Computational Design of Low Thermal Conductivity TBC Microstructures

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National Institute of Standards and Technology

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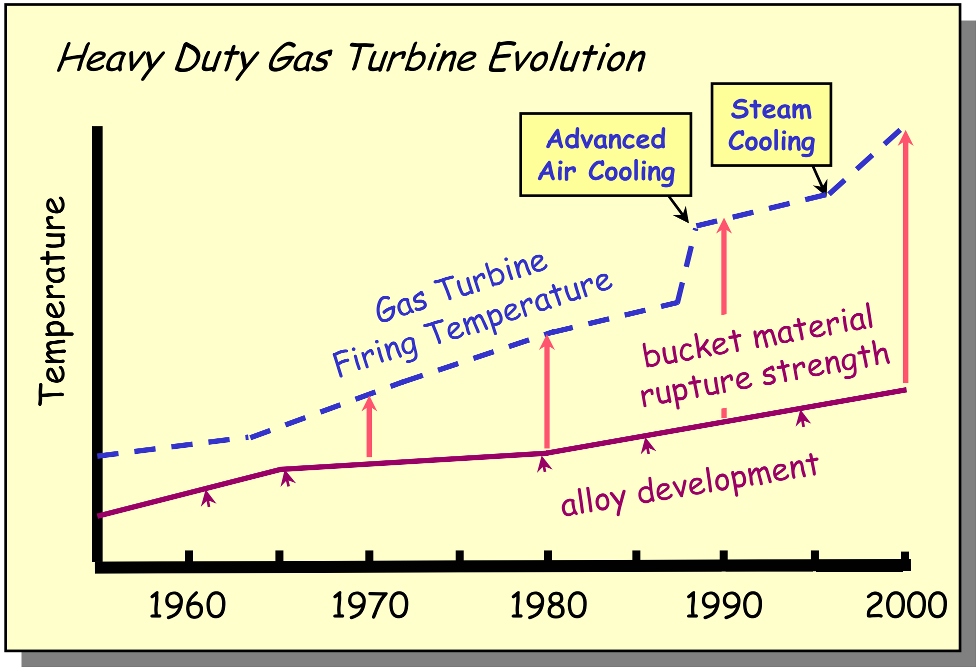
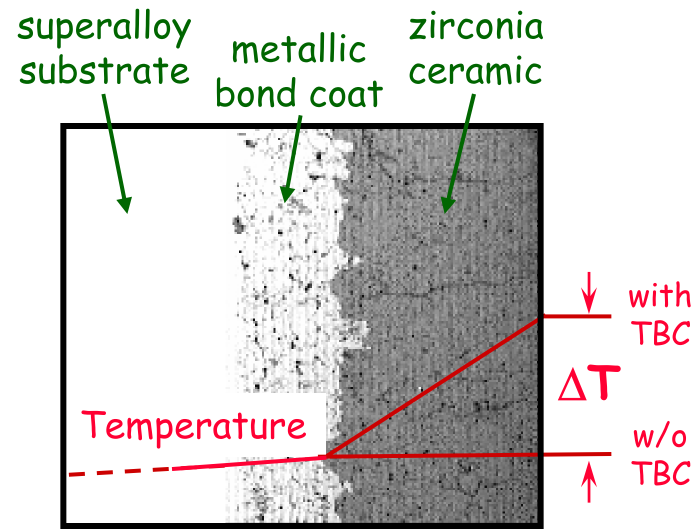
Thermal Barrier Coatings





Benefits of TBCs:

- *Higher firing temperature*
- *Reduced cooling air required*
- *Longer component life.*

TBCs are needed as the gap between the turbine firing temperature and substrate alloy capability increases

Courtesy of GE Power Systems

Motivation for predicting thermal conductivity, k, 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 TBCs for thermal conductivity

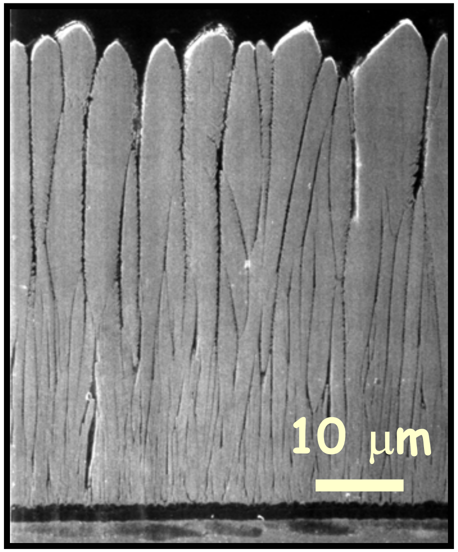
Computational Design of Low Thermal Conductivity TBC Microstructures

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

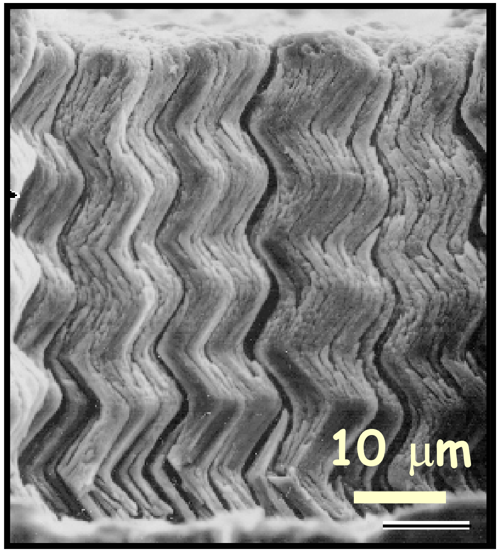
CONTENTS:

- EB-DVD TBC Microstructures
- Microstructural Simulation Approach *(OOF)*
- Thermal Conductivity Simulations
  - Model Zig-Zag Geometries
  - Monte Carlo Generated Microstructures

Types of Thermal Barrier Coatings and Deposition Processes



EB-PVD TBCs

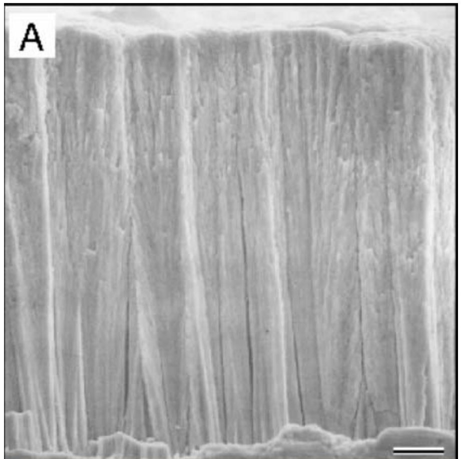


EB-DVD TBCs

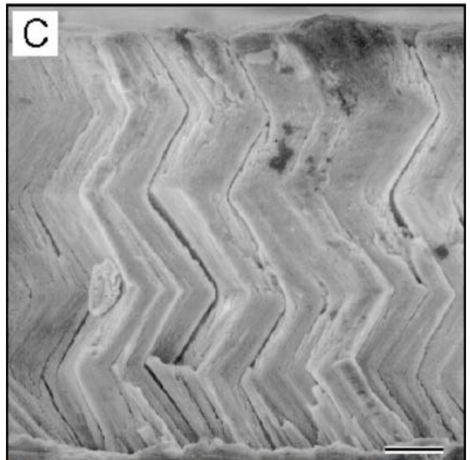
Selected Deposition Processes for the yttria stabilized zirconia (YSZ) ceramic top coat

- electron-beam physical vapor deposition (EB-PVD)
- electron-beam directed vapor deposition (EB-DVD)

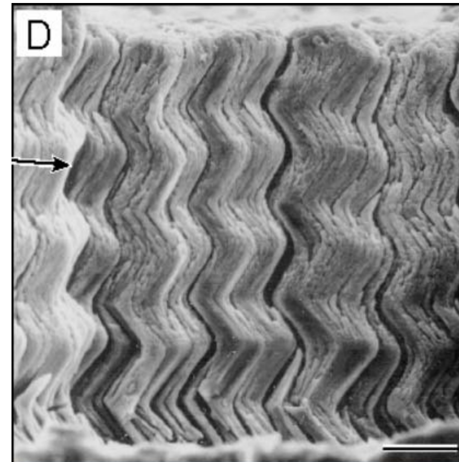
EB-DVD Zig-Zag Microstructures



Stationary Substrate 10μm

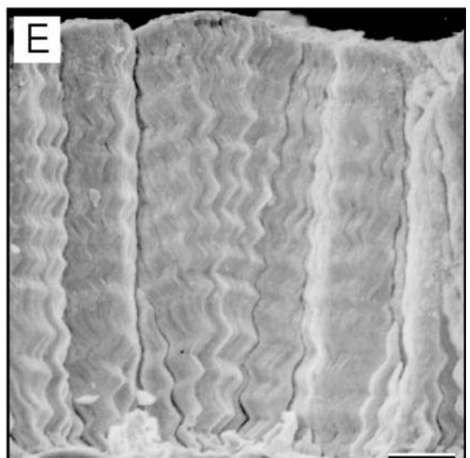


Zig-Zag (λ = 31.7μm) 10μm

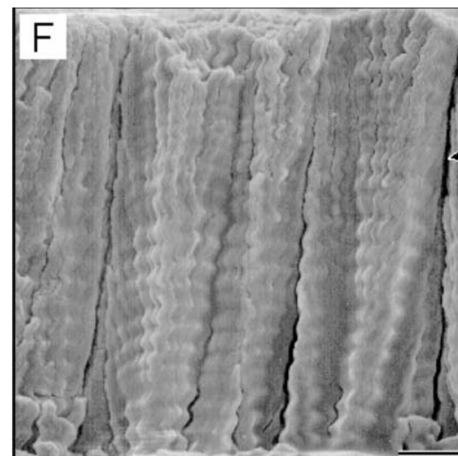


Zig-Zag (λ = 13.4μm) 10μm

D. D. Hass, A. J. Slifka & H. N. G. Wadley, "Low Thermal Conductivity Vapor Deposited Zirconia Micro-structures," *Acta mater.* **49**, 973-983 (2001)

