Predicting Physical Properties From Microstructures

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Symposium on
Multifunctional Materials and Structures
In honor of *Anthony G. Evans*
Max-Planck-Institut für Metallforschung
Stuttgart — March 19, 2003

National Institute of Standards and Technology

Collaborators & Acknowledgments

- Stephen A. Langer, Information Tech. Lab, NIST
- Andrew C. E. Reid & David M. Saylor, MSEL, NIST
- Bhavesh Patel, K. K. Chawla, Mark Koopman, X. Deng, B. R. Patterson, Univ. of Alabama Birmingham
- Scott Terry & Carlos Levi, Univ. Calif. Santa Barbara
- Marion Bartsch & Uwe Schulz, DLR, Germany
- Jean Marc Dorvaux, Odile Lavigne, & Rémy Mevrel, ONERA, France
- James Ruud, N. S. Hari, James C. Grande, & Antonio Mogro-Campero, GE Global Research
- Yougen Yang, Derek Hass, & Haydn N. G. Wadley, Univ. of Virginia
- Venkata R. Vedula, Shekhar Kamat & S. Jill Glass, Sandia Natl. Labs
- André Zimmermann, PML, Max-Planck-Institut & Bosch GmbH, Germany
- Susan Galal Yousef & Jürgen Rödel, T-U Darmstadt, Germany
- Thomas Weiß & Siegfried Siegesmund, Universität Göttingen, Germany
- Hannes Kessler and Herbert Balke, T-U Dresden, Germany

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MATERIALS MOTIVATION

- Elucidate the role of *heterogeneous, stochastic* microstructures on bulk physical properties and microstructural damage evolution.
- Correlate physical properties and damage evolution with microstructure
  - to shorten the materials development cycle
  - to improve materials & processing
  - to enable more reliable design

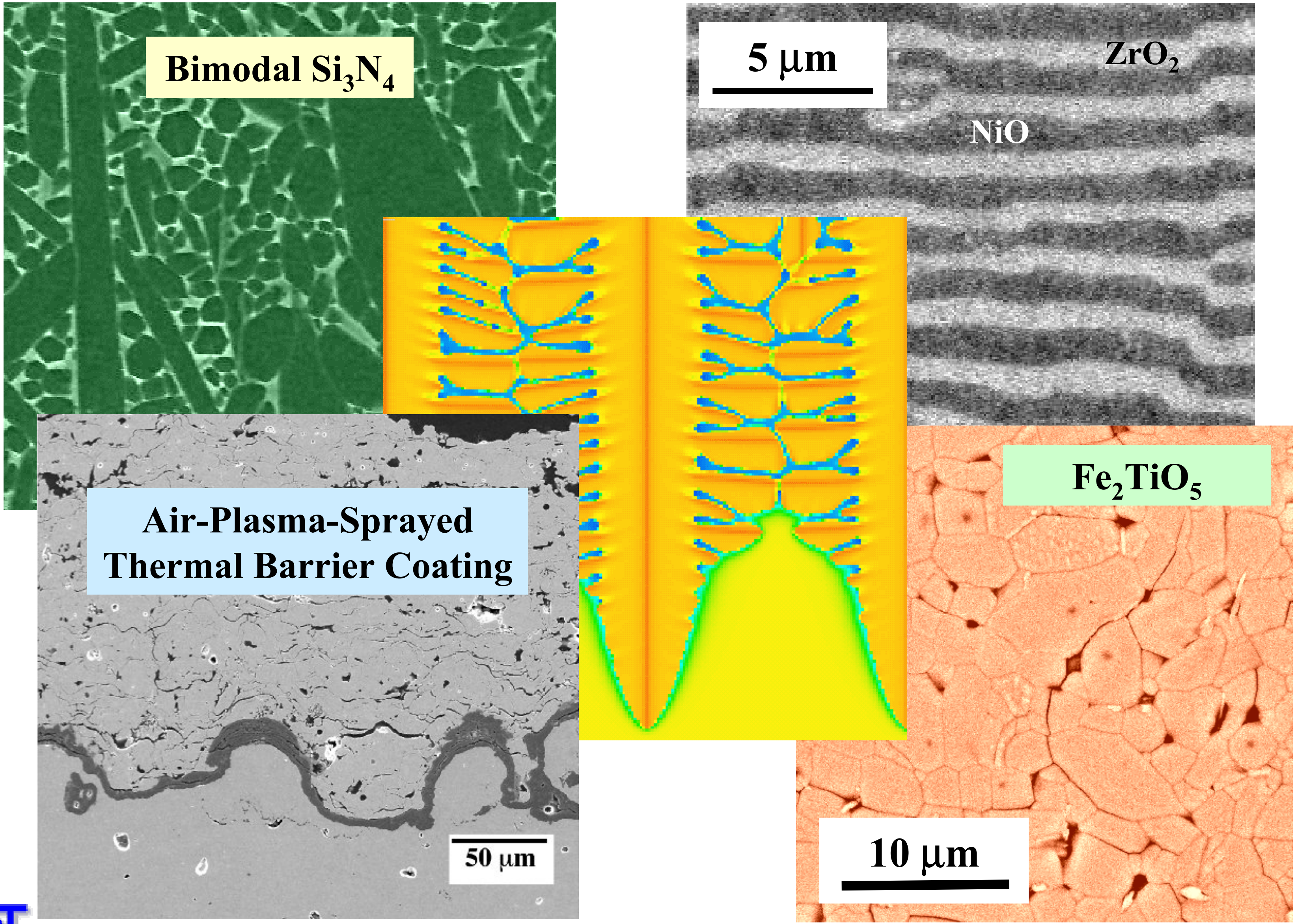
APPROACH: Develop computational tools for simulating ***multifunctional*** *properties & elucidating influences of stochastic, anisotropic microstructural features on physical properties and damage evolution processes.*

Predicting Physical Properties From Microstructures

CONTENTS:

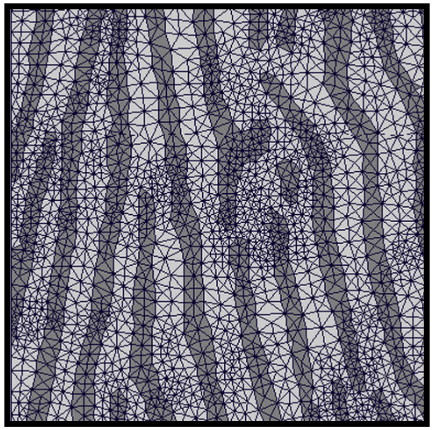
- Microstructural Finite-Element Analysis
- Physical Property Simulations
    - Coefficient of Thermal Expansion
    - Elasticity
    - Thermal Conductivity
- Residual Stresses & Nonlinear Processes
    - TEA induced residual stresses
    - damage simulations
    - domain switching in ferroelectrics

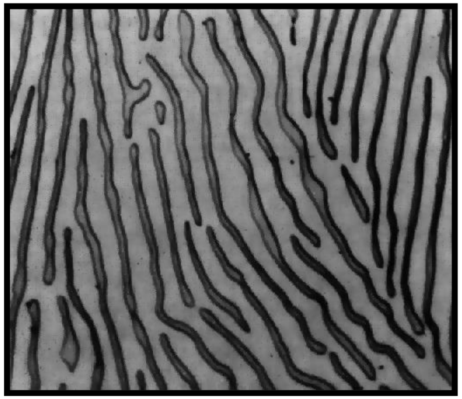
Material Microstructures: Heterogeneous & Stochastic

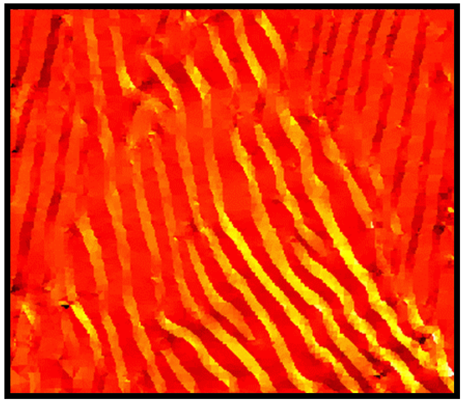


Object Oriented Finite Element Analysis for Materials Science and Engineering

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







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

Building a Microstructural Model

Experiments

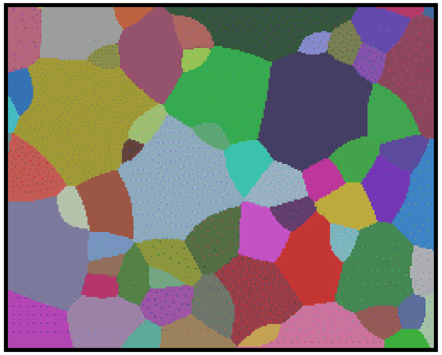
Simulations

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

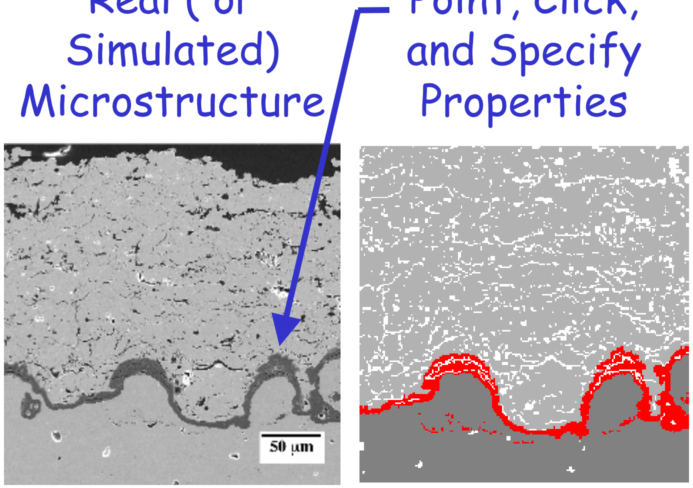
Effective Macroscopic Physical Properties

Finite Element Analysis of Real Microstructures

a tool for materials scientists to design and analyze advanced materials

Real (or Simulated) Microstructure

Point, Click, and Specify Properties

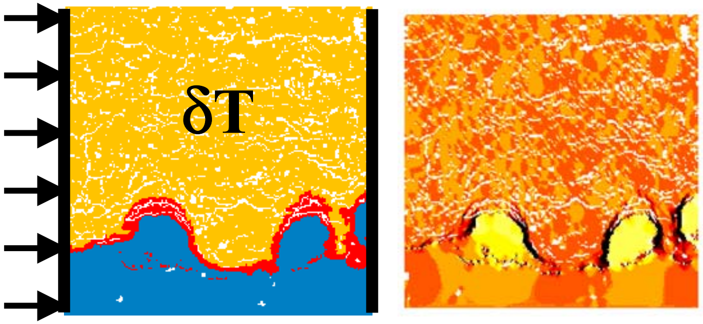


ppm2oof: a tool to convert a micrograph or image of a complex, heterogeneous microstructure into a finite element mesh with constitutive properties specified by the user.

oof: a tool to perform virtual experiments via finite element analysis to elucidate microstructural properties and macroscopic behavior.

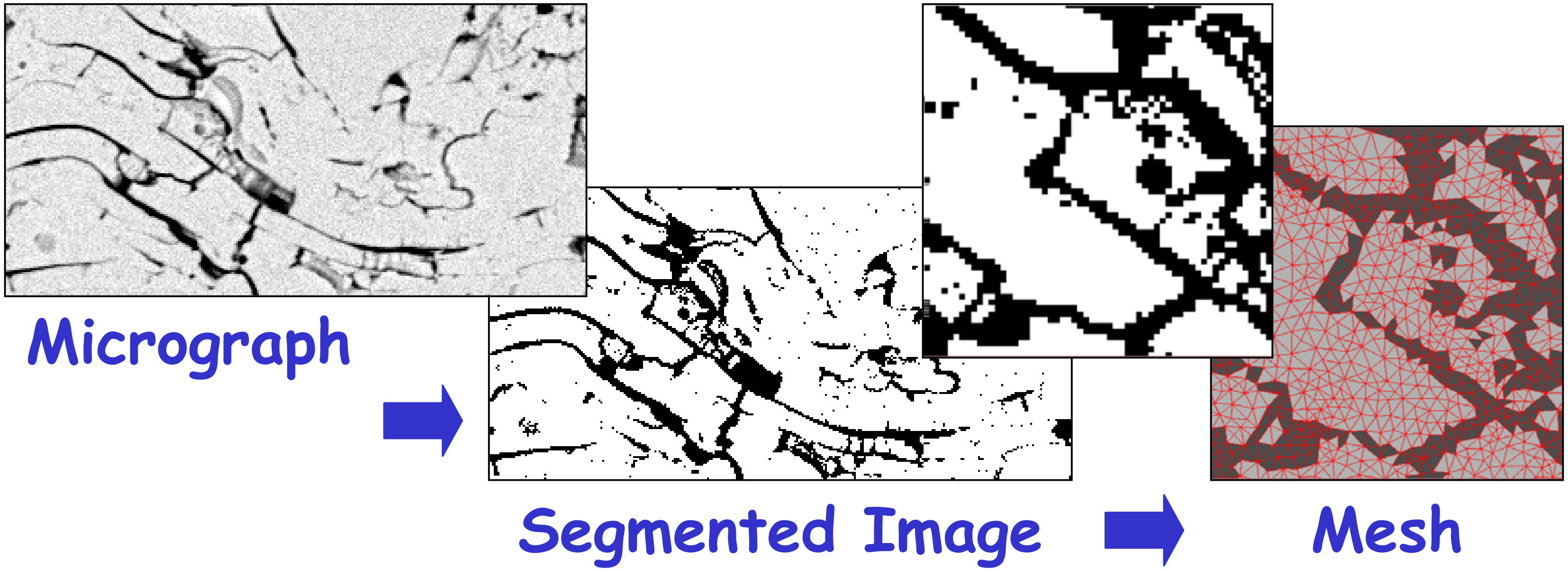
Virtual Test

Visualize and Quantify



oof2abaqus: converts PPM2OOF or OOF data files into input files for ABAQUS™.

