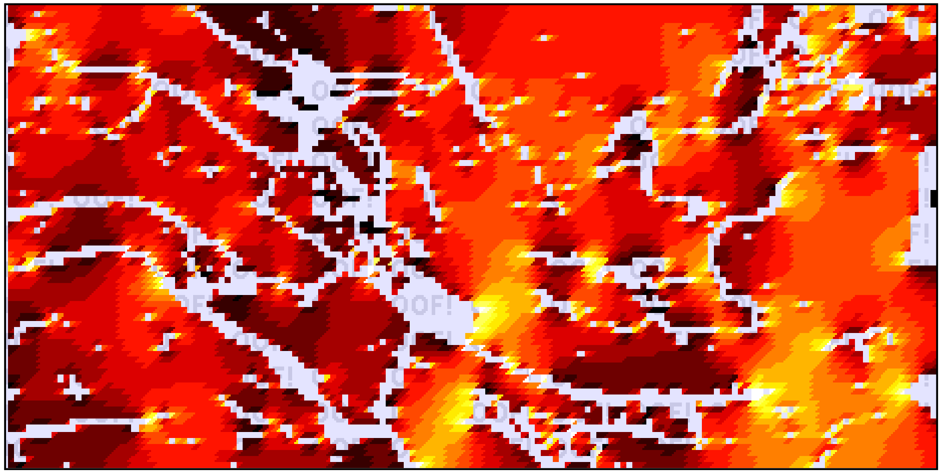
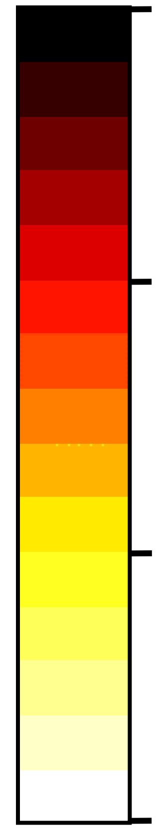