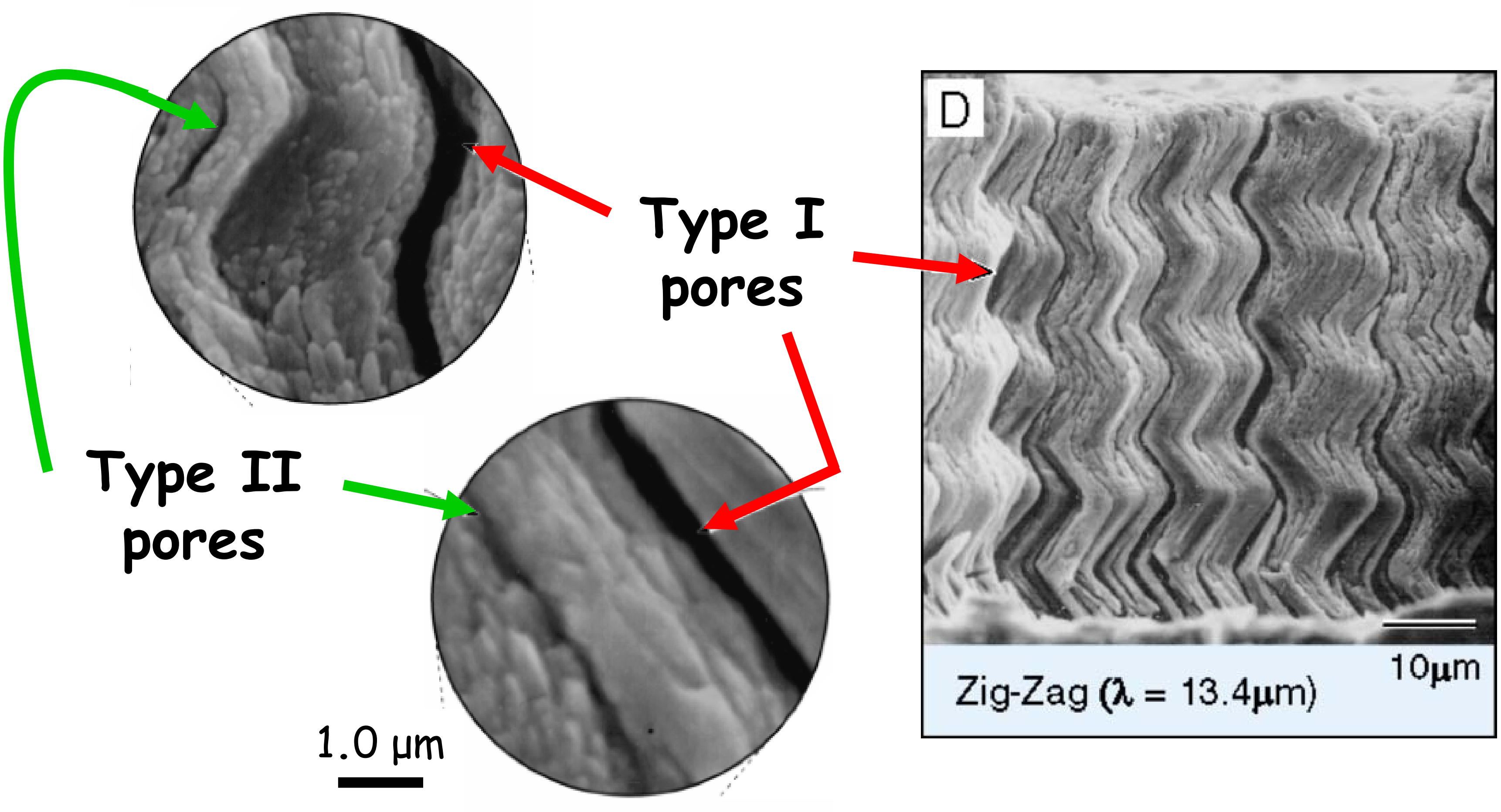


Zig-Zag (λ = 6.6μm) 10μm

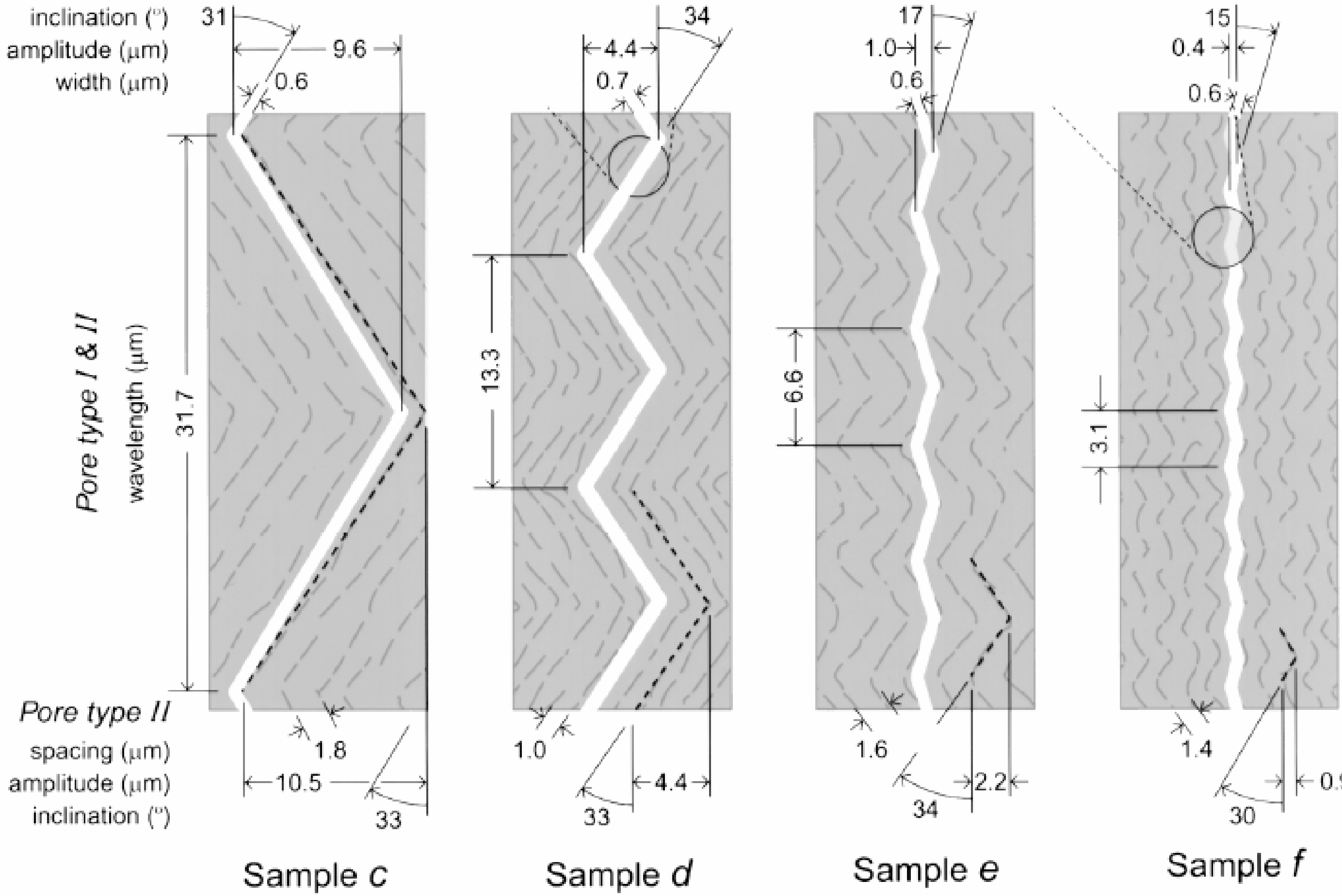


Zig-Zag (λ = 3.1μm) 10μm

Types of Porosity in EB-DVD's

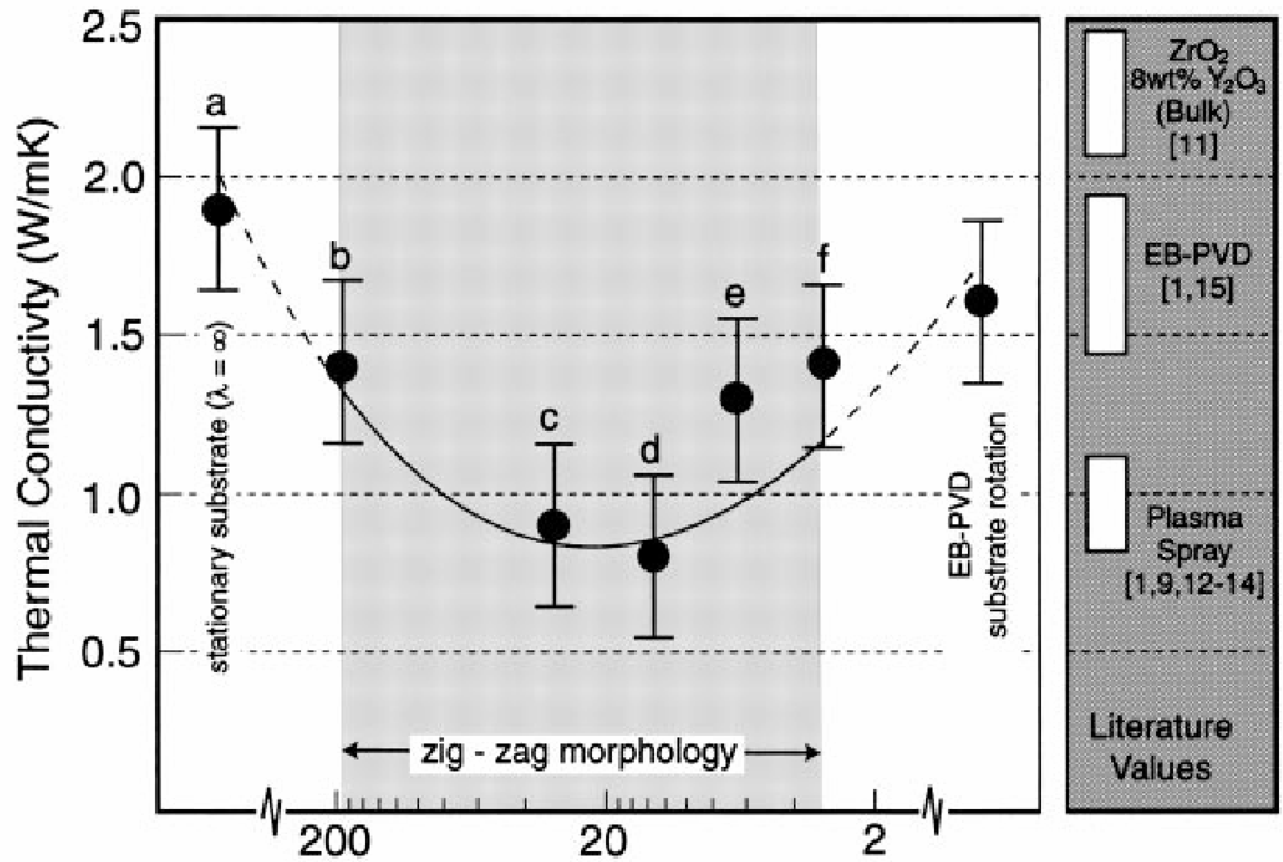


EB-DVD Zig-Zag Microstructures



D. D. Hass, A. J. Slifka & H. N. G. Wadley, "Low Thermal Conductivity Vapor Deposited Zirconia Micro-structures," Acta mater. **49**, 973–983 (2001)

Thermal Conductivities of EB-DVD Zig-Zag Microstructures



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Computational Design of Low Thermal Conductivity TBC Microstructures