PPM2OOF Tool



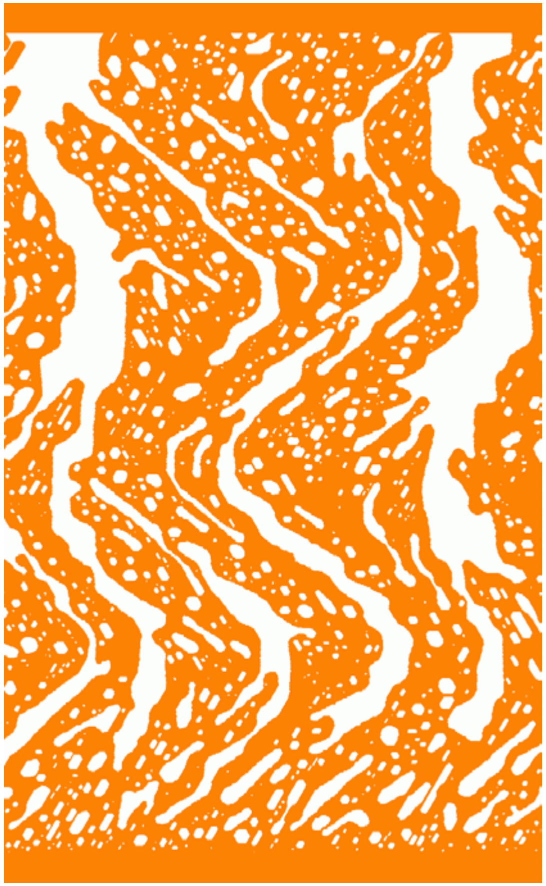
Micrograph

Segmented Image

Mesh

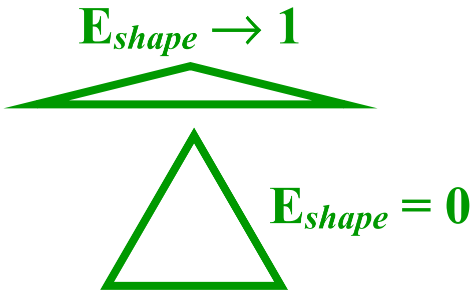
- Convert micrograph to ".ppm" (portable pixel map) file
- Select & identify phases to create segmented image
- Assign constitutive physical properties to each phase
- Mesh in PPM2OOF via "Simple Mesh" or "Adaptive Mesh" – multiple algorithms that allow elements to adapt to the microstructure

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



image

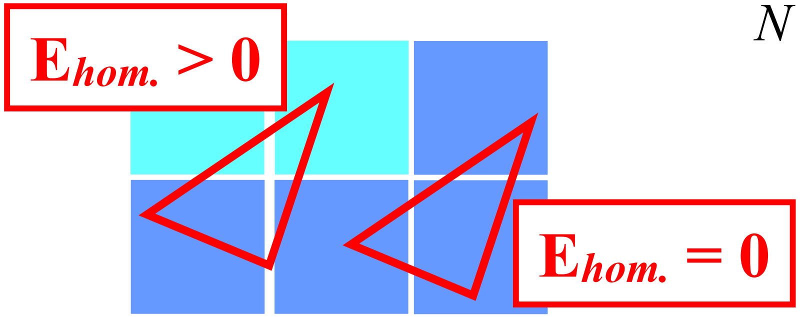
$$E_{shape} = 1 - \frac{36A}{\sqrt{3}L^2}$$



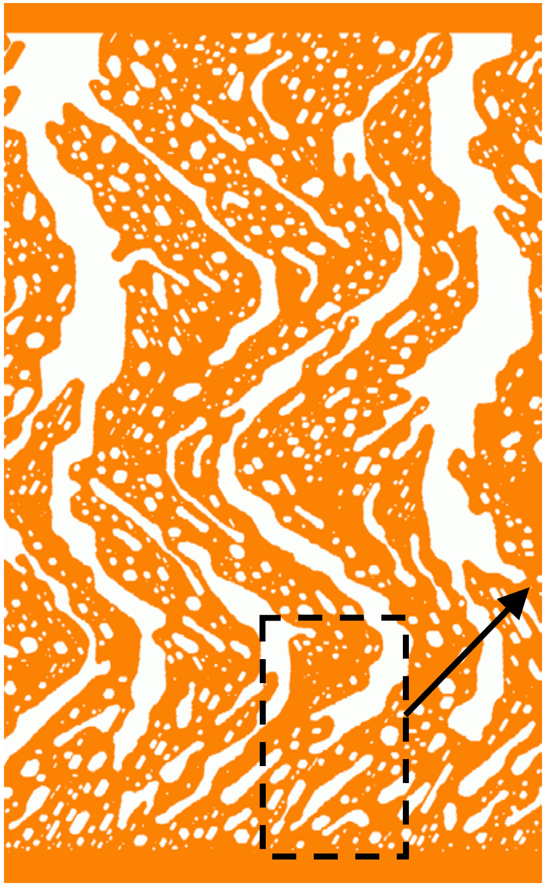
$$E_{homogeneity} = \prod_{i=1}^{N}\left[\frac{(1-a_i)}{(1-1/N)}\right]$$

a_i = fractional area of pixel type i

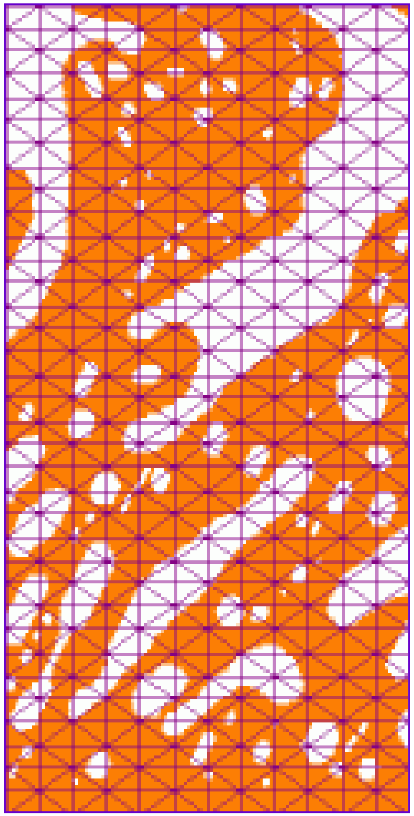
N = number of pixel types



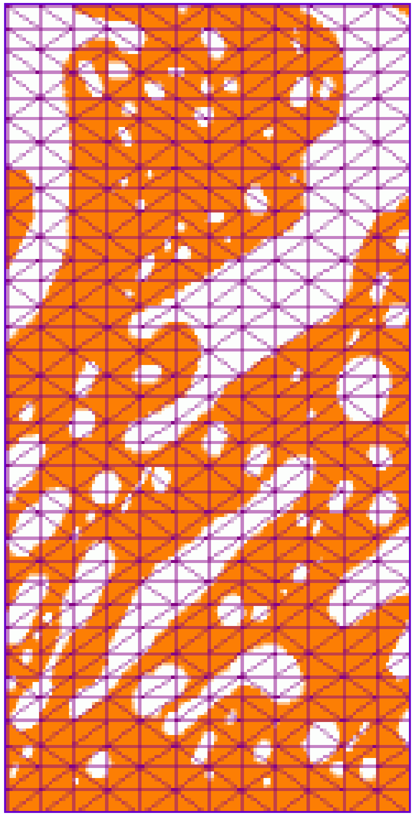
Adaptive Meshing by Components: refine elements and move nodes via Monte Carlo *annealing* to reduce $E = (1-\alpha)E_{shape} + \alpha E_{homogeneity}$



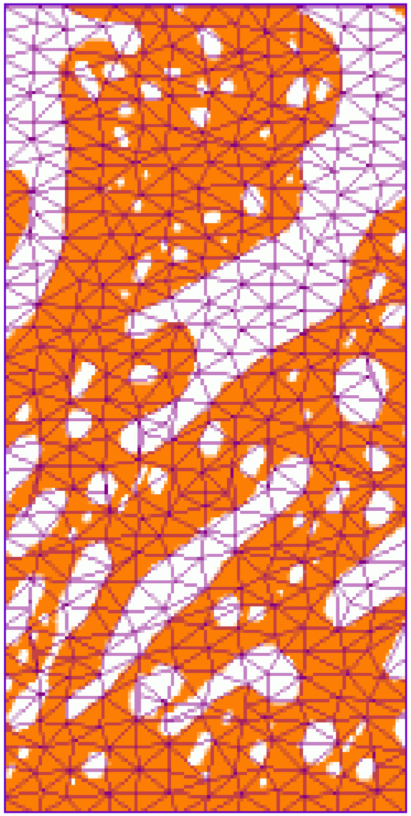
image



create
mesh

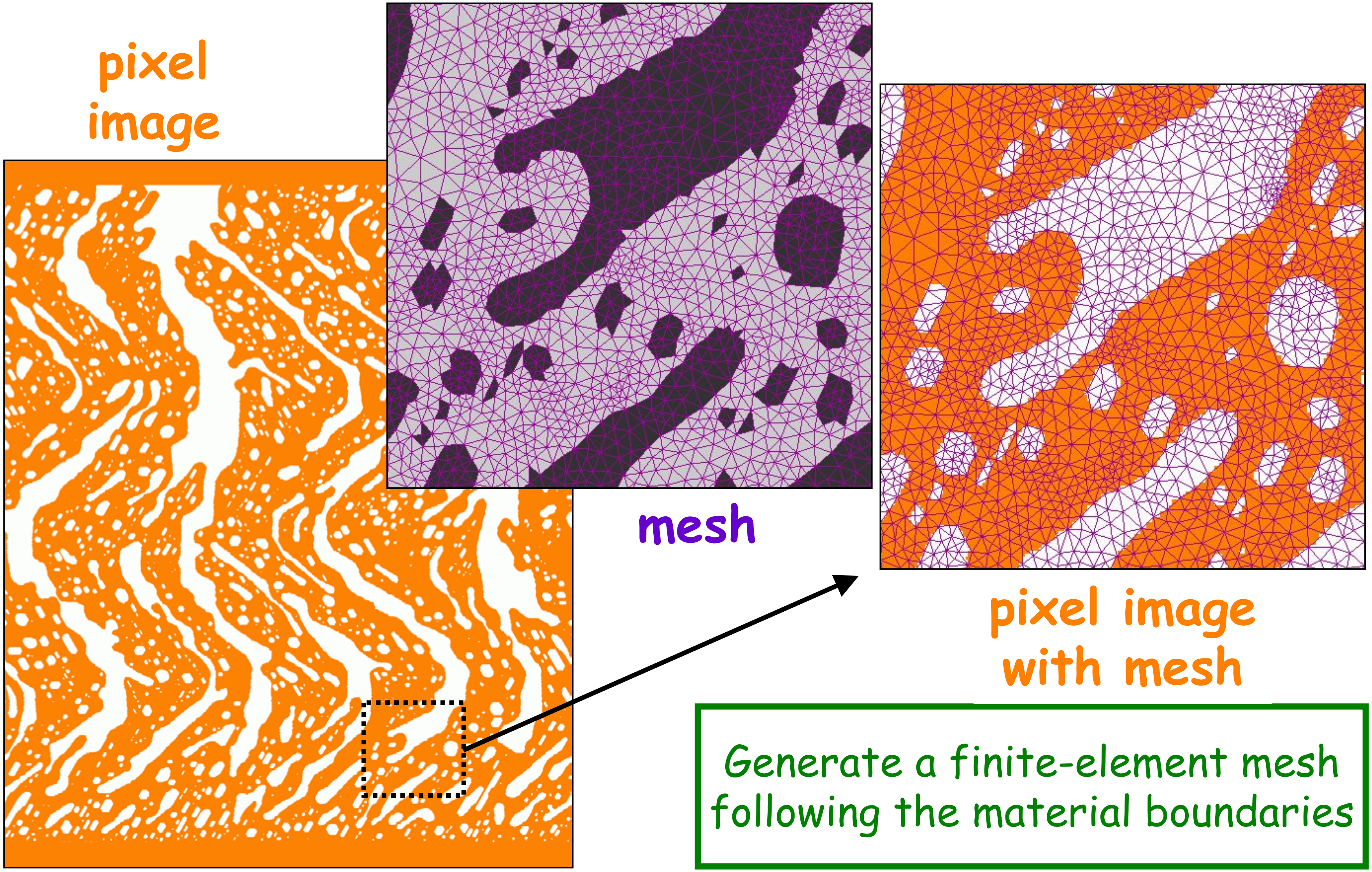


swap worst
to reduce E



anneal to
reduce E

Adaptive Meshing by Components

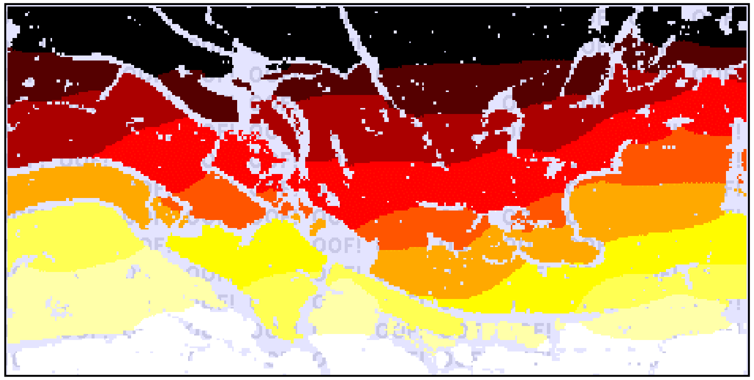


Generate a finite-element mesh following the material boundaries

OOF Tool

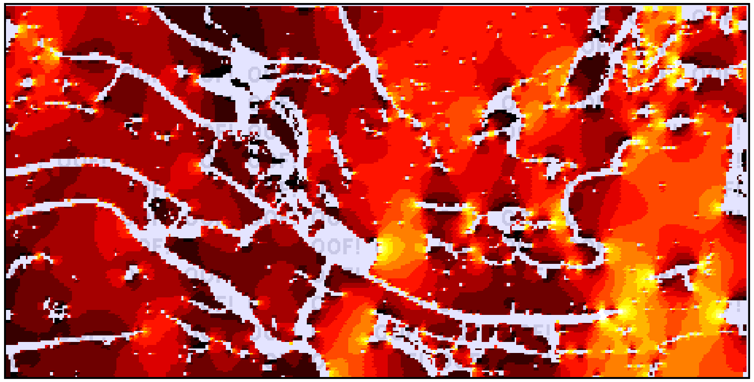
Virtual Experiments:
Temperature Gradient