Image Resolution: 0.428 μm/pixel



0.940 W/m·K

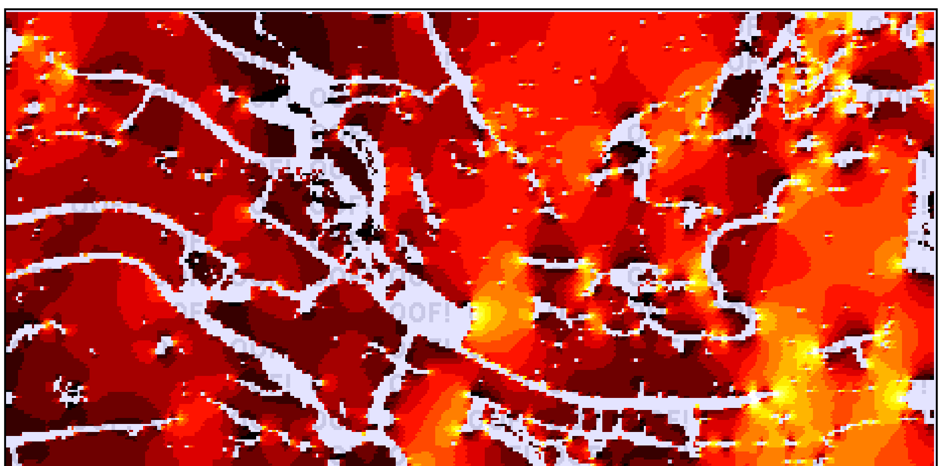
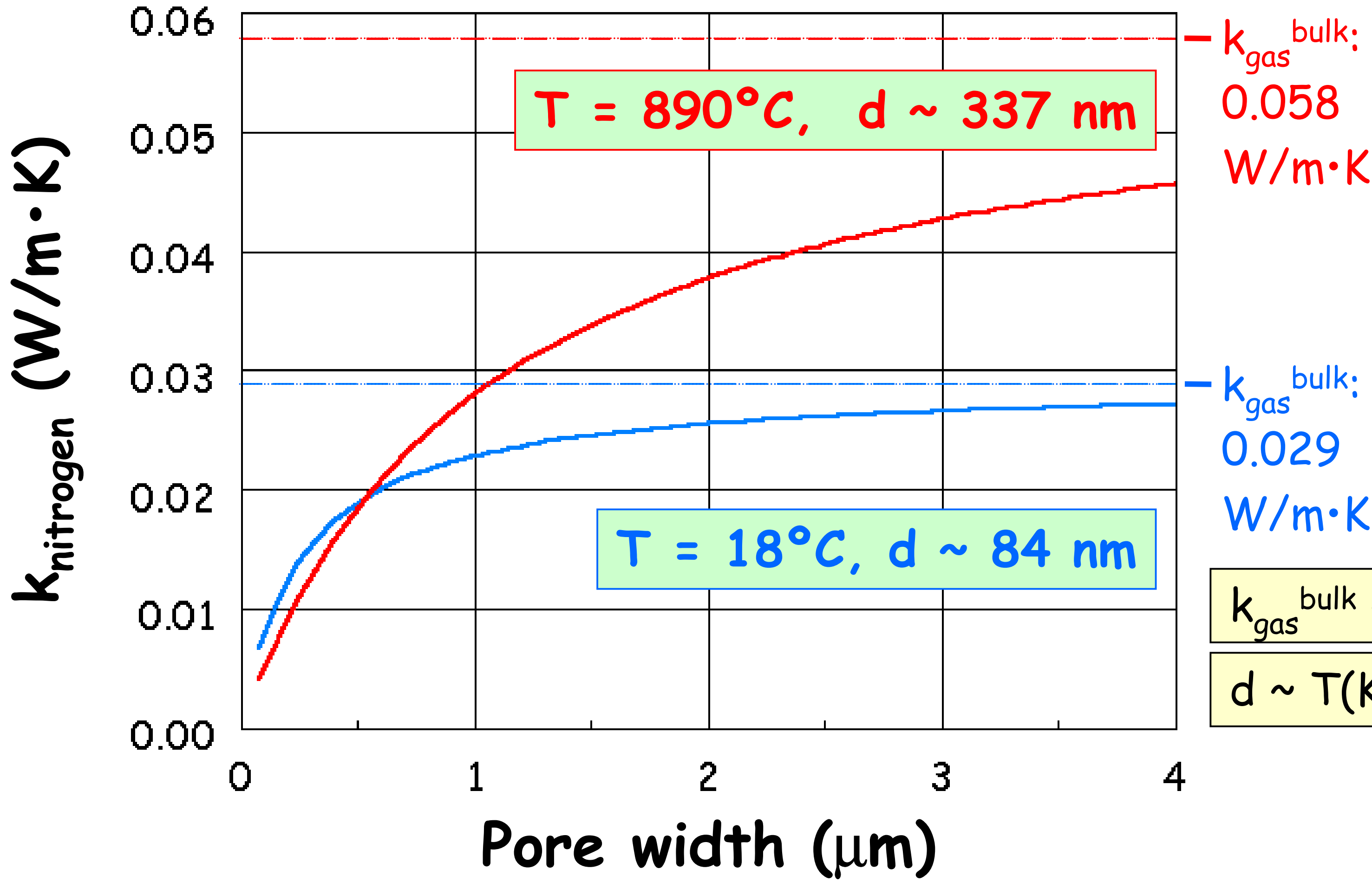


Image Resolution: 0.214 μm/pixel

64.2 μm × 32.1 μm

Influences of Feature Size

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



$k_{gas}^{bulk} \sim \sqrt{T(K)}$

$d \sim T(K)$

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

Predicting Thermal Properties From Microstructures

SUMMARY:

- Microstructure-based, finite-element simulations provide a new paradigm for property measure- ments 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.

Abstract

PREDICTING THERMAL PROPERTIES FROM MICROSTRUCTURES

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.

Point-to-point knowledge of the thermal properties of thermal barrier coatings (TBC's) is crucial in the design of advanced turbine airfoils to allow more precise component temperature evaluation and more reliable life assessment. However, laser flash measurements for determining thermal diffusivity are generally time consuming and expensive, and require special expertise. An alternate stratagem is to develop finite-element schemes for calculating thermal properties directly from coating microstructures. Such a computational tool, called OOF for Object Oriented Finite element analysis, is used to determine thermal conductivity of TBC's. Simulations are performed for thermal-spray (TS), electron-beam physical vapor deposition (EB-PVD), and electron-beam directed vapor deposition (EB-DVD) microstructures. Laser flash measurements of thermal diffusivity are used to validate the microstructural simulations for a range of thermal-spray microstructures. This validation procedure has indicated many aspects of the image analysis and thermal conductivity physics that must be considered for elucidating the influence of fine microstructural features, such as microcracks.