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Building a Microstructural Model

Experiments

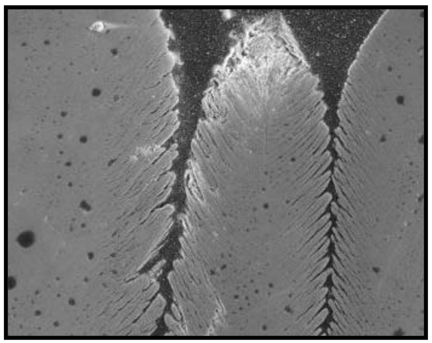
Simulations

Microstructure Data (micrographs)

Fundamental Materials Data

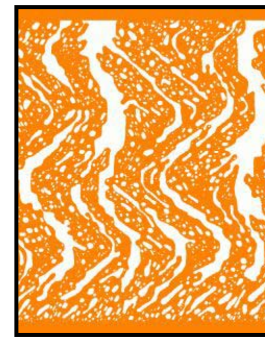
Materials Physics

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

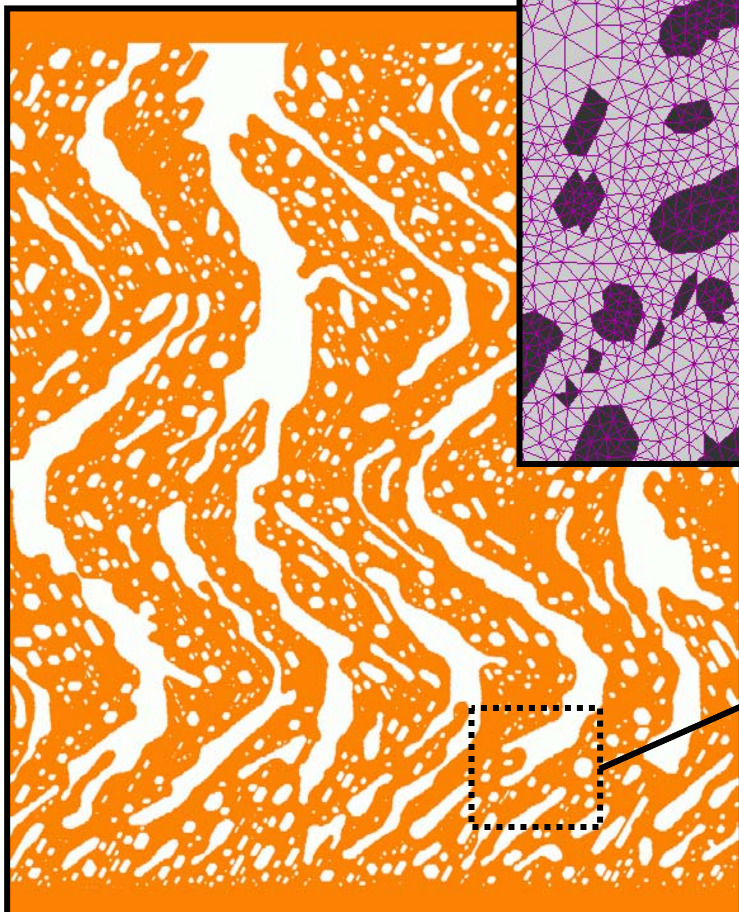
Virtual Parametric Experiments

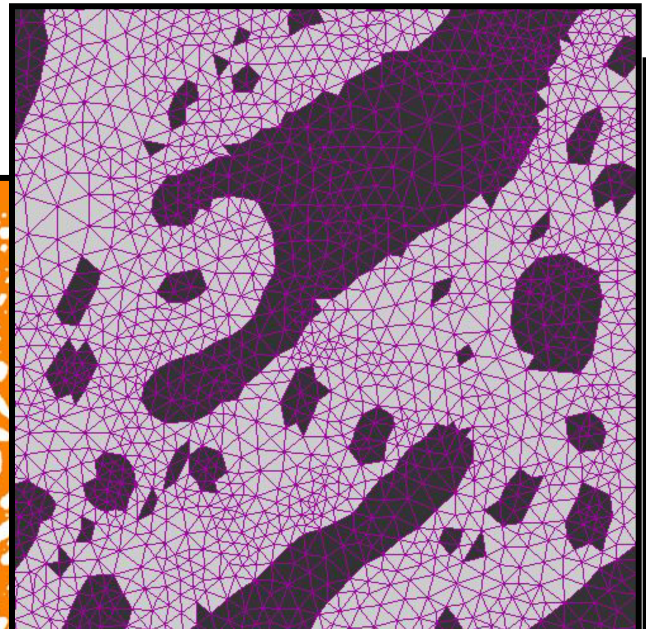
Visualization of Microstructural Physics