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

OOF 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.: $\nabla \cdot \Psi = f$	Constitutive Eq.: $\Psi = \sum c \cdot \nabla \phi$

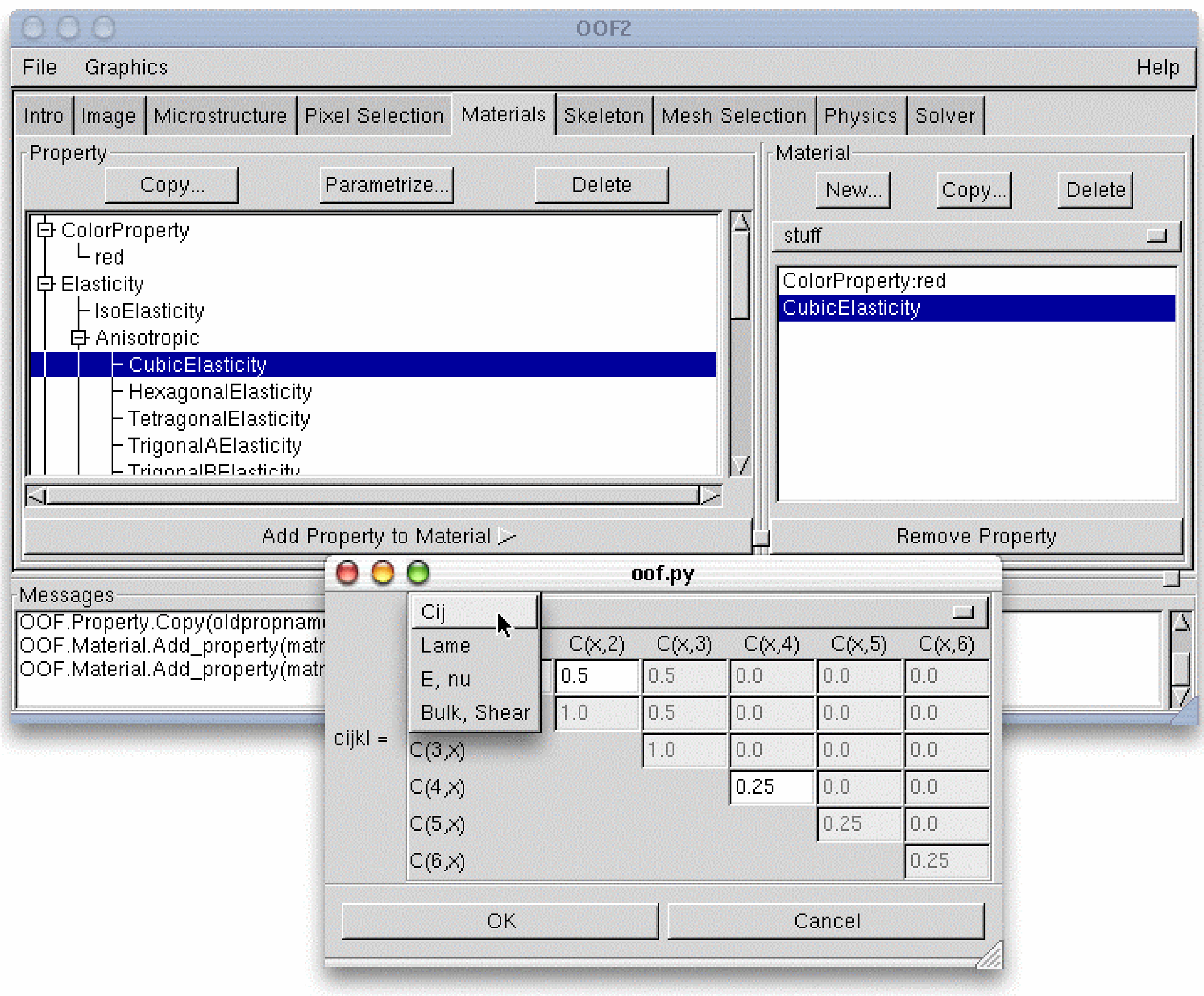
- Linear and nonlinear solvers

  with automatic mesh refinement

Planned Additions

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

OOF2 Materials Menu



OOF.Property.Copy(oldpropnam
OOF.Material.Add_property(matr
OOF.Material.Add_property(matr

	C(x,2)	C(x,3)	C(x,4)	C(x,5)	C(x,6)
	0.5	0.5	0.0	0.0	0.0
	1.0	0.5	0.0	0.0	0.0
C(3,x)		1.0	0.0	0.0	0.0
C(4,x)			0.25	0.0	0.0
C(5,x)				0.25	0.0
C(6,x)					0.25

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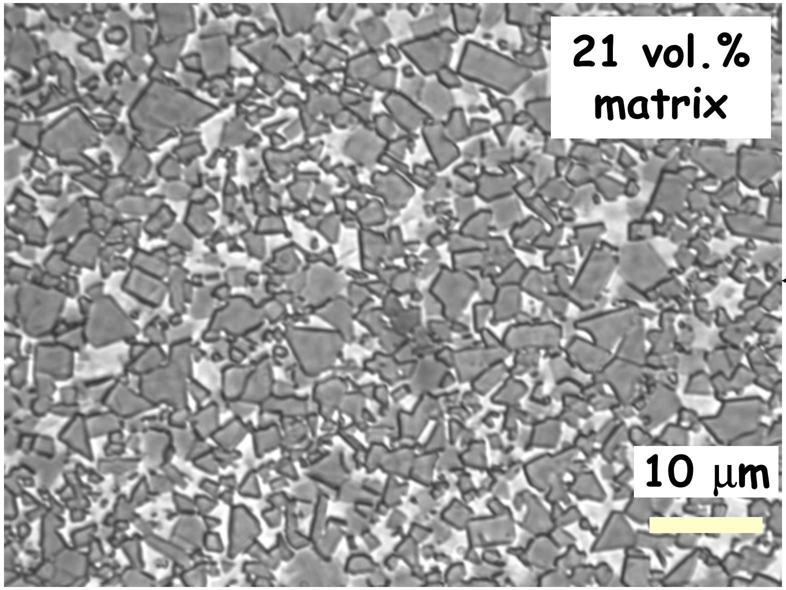
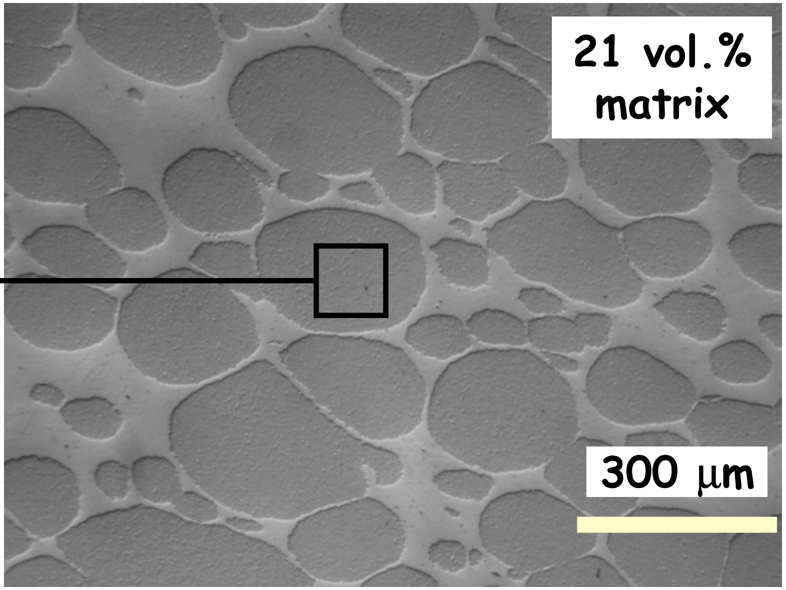
Elastic Modulus and CTE of Double Cemented Carbides



conventionally cemented
carbide microstructure

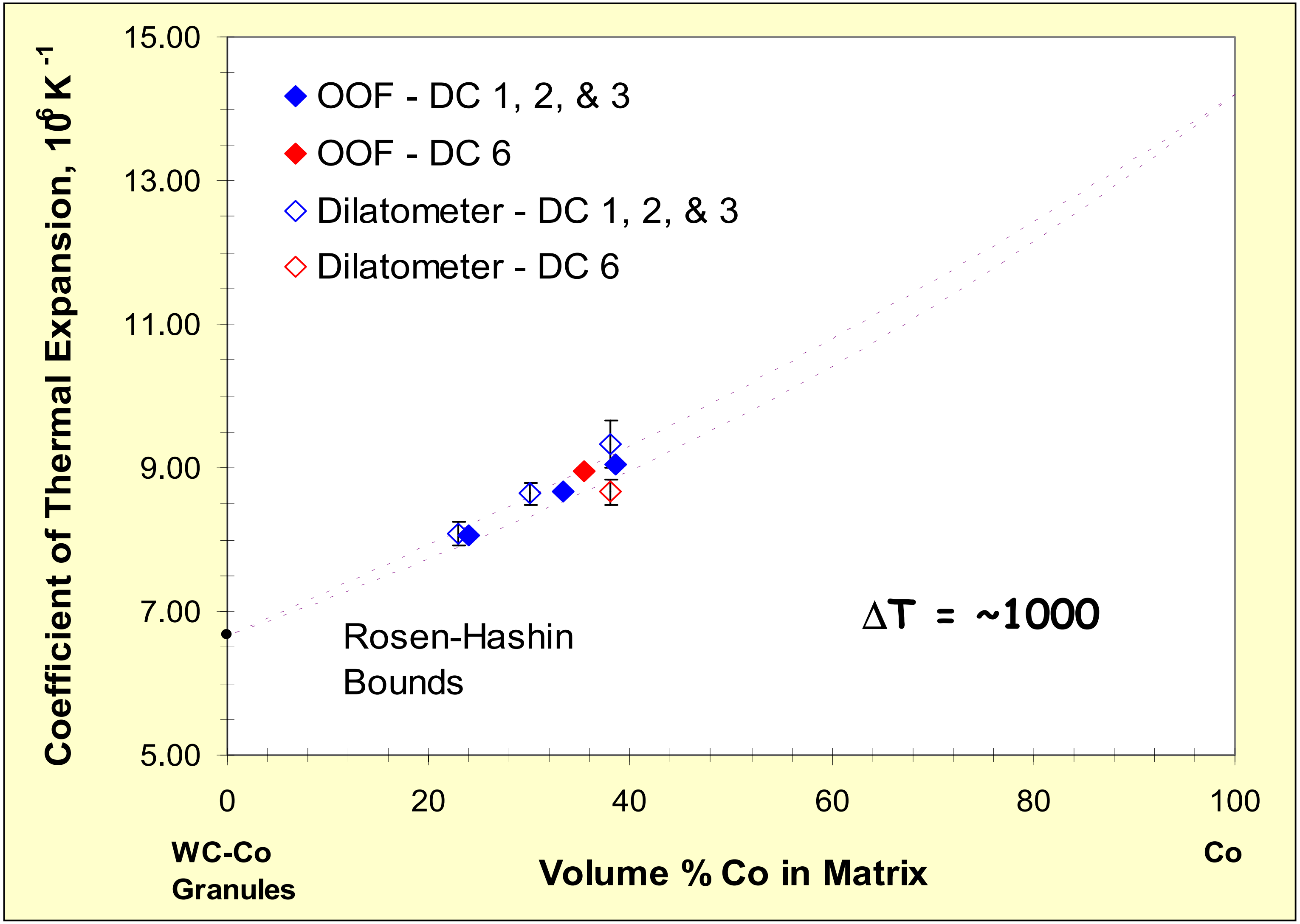


double cemented
carbide microstructure

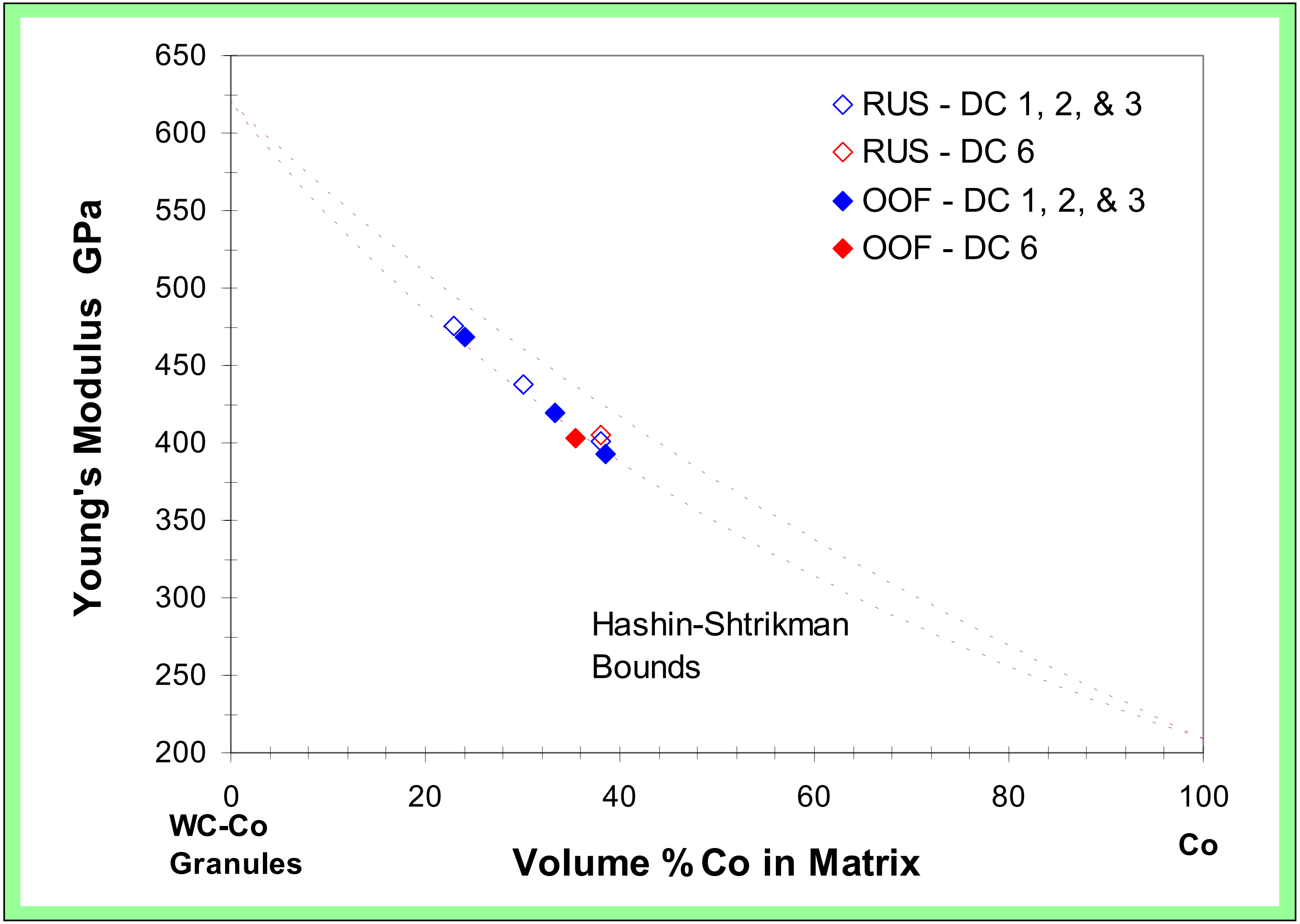
Motivation: Accelerated development of advanced material microstructures for drilling applications (Smith International, Houston)

B. V. Patel, K. K. Chawla, M. Koopman, X. Deng, B. R. Patterson
Univ. of Alabama at Birmingham

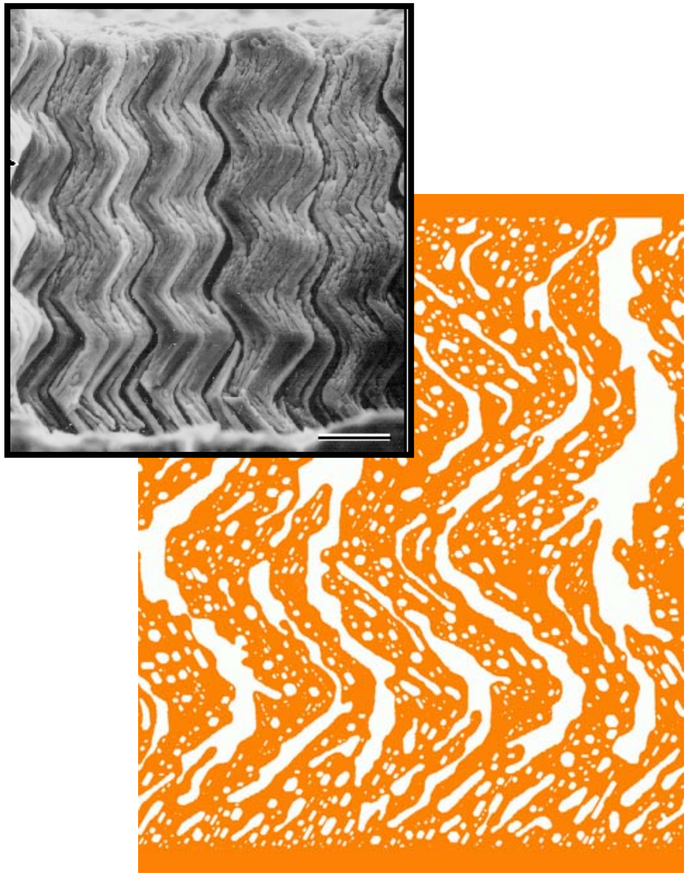
Coefficient of Thermal Expansion (CTE) Dilatometer & OOF



Elastic Modulus
Resonance Ultrasound Spectroscopy & OOF



Optimization of Low Conductivity EB-DVD Microstructures



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

- ☐ **Deposition at**

  $T/T_m = 0.23$

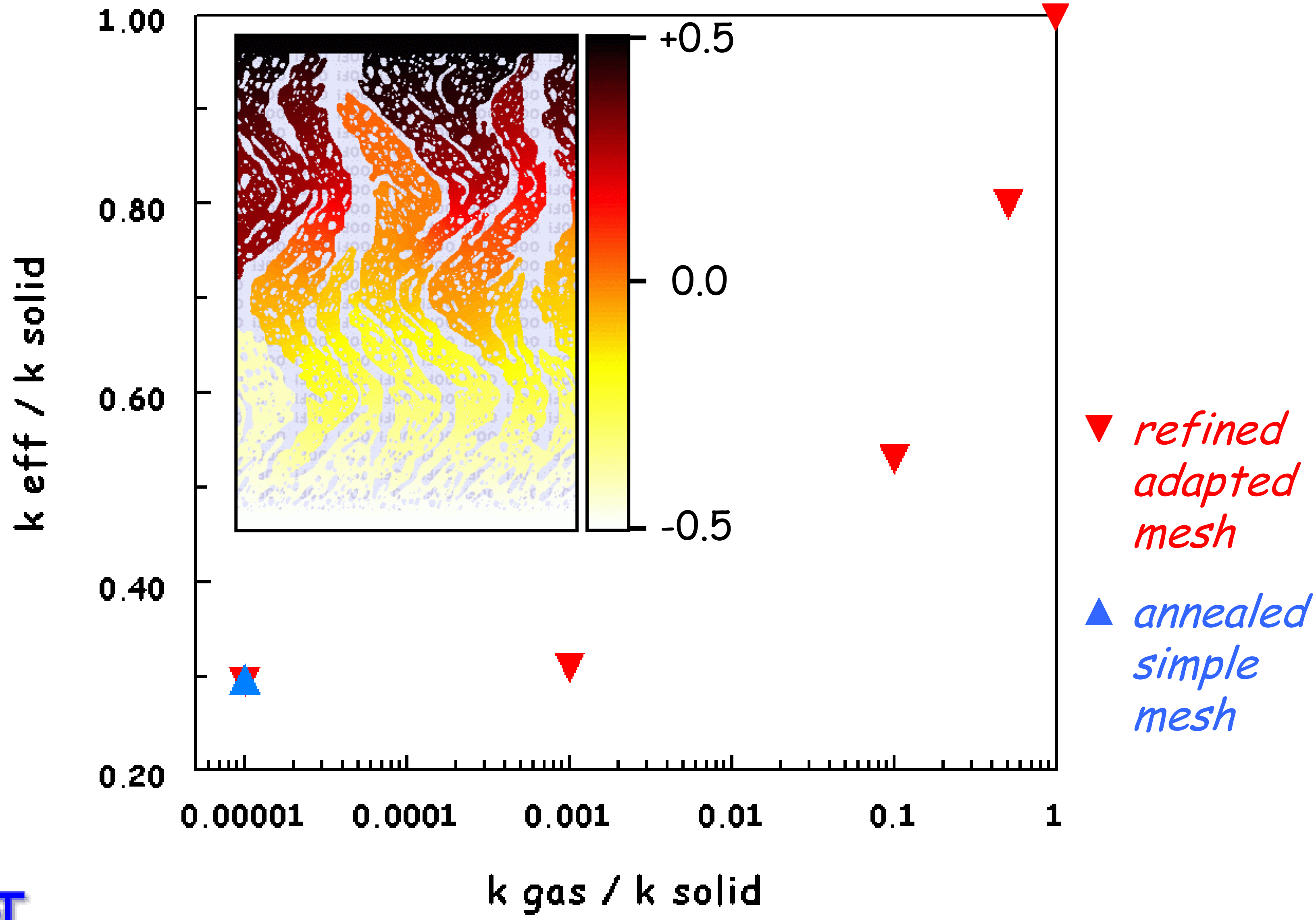
- ☐ **Annealed at**

  $T/T_m = 0.43$

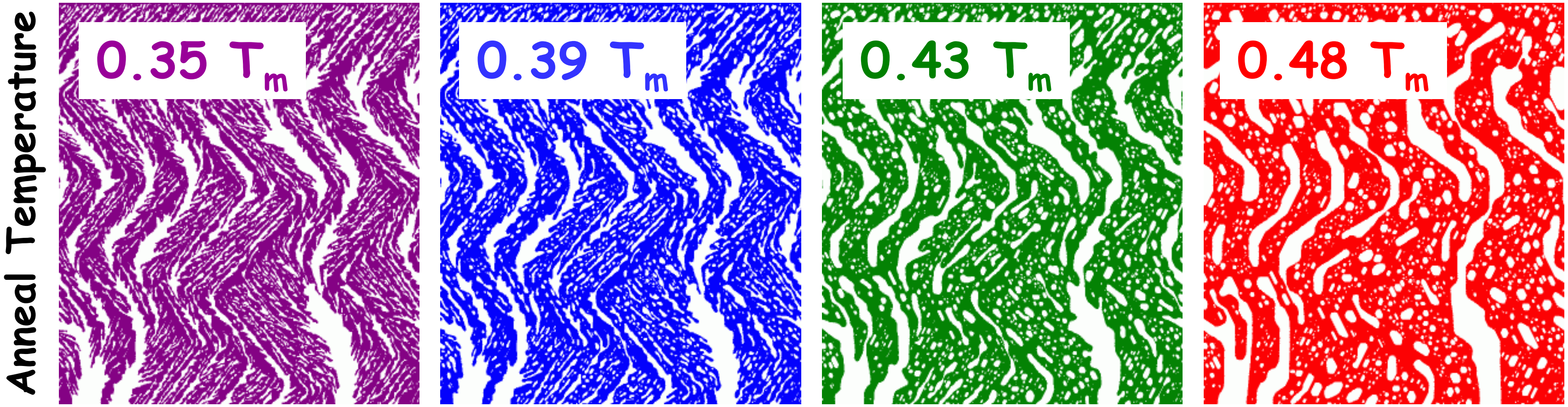
substrate was periodically inclined to the vapor flux

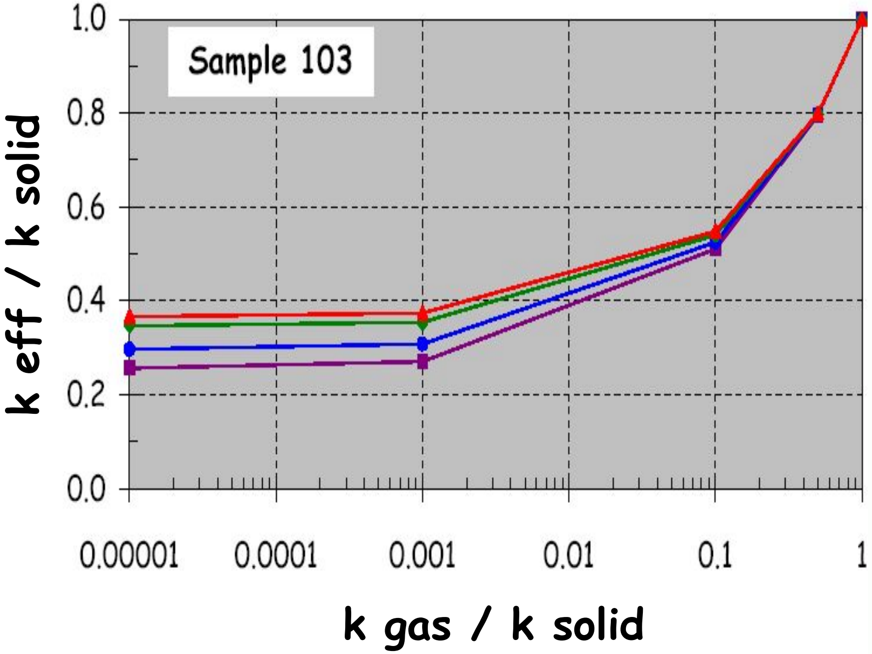
Yougen Yang, Derek D. Hass, & Haydn N. G. Wadley, Univ. of Virginia