Effective Macroscopic Physical Properties

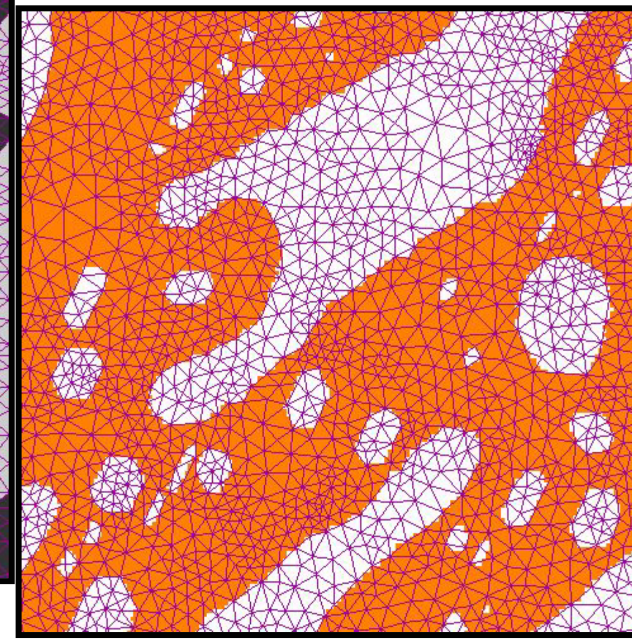
Adaptive Meshing by Components

pixel
image





mesh



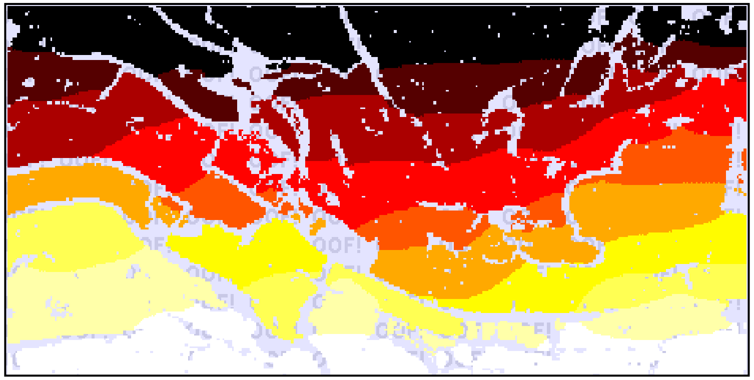
pixel image
with mesh

Generate a finite-element mesh
following the material boundaries

OOF Tool

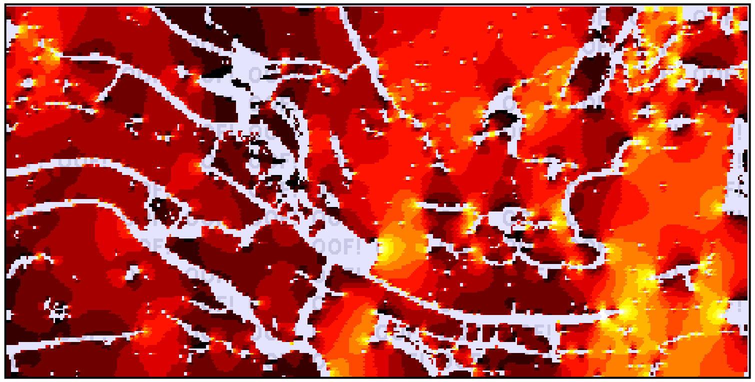
Virtual Experiments:
Temperature Gradient

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

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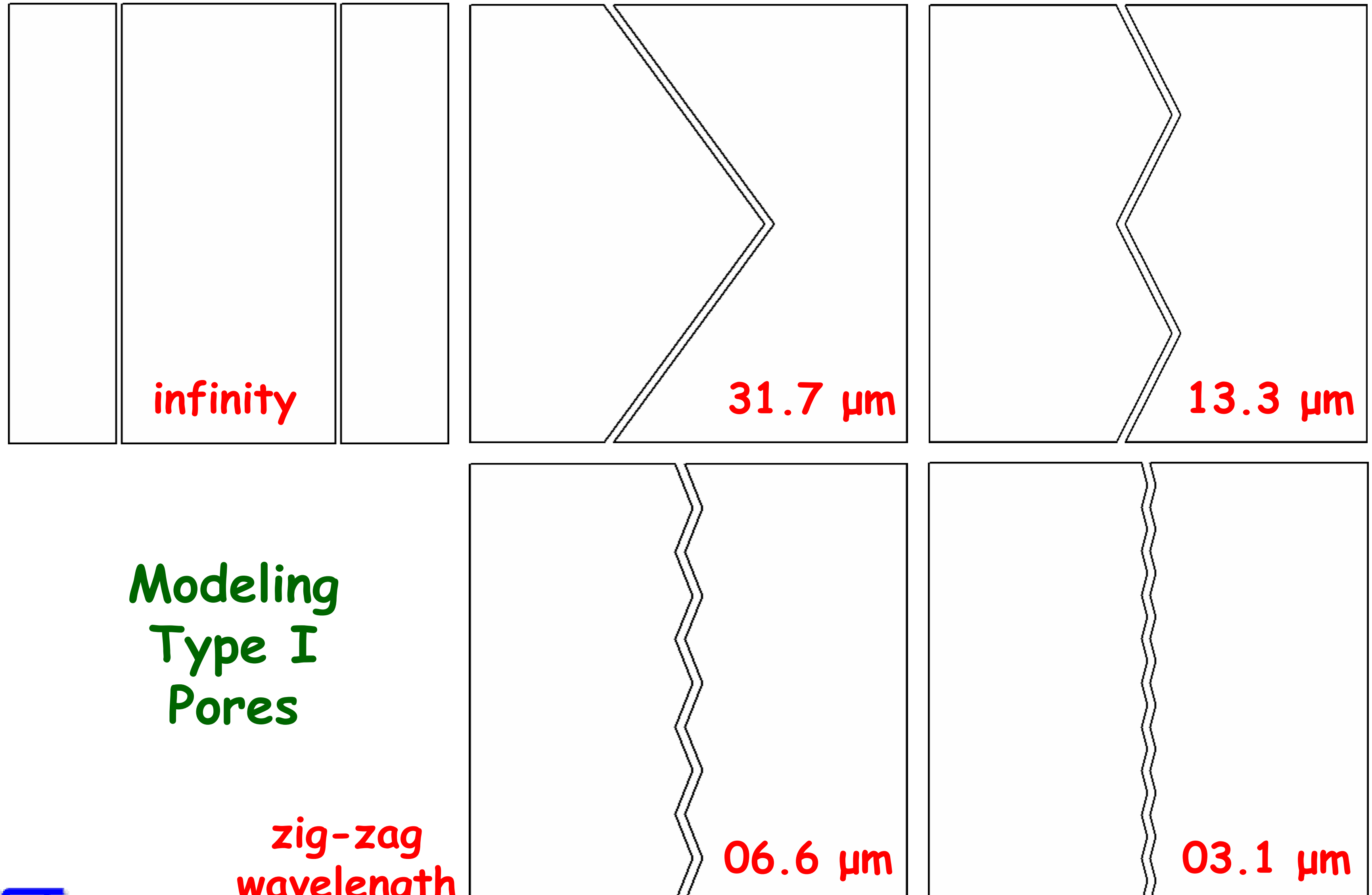
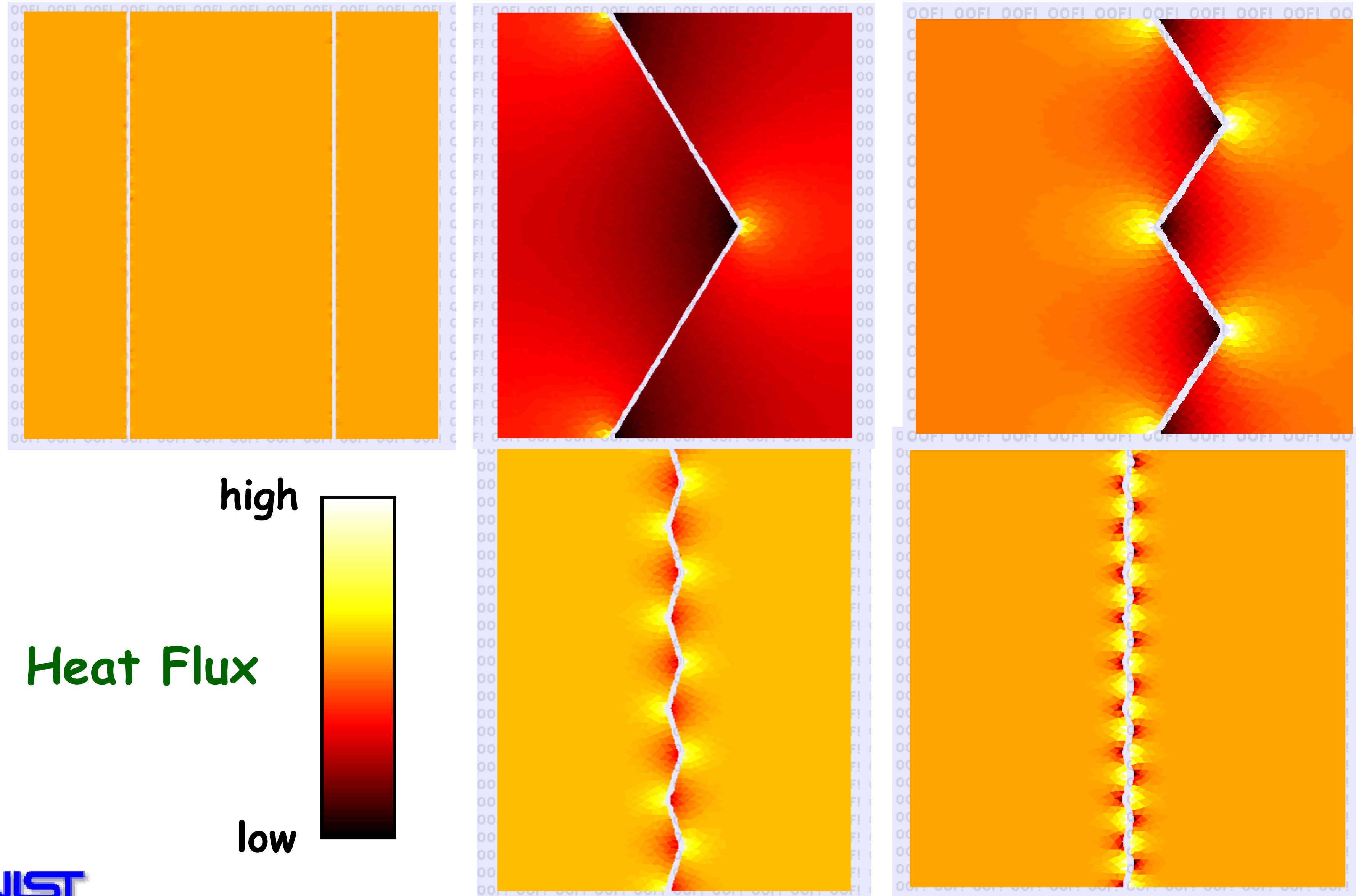
EB-DVD Zig-Zag Microstructures