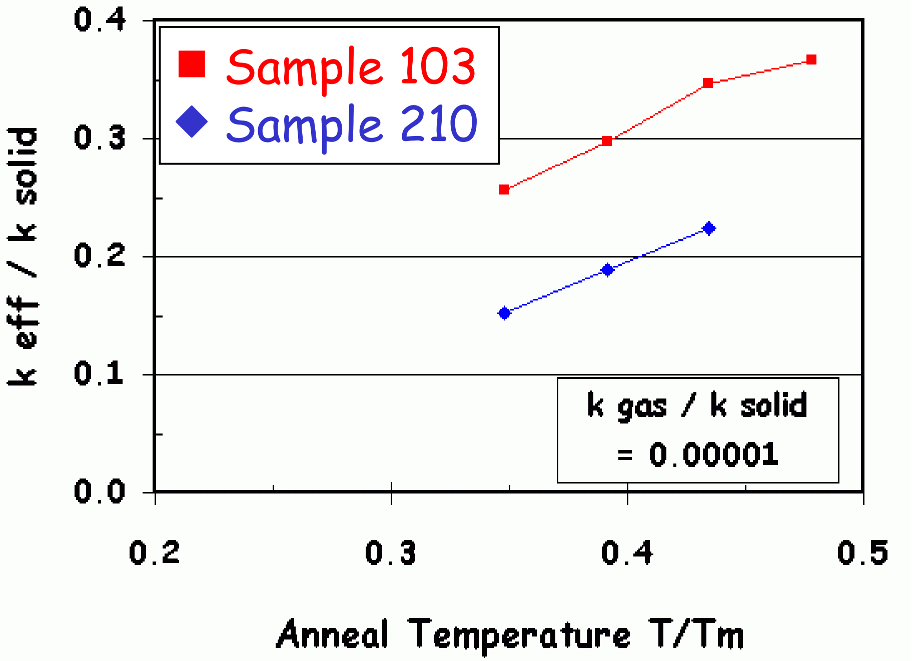
Effective Thermal Conductivity



Thermal Conductivity Simulations







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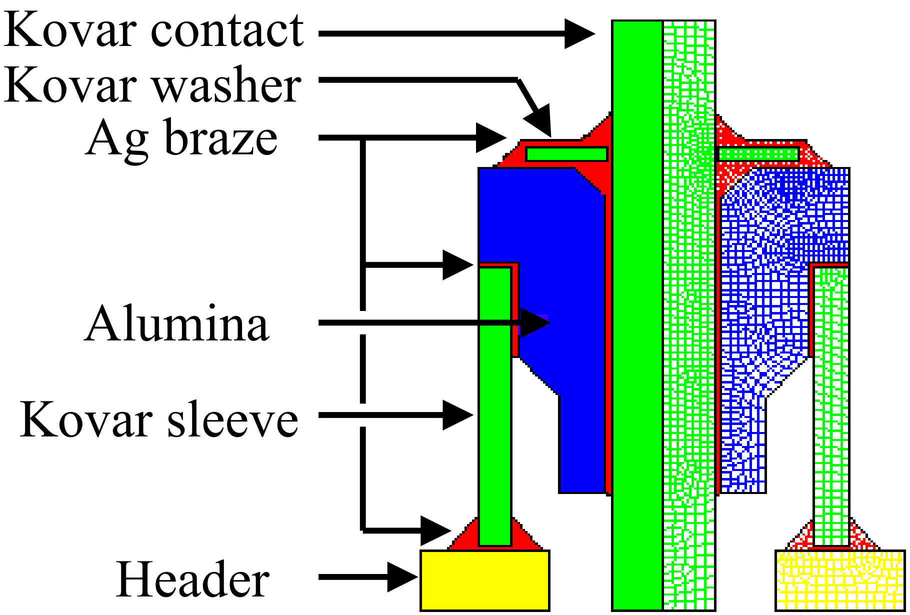
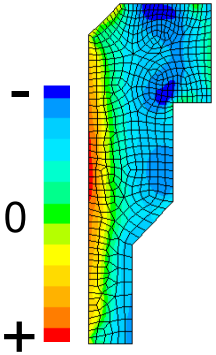
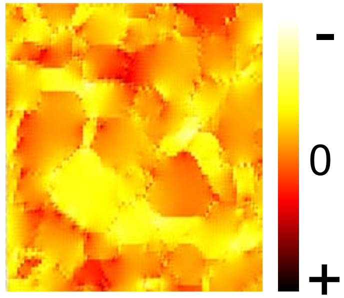
Residual Stress Distributions



Residual Stresses:

- Due to CTE-mismatch
- Due to CTE-anisotropy



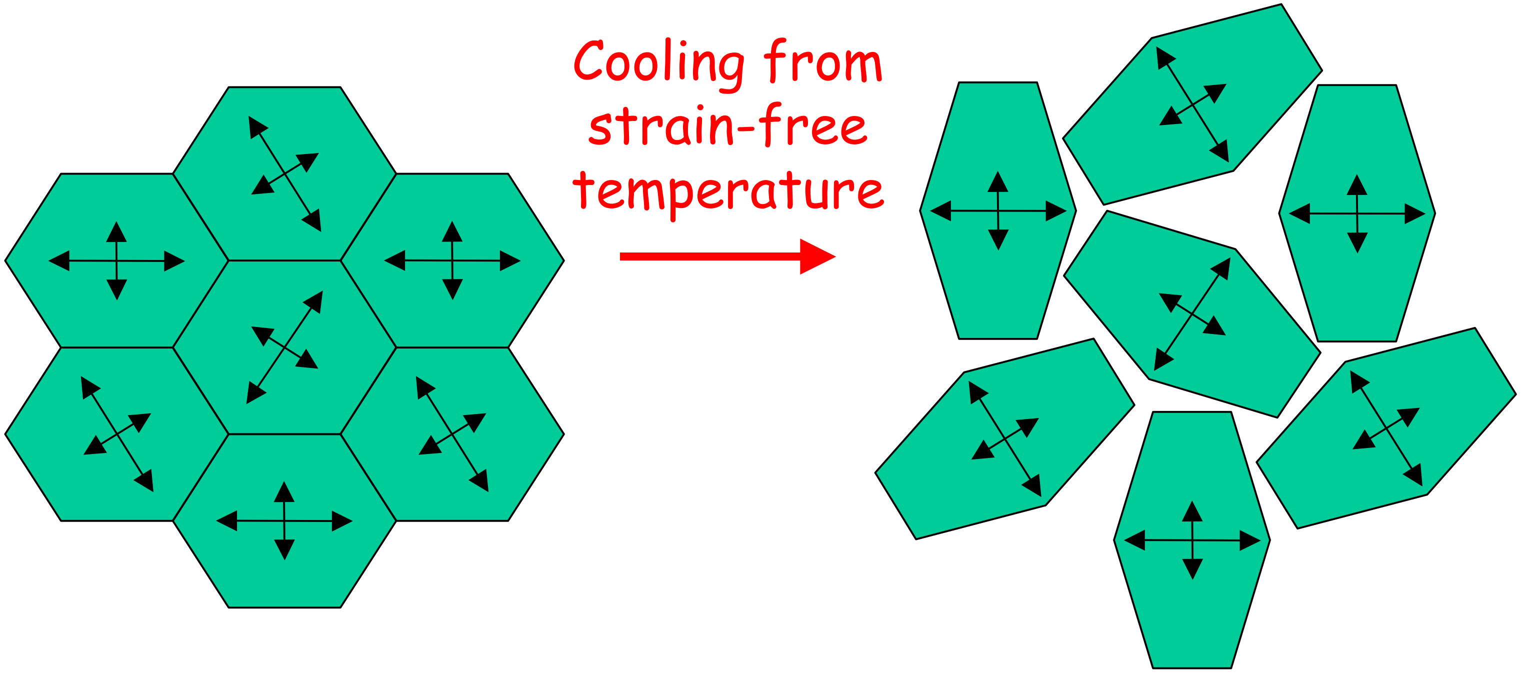


Motivation: Reliability of Ceramic-Containing Components

(*residual stresses can cause spontaneous microcracking and influence R-curve behavior & crack propagation under applied loads*)

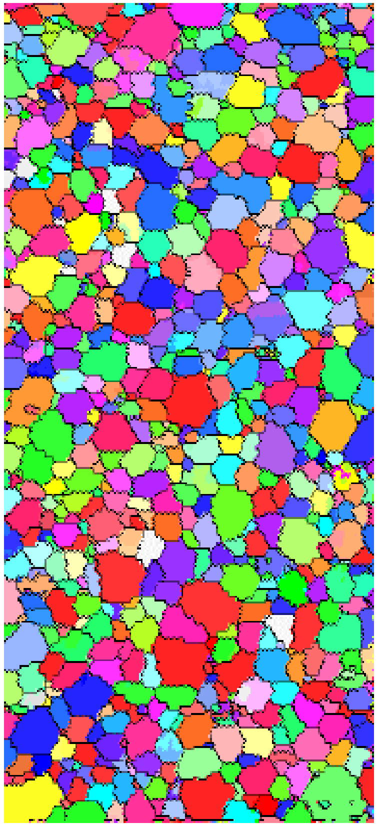
Venkata R. Vedula, Shekhar Kamat & S. Jill Glass, Sandia National Laboratories

Origin of Microstructural Stresses: Thermal Expansion Anisotropy Misfit Strains

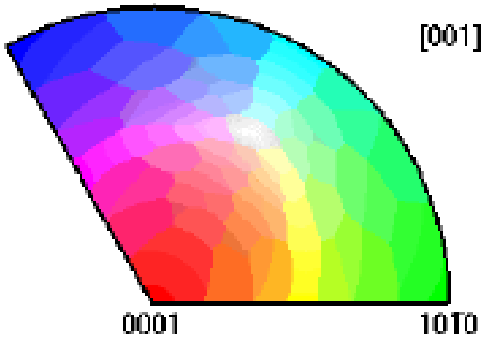


‹ Microstresses are independent of grain size ›

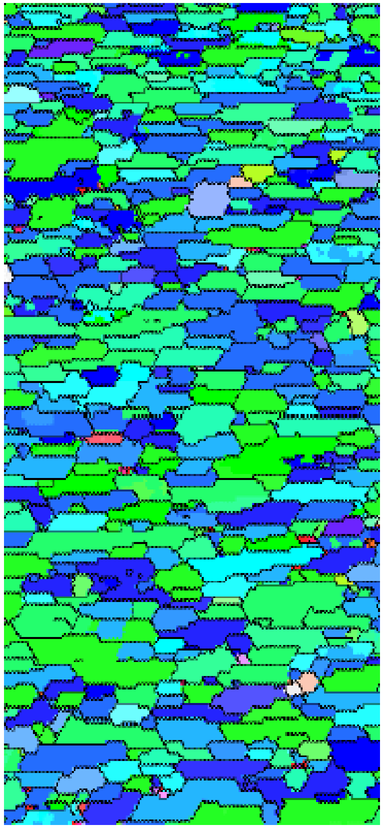
Alumina Microstructure via *OIM*



Untextured
(MRD=2)



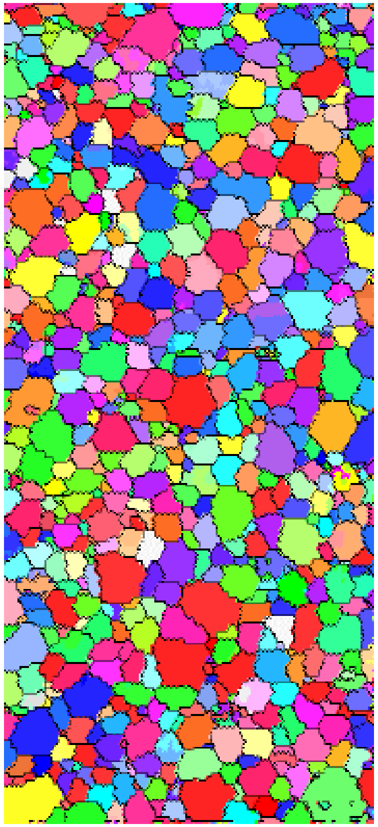
Grain Normals



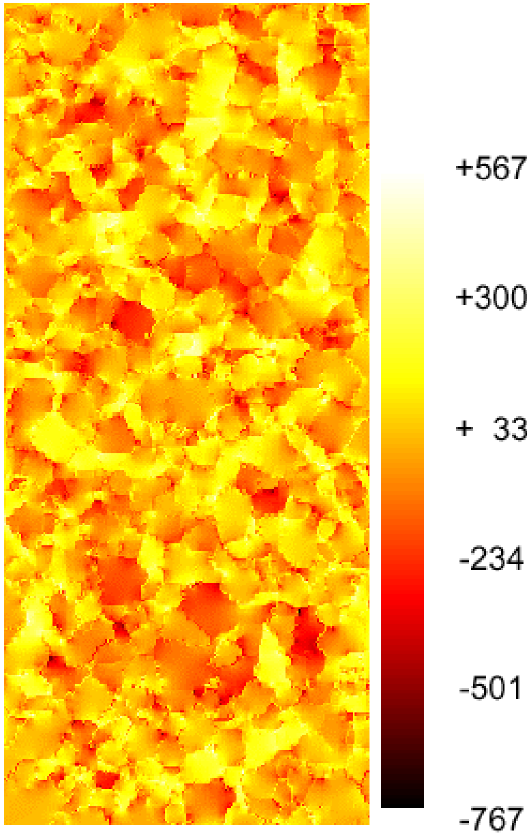
Textured
(MRD=90)

V.R. Vedula, S.J. Glass, D.M. Saylor, G.S. Rohrer, W.C. Carter, S.A. Langer, and E.R. Fuller, Jr., J. Am. Ceram. Soc., **84** [12], 2947-2954 (2001).

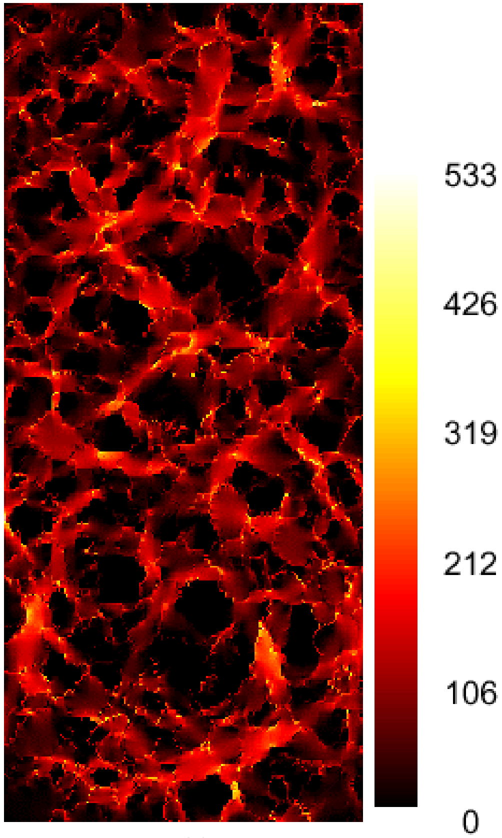
Residual Stress Distribution in Untextured Alumina (ΔT = -1500°C)



OIM microstructure



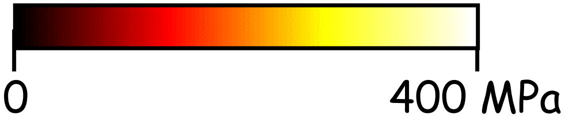
$[\ \sigma_{xx} + \sigma_{yy}\ ]$ (MPa)

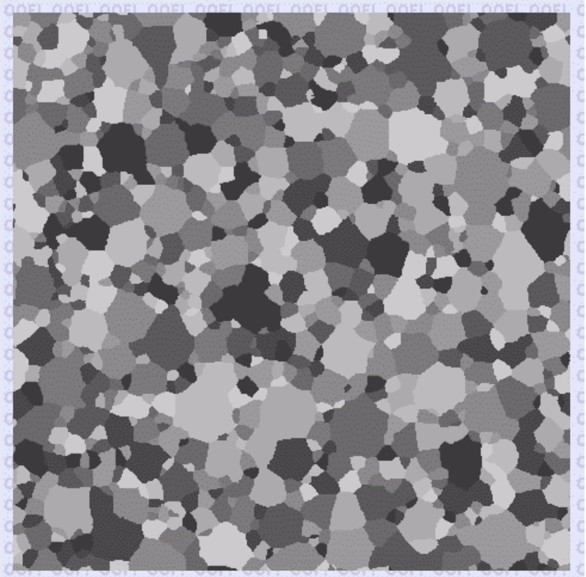


Max. Principal Stress (MPa)

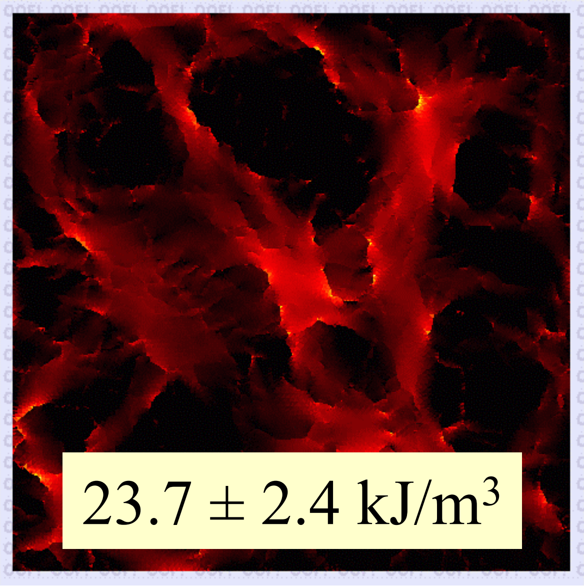
Influence of Grain Misorientation Distribution Function

maximum principal stress for a random grain orientation distribution function



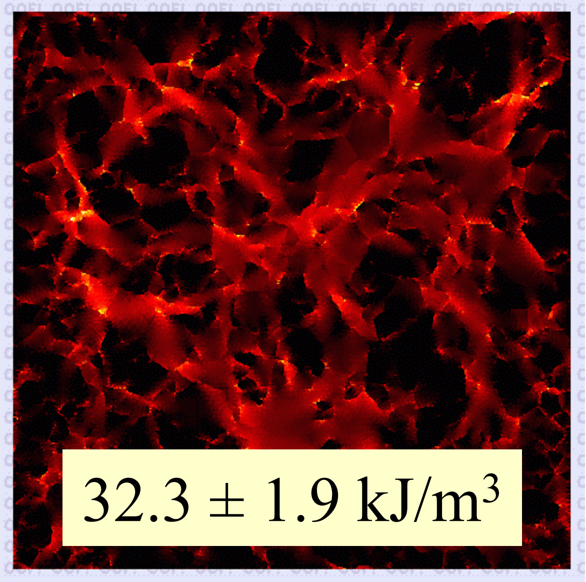


low-angle GB's

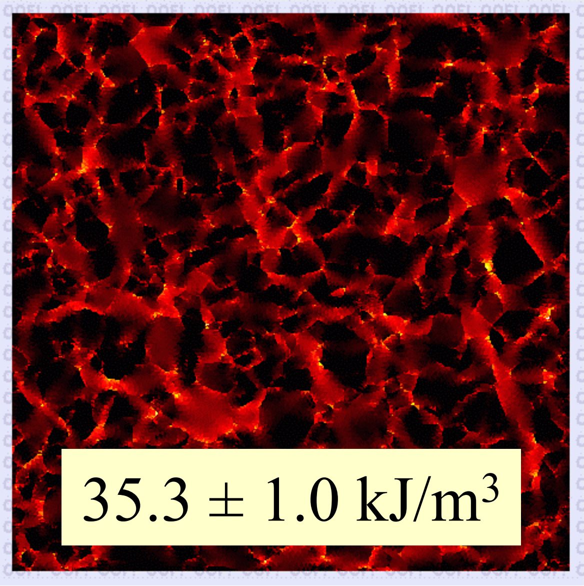


23.7 ± 2.4 kJ/m^3

uniform



32.3 ± 1.9 kJ/m^3



35.3 ± 1.0 kJ/m^3

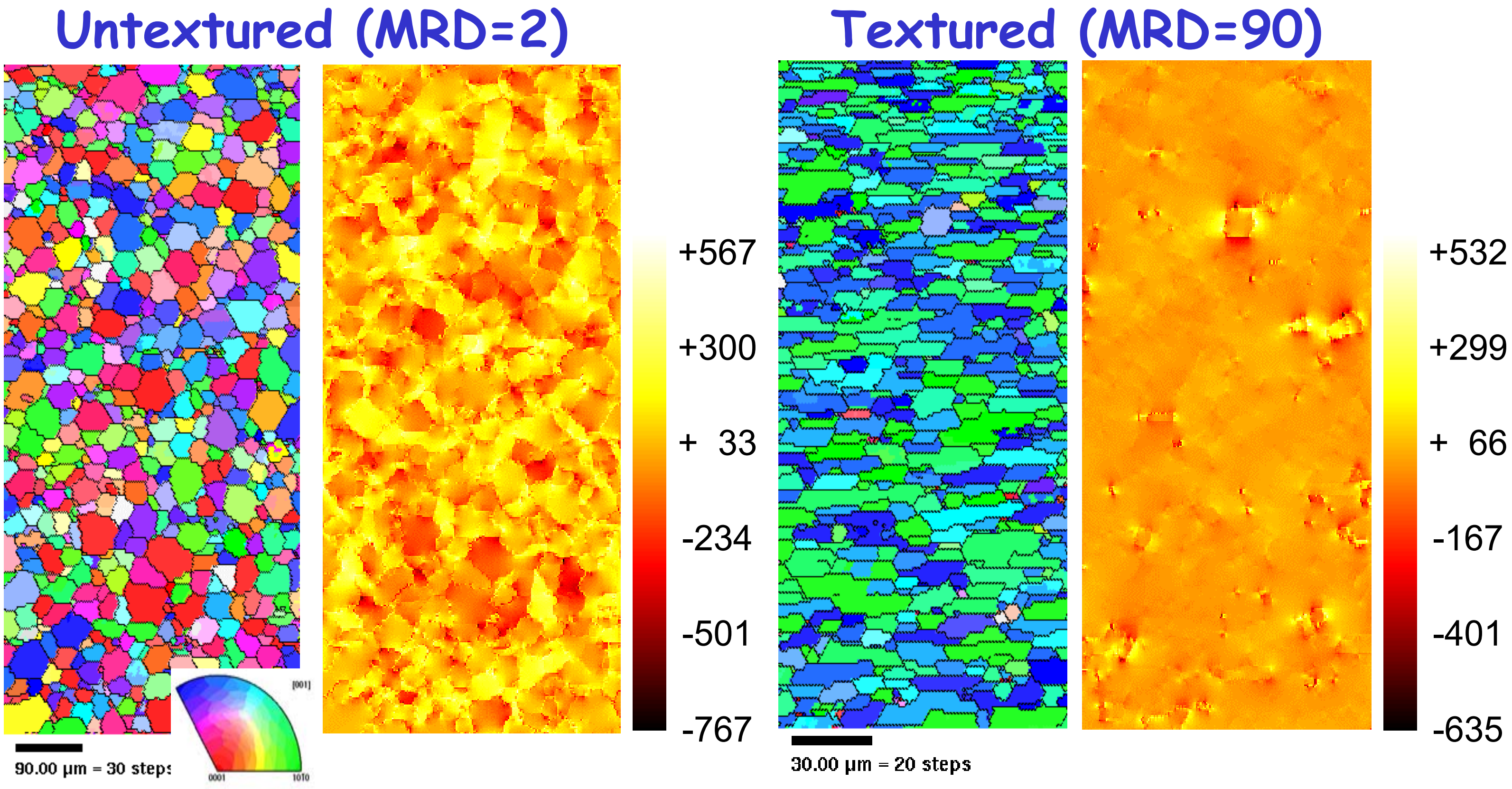
high-angle GB's

David M. Saylor, NIST & Thomas Weiß, Universität Göttingen,

NIST
National Institute of Standards and Technology

Materials Science & Engineering Laboratory

Residual Stresses in Alumina



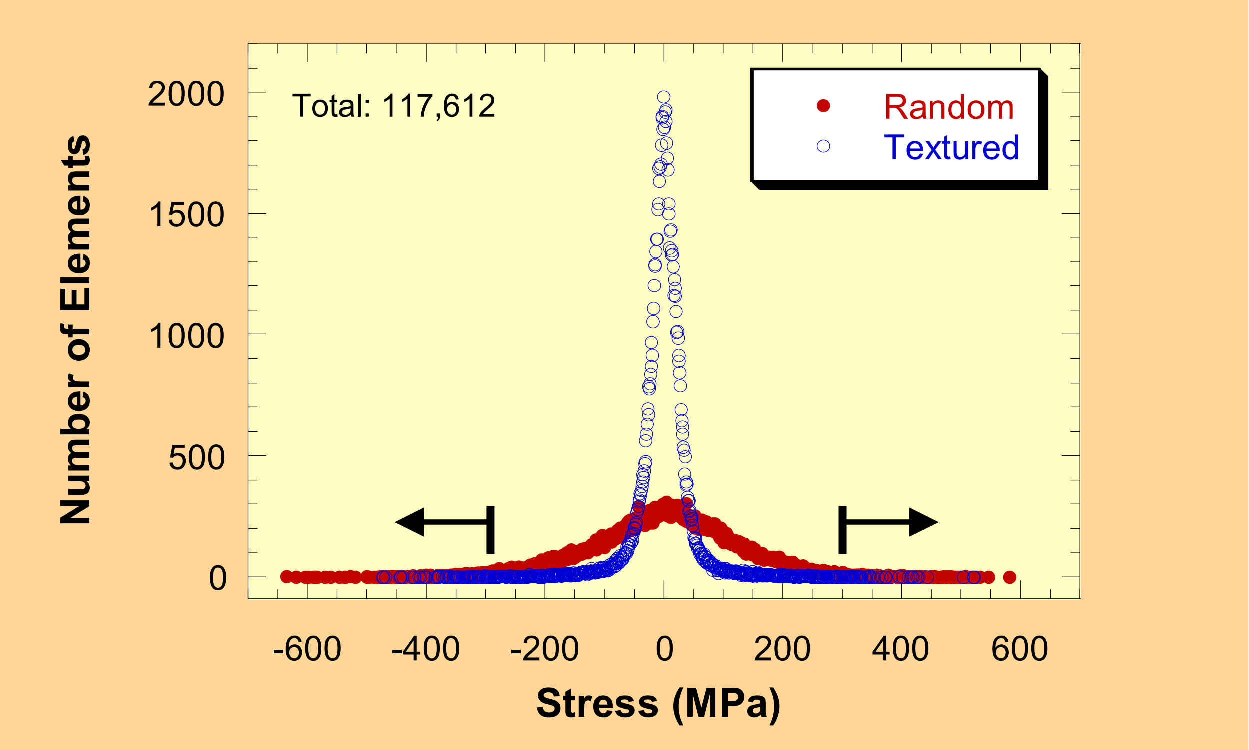
Untextured (MRD=2)