Modeling Type I Pores

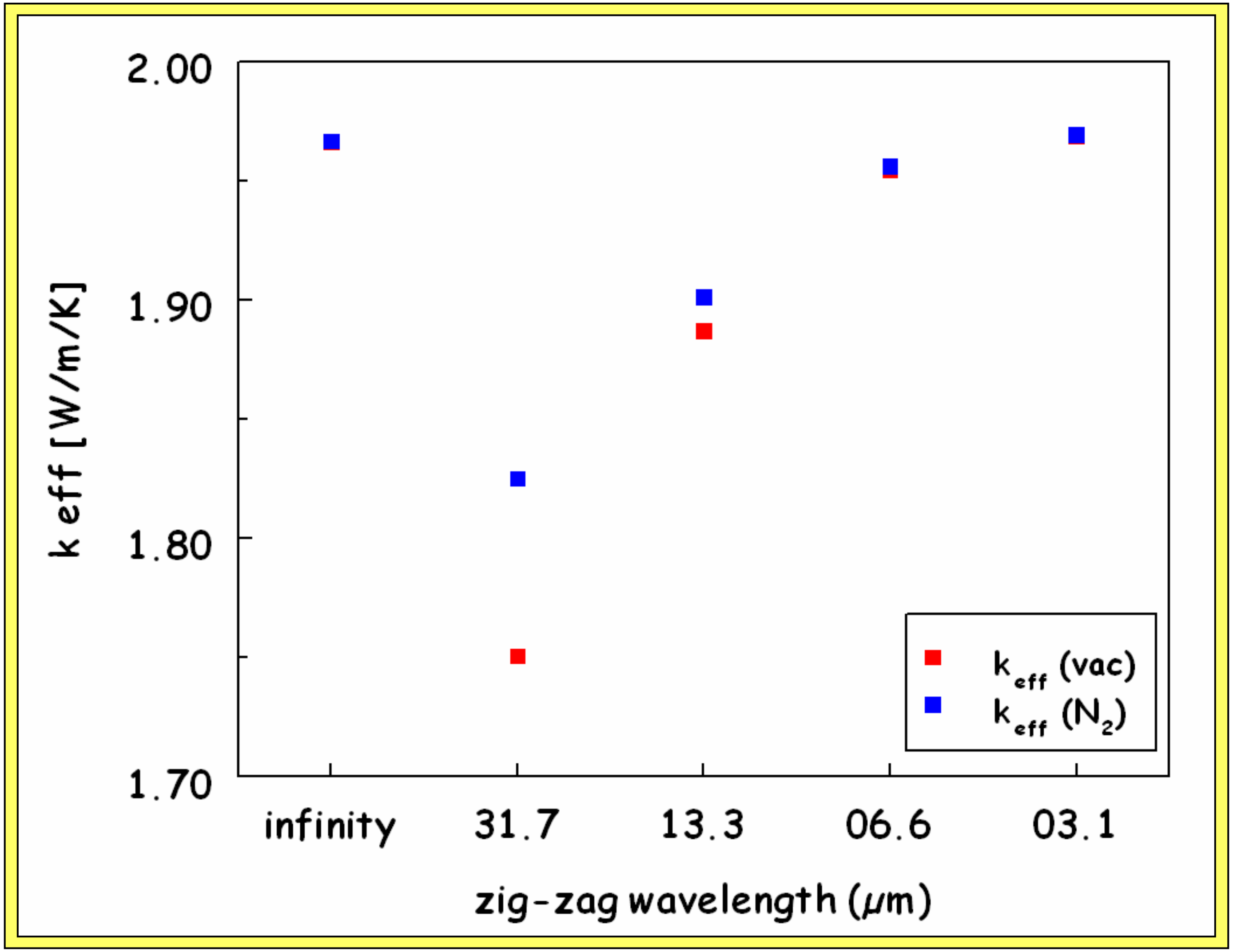
EB-DVD Zig-Zag Microstructures



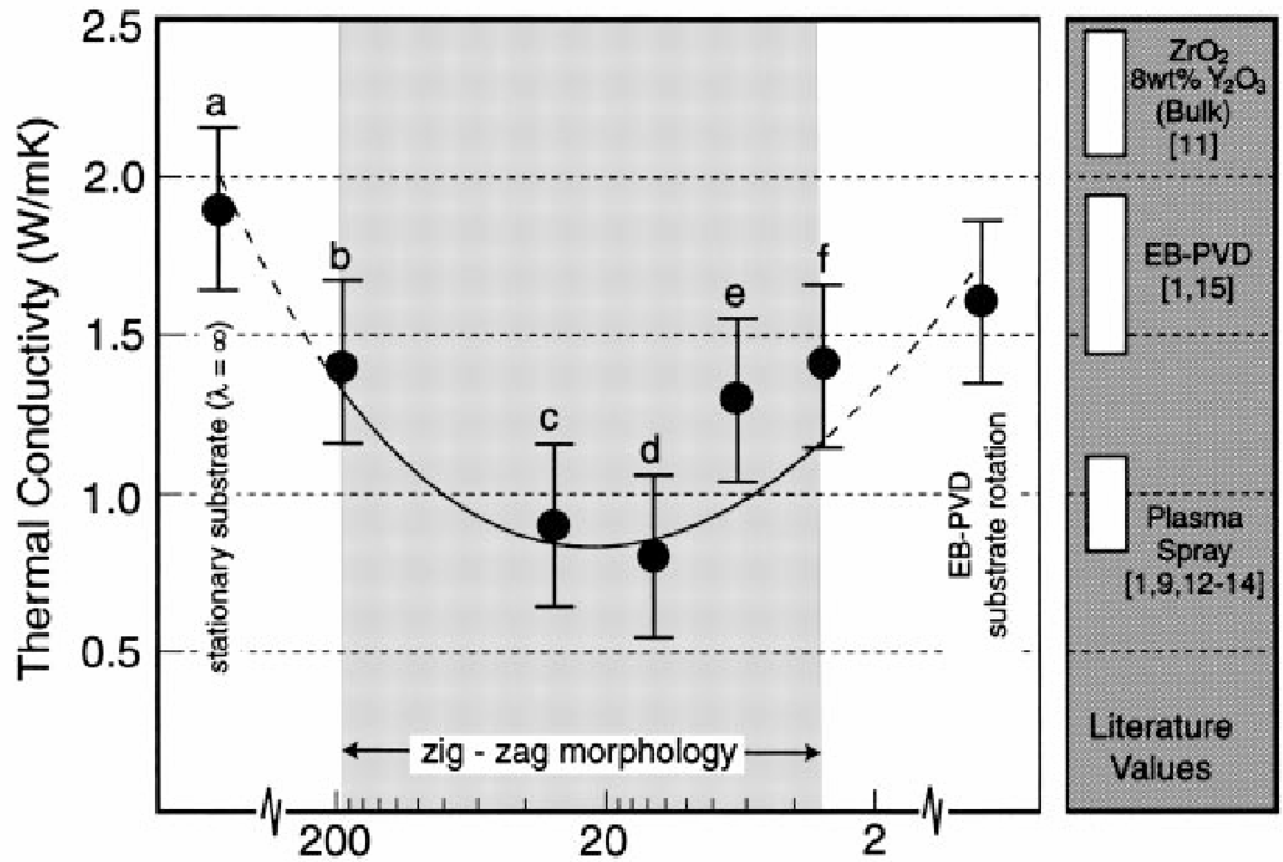
National Institute of Standards and Technology