Textured (MRD=90)

Stress Invariant ($\sigma_{11} + \sigma_{22}$) for ΔT = -1500 °C

plane stress with free boundary conditions
total number of elements = 117,612

Residual Stress Distributions

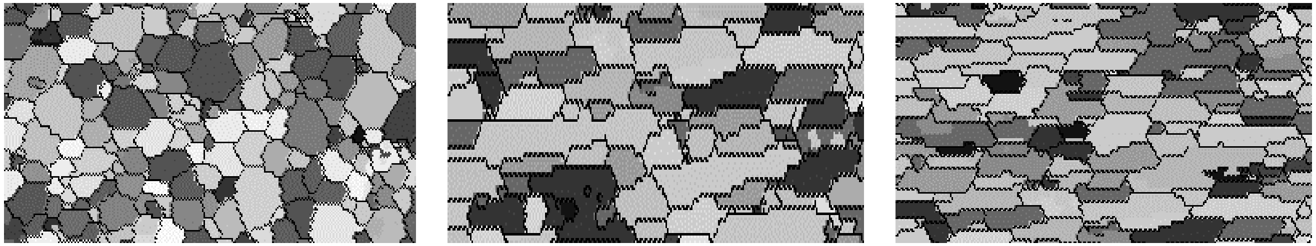


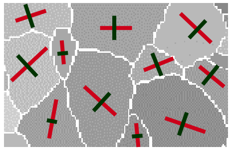
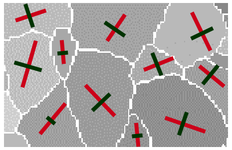
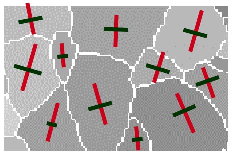
# of Elements with $|\sigma_{11}+\sigma_{22}|$ > 300 MPa

Random = 2563 (≅ 2.2%)

Textured = 221 (≅ 0.2%)

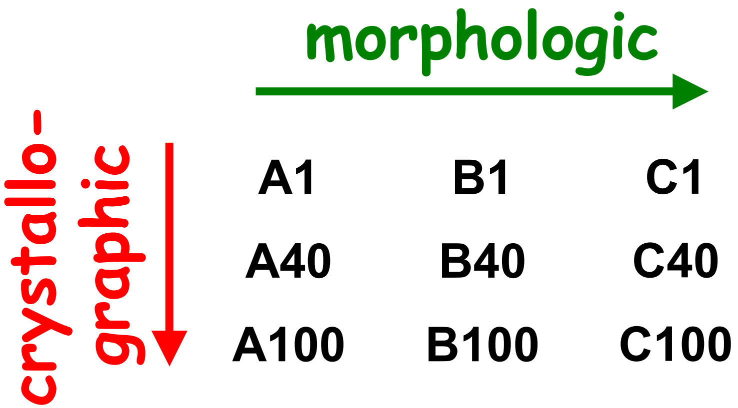
Morphologic versus Crystallographic Texture in Alumina



	Aspect Ratio:	1:1	4:1	8:1
	MRD:			
	1	A1	B1	C1
	40	A40	B40	C40
	100	A100	B100	C100

◯ Experimental Microstructures

Residual Stress Distributions



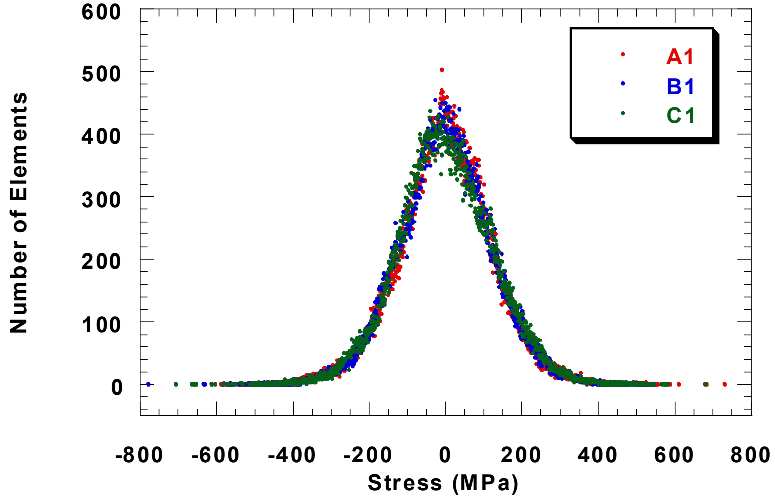
morphologic

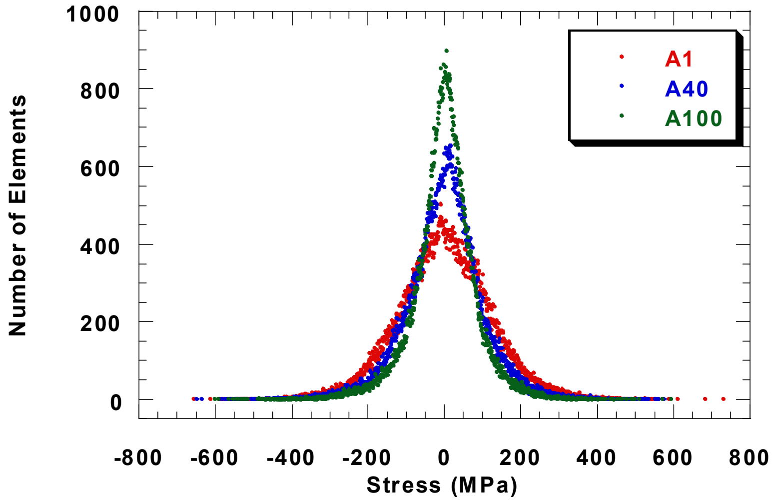
crystallo-graphic

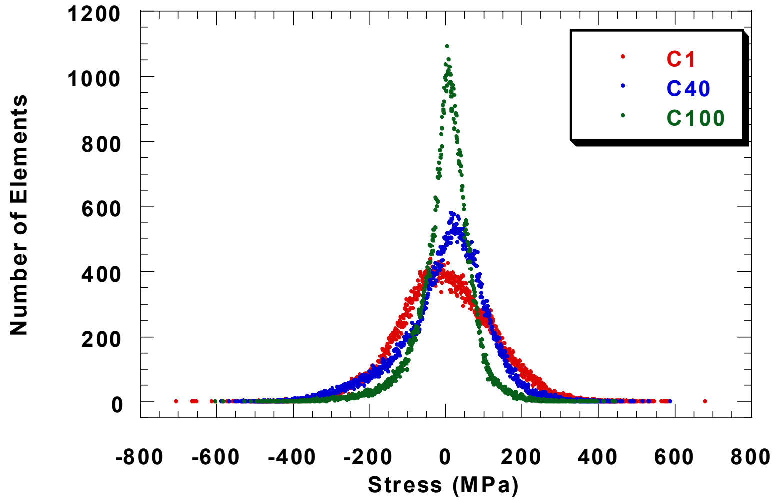
A1 B1 C1

A40 B40 C40

A100 B100 C100



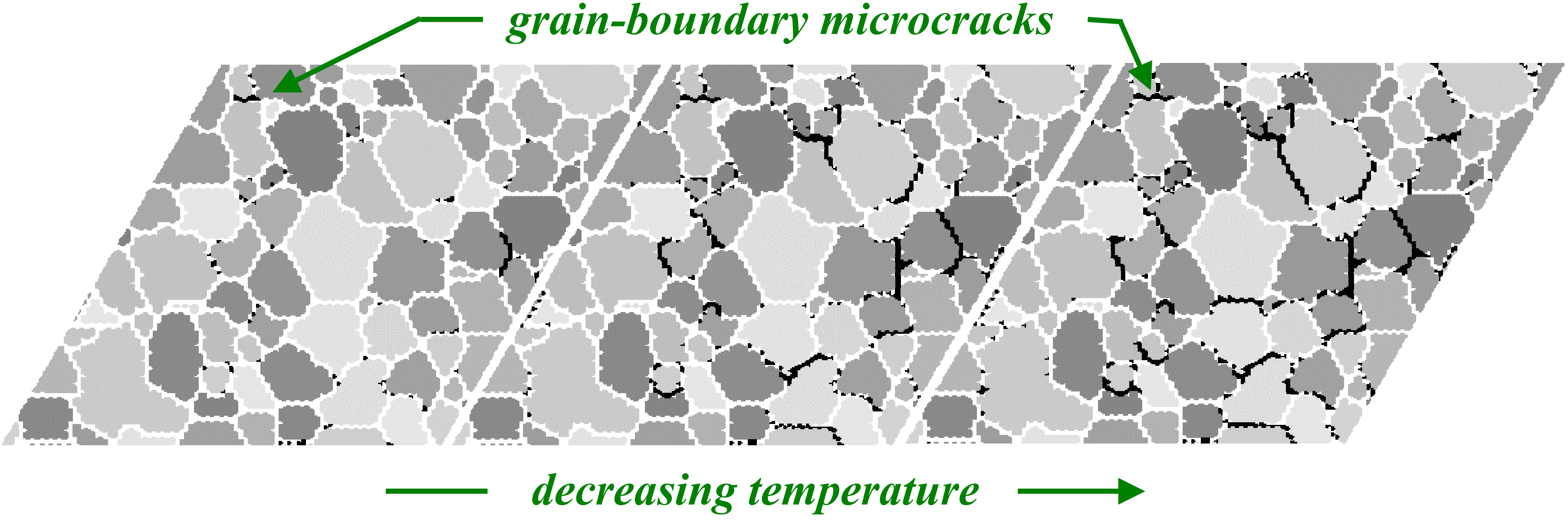




Nonlinear Simulations

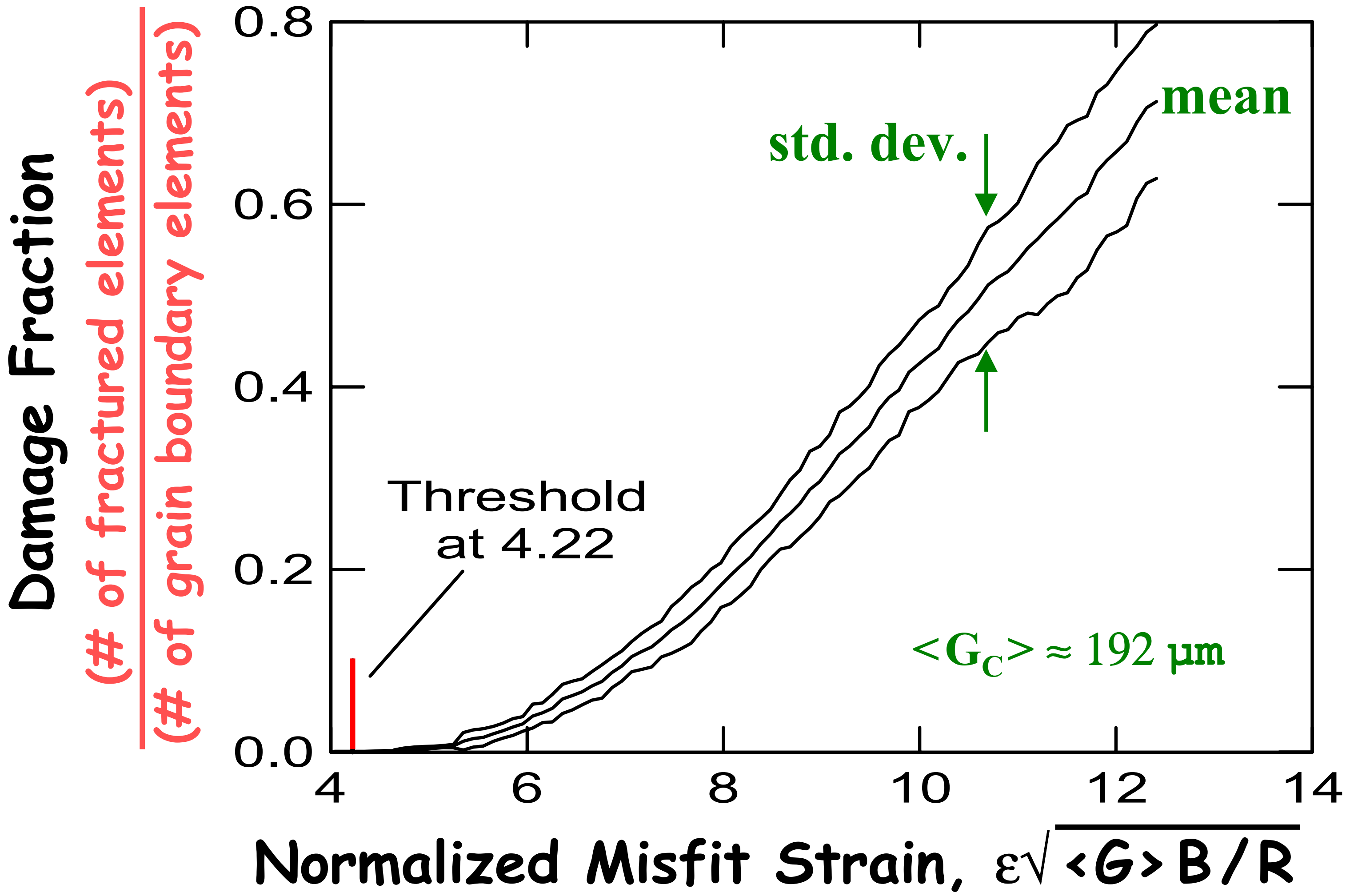
elucidate dependence of nonlinear processes in heterogeneous, stochastic microstructures on crystalline properties, morphology and texture

Microcrack Formation in Alumina

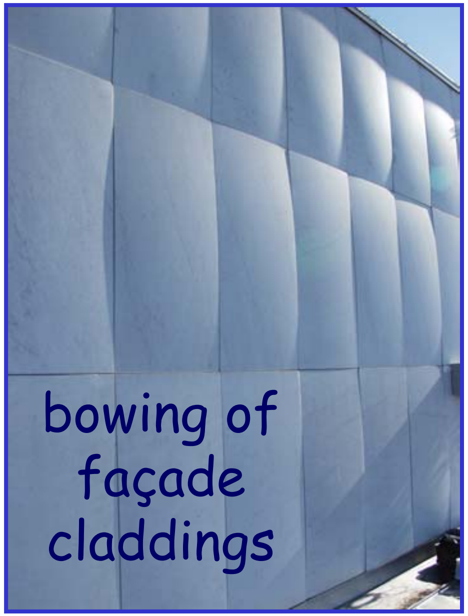


André Zimmermann, W. Craig Carter, and Edwin R. Fuller, Jr.,
Acta Materialia, **49** [1], 127-137 (2001).