Ceramics Division

Thermal Conductivities of Model Zig-Zag Microstructures

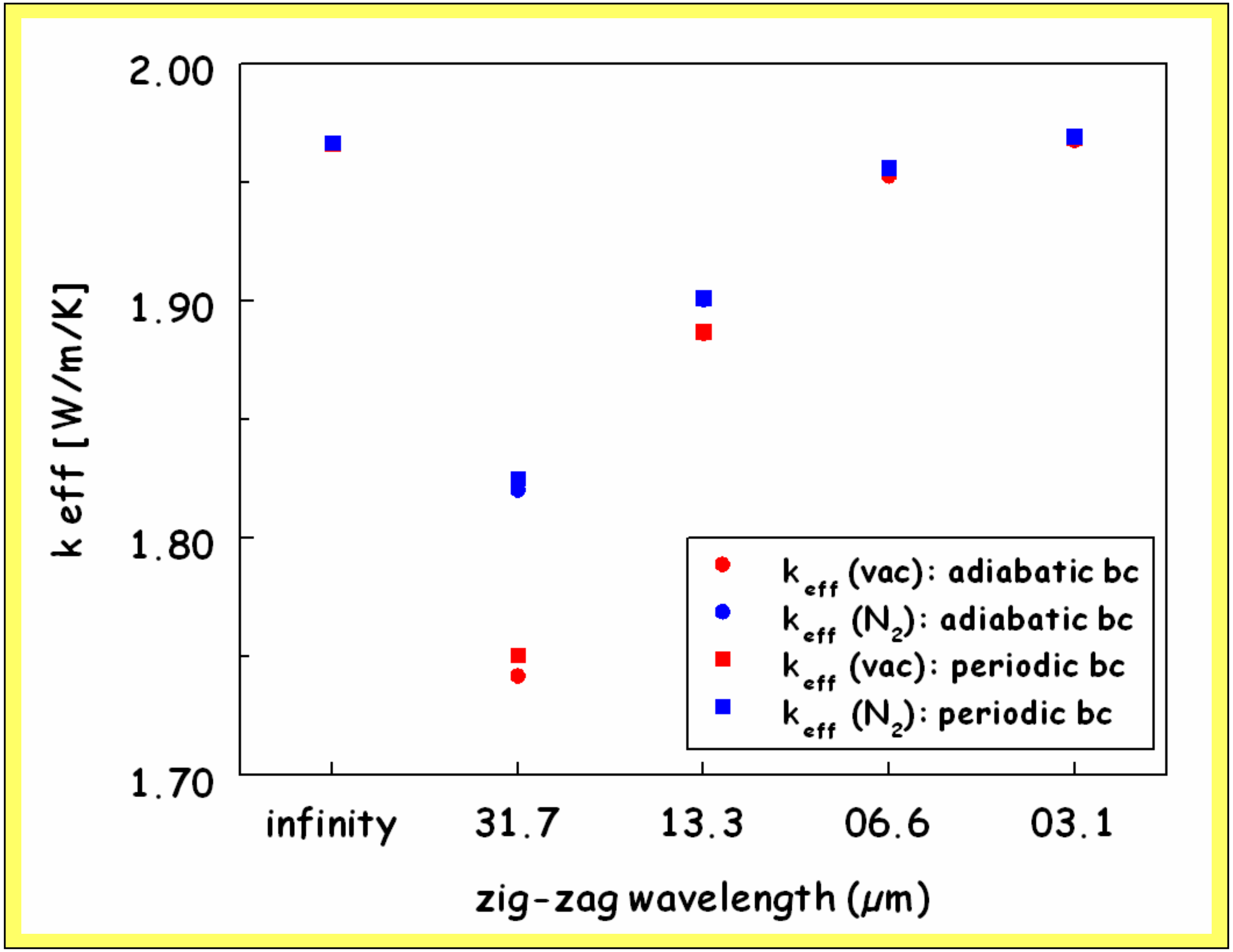


Thermal Conductivities of EB-DVD Zig-Zag Microstructures

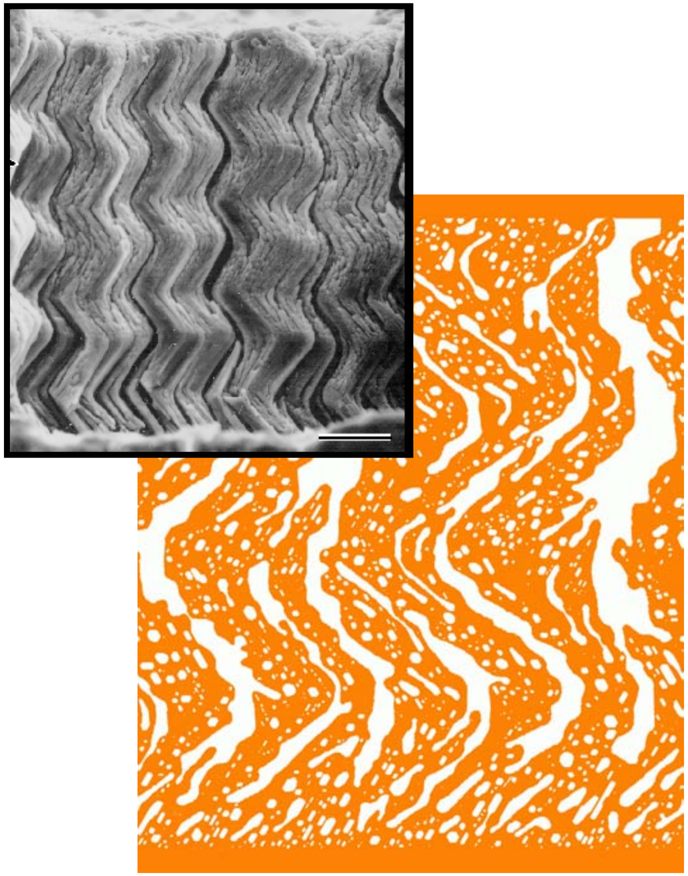


D. D. Hass, A. J. Slifka & H. N. G. Wadley, "Low Thermal Conductivity Vapor Deposited Zirconia Micro-structures," Acta mater. **49**, 973–983 (2001)

Effect of Boundary Conditions



Optimization of Low Conductivity EB-DVD Microstructures



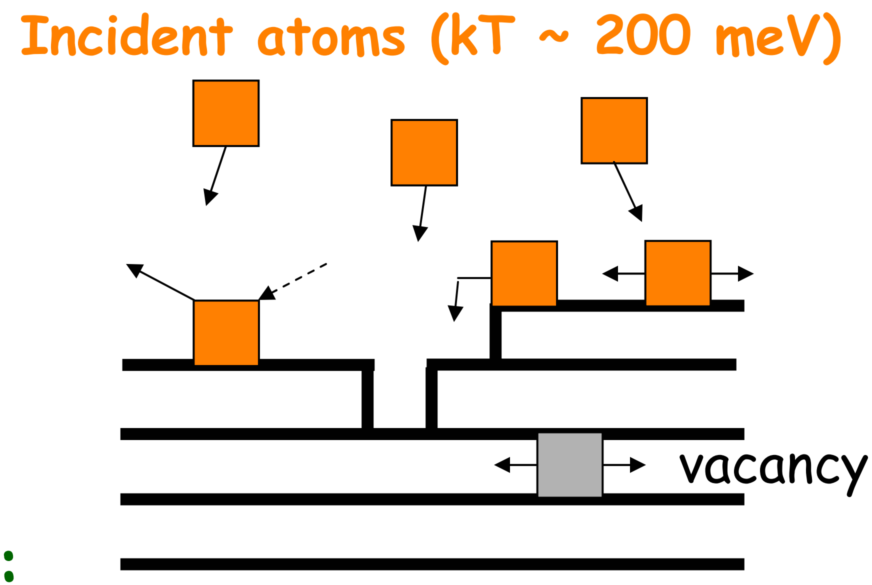
Electron-Beam Directed Vapor Deposition coating microstructure via kinetic Monte Carlo simulation

- 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



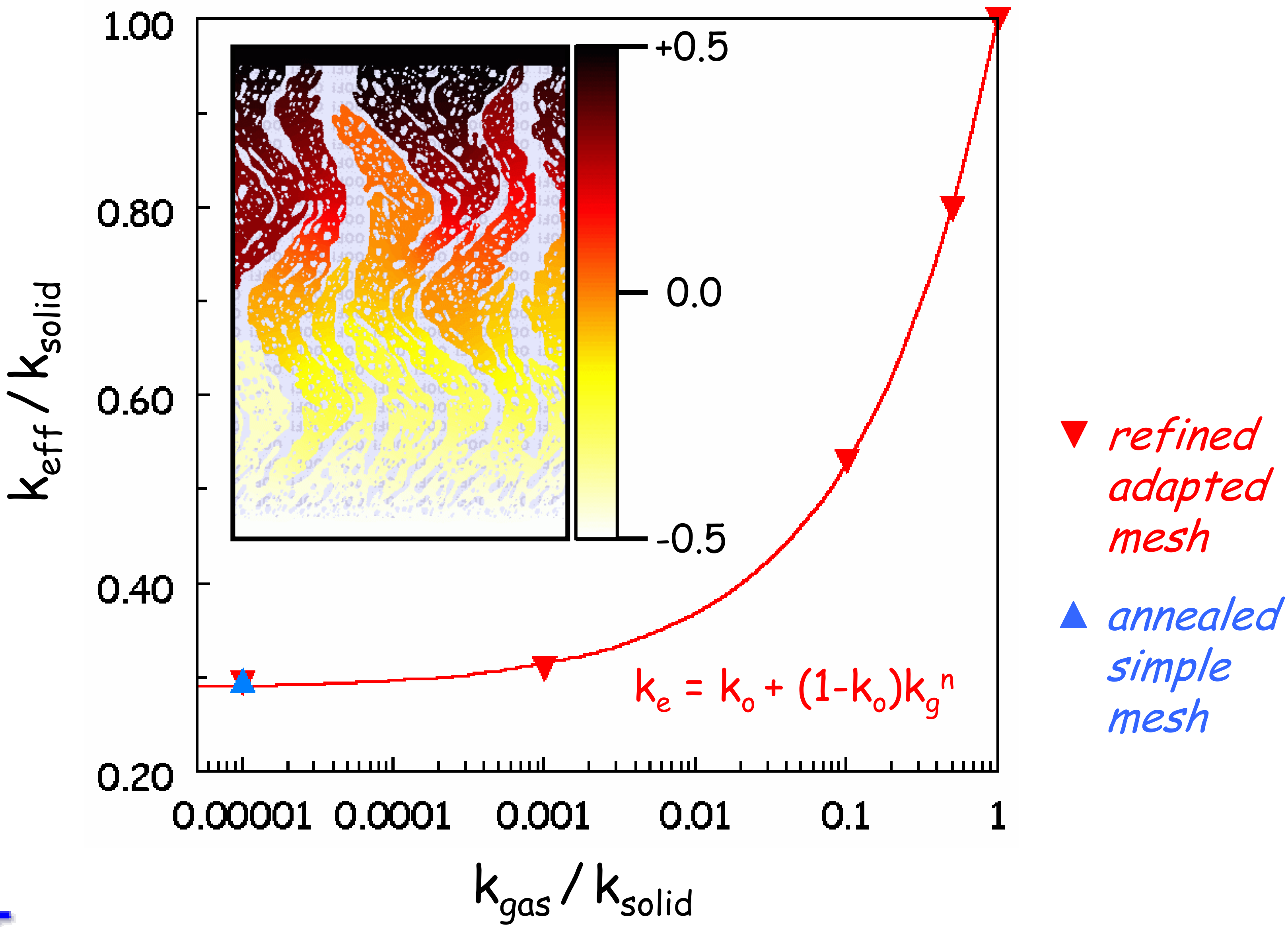
Physical Vapor Deposition

Assembly Process:

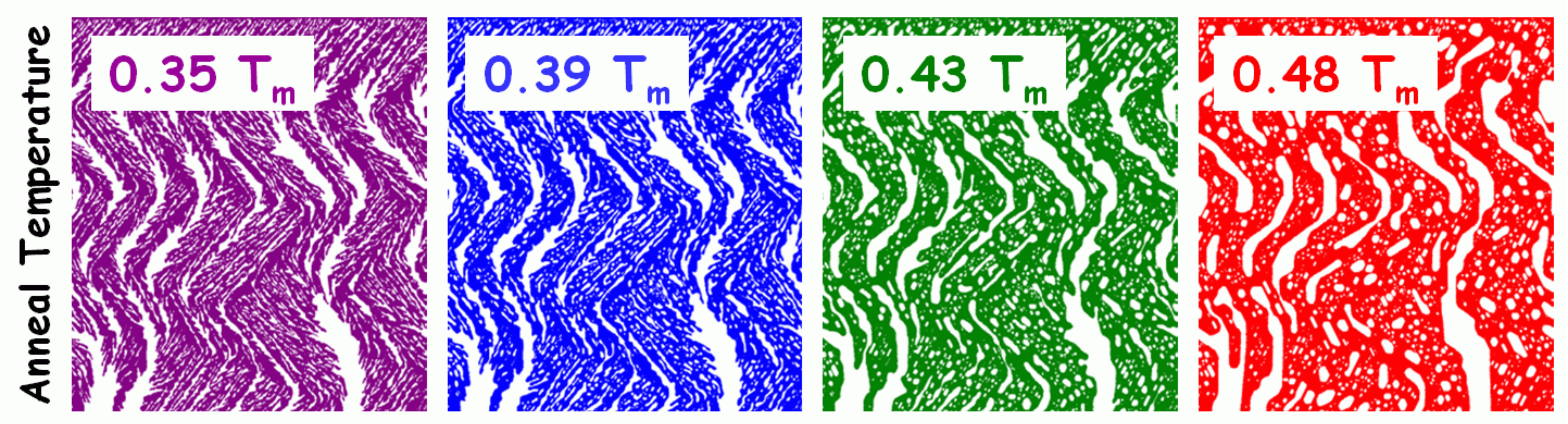
- Condensation
- Thermal diffusion (surface, bulk)
- Incident atom-growing surface interactions, including reflection, resputtering, etc.

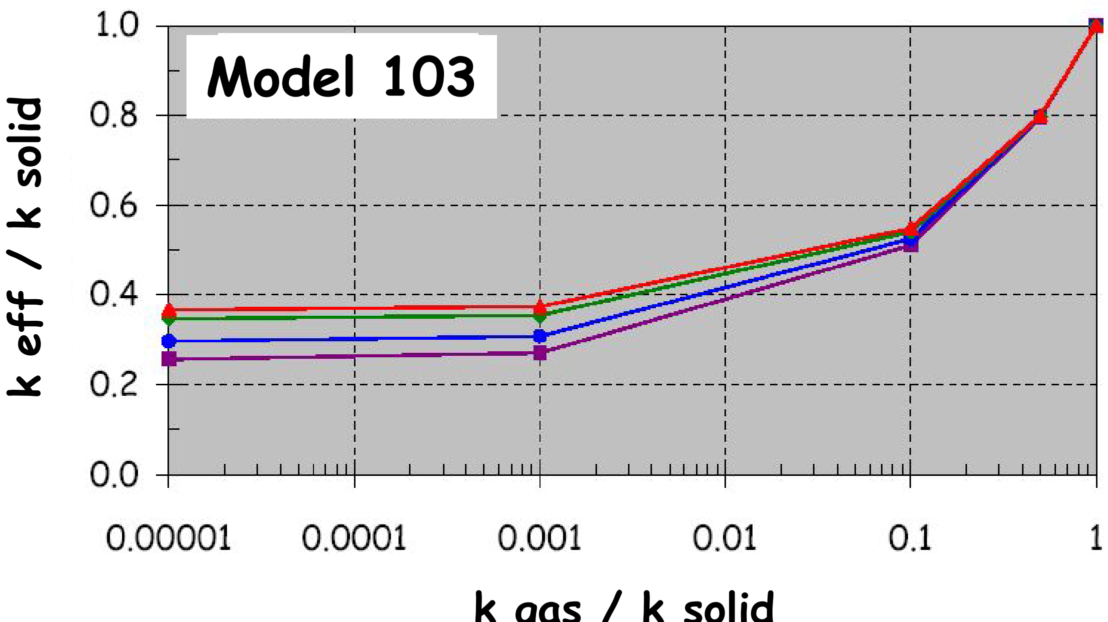
kinetic Monte Carlo (kMC) for diffusion
Molecular Dynamics (MD) for effects of energy

Effective Thermal Conductivity



Thermal Conductivity Simulations





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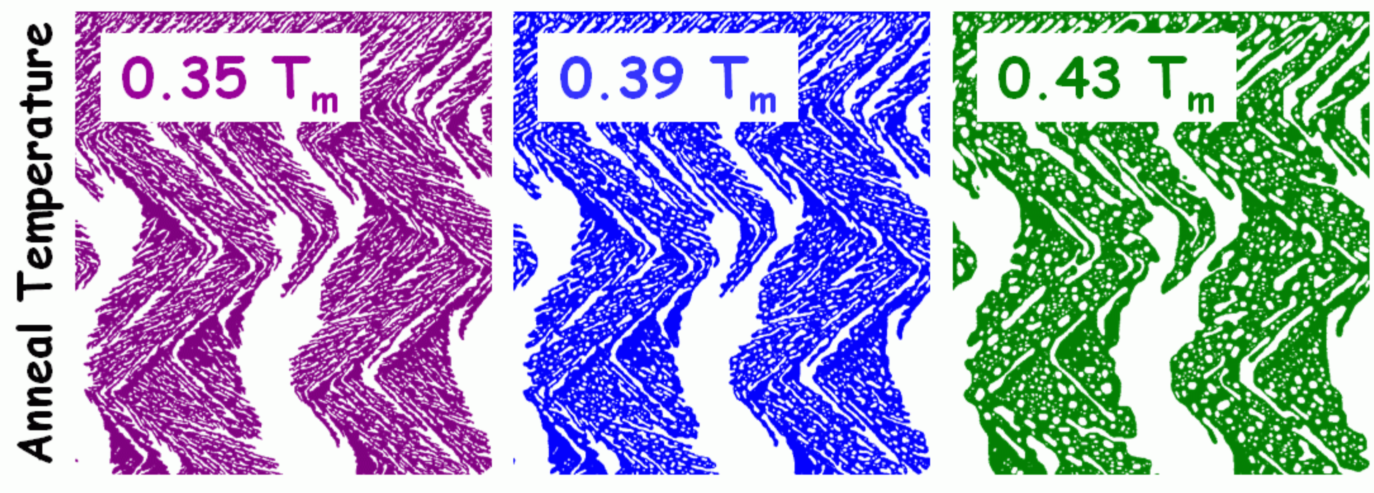
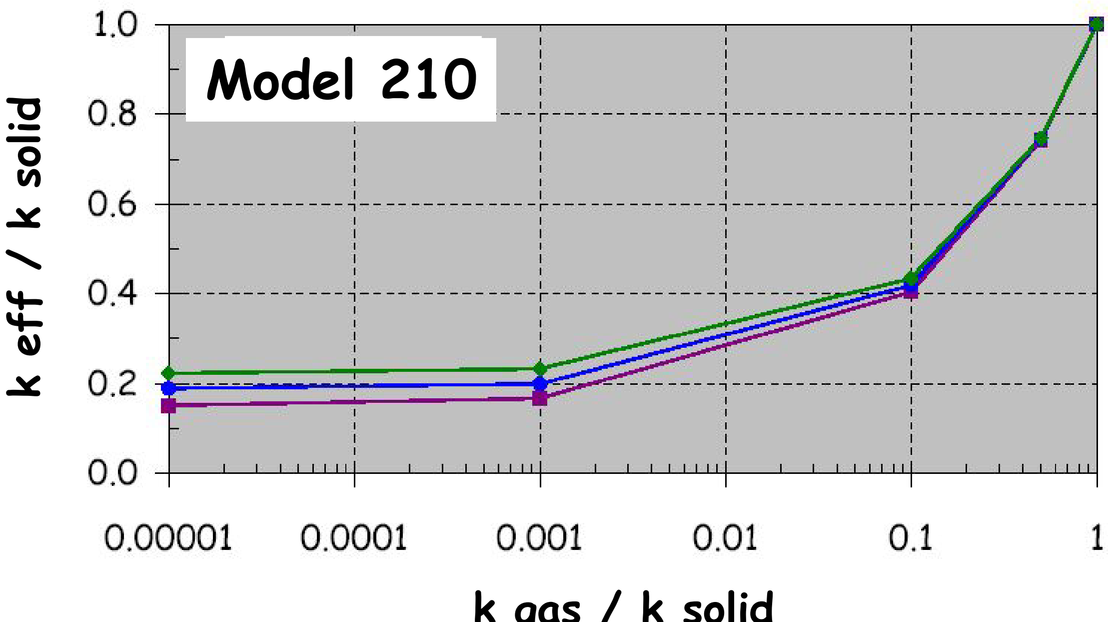
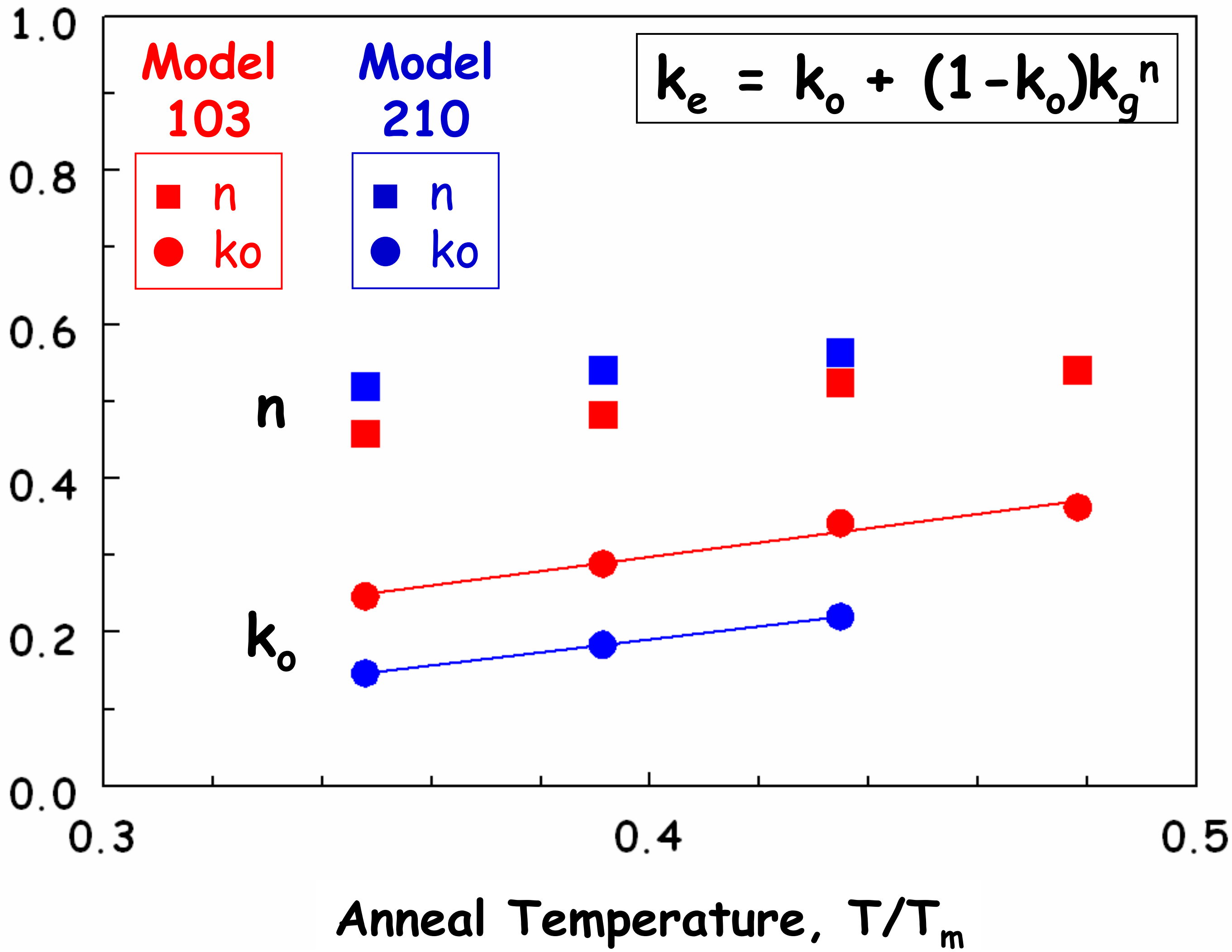




Thermal Conductivity Simulations



Computational Design of Low Thermal Conductivity TBC Microstructures

SUMMARY:

- Microstructure-based, finite-element simulations are used to elucidate the thermal conductivity of complex TBC microstructures.
- Microstructures include actual EB-DVD microstructures, model microstructures, and kinetic Monte Carlo generated microstructures.
- Effective thermal conductivity is a simple function of gas conductivity with microstructure-dependent properties.

Acknowledgments

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  Information Tech. Lab, NIST
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Abstract

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Lowering the thermal conductivity of thermal barrier coatings (TBCs) is an important design aspect in the improvement of advanced turbine airfoils. While much research is ongoing in development of alternative materials to yttria-stabilized zirconia with lower intrinsic thermal conductivity, many advantages can be made through microstructural design of pore morphology and pore distribution [e.g., see T. J. Lu et al., J. Am. Ceram. Soc., 84 [12]: 2937-2946 (2001)]. Electron-Beam Directed Vapor Deposition (EB-DVD) provides a fabrication process by which the pore morphology and distribution can be tailored through the development of zigzag columnar TBC microstructures. However, optimization of these zigzag microstructures entails depositing and testing many coatings via myriad processing variables. Computational simulations are used to accelerate this process. EB-DVD zigzag microstructures are generated via kinetic Monte Carlo and molecular dynamics (MD) simulations, in which the substrate is periodically inclined to the vapor flux. The generated microstructures are annealed via similar computational processes. Effective thermal conductivity of real and simulated microstructures is computed via microstructure-based finite-element simulations. Effects of coating design and annealing temperature are systematically explored.