Damage versus Misfit Strain

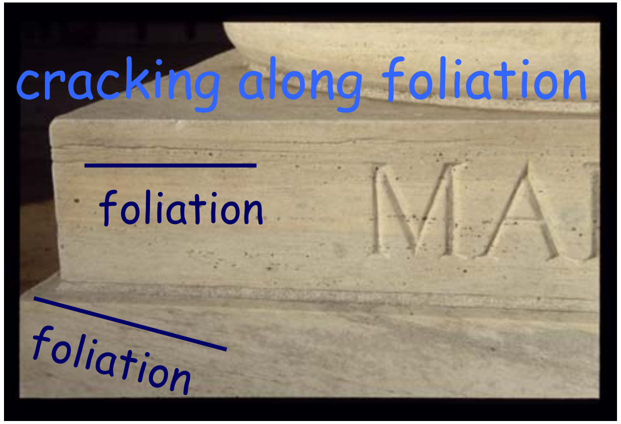


Thermal Degradation of Marbles

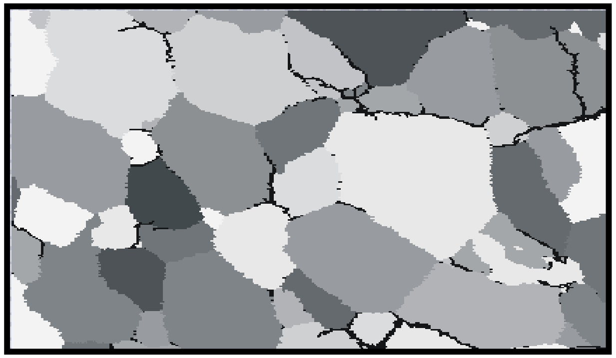


bowing of façade claddings

dolomite marble microstructure



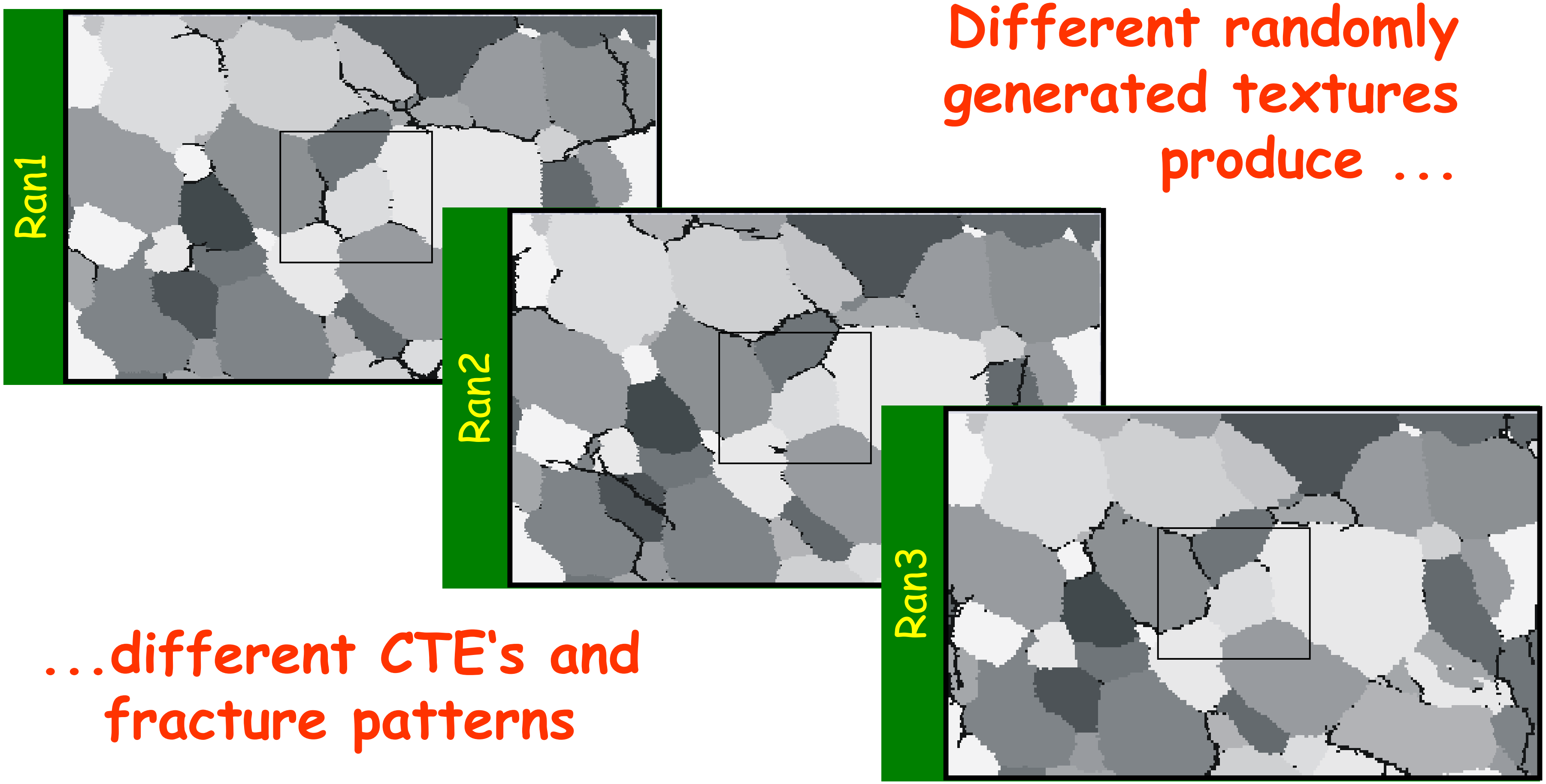
cracking along foliation



microcracking in calcite marble for ΔT = +100°C

Thomas Weiß and Siegfried Siegesmund, Universität Göttingen, Germany

Texture Effects

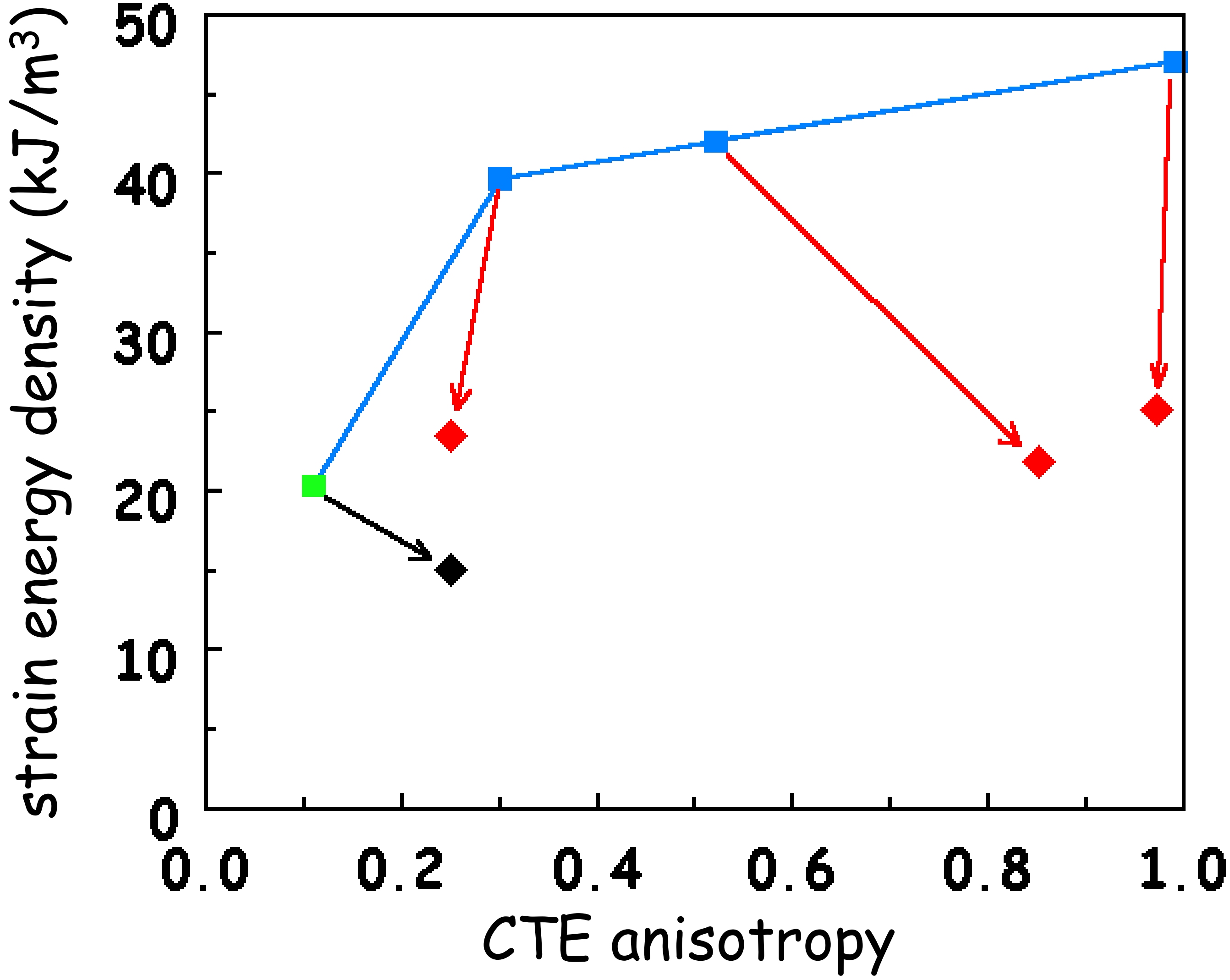


Different randomly generated textures produce ...

...different CTE's and fracture patterns

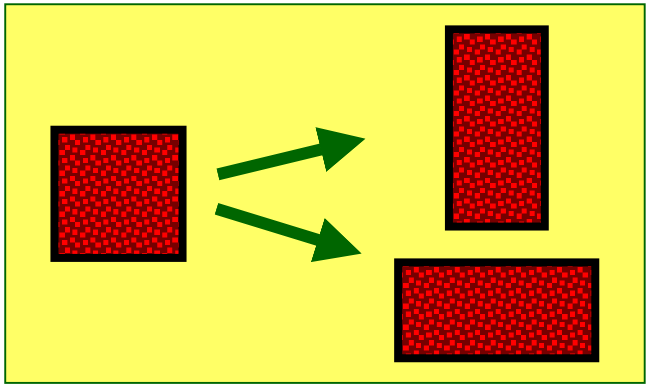
T. Weiss, S. Siegesmund, and E.R. Fuller, Jr., in "Natural Stone, Weathering Phenomena, Conservation Strategies and Case Studies," Geological Society London Special Publication, No. 205, edited by S. Siegesmund, A. Vollbrecht and T. Weiss, (The Geological Society of London, 2003). pp. 81-94.

Influence of texture & microcracking on strain energy density

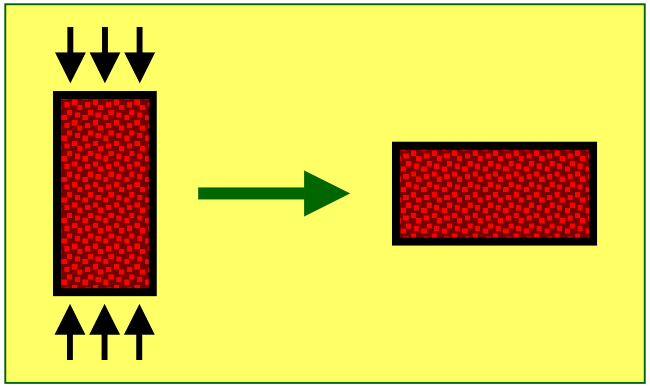


Definition of a Ferroelastic Crystal

"a crystal is said to be *ferroelastic* when it has two or more orientation states in the absence of mechanical stress and can be shifted from one to another of these states by mechanical stress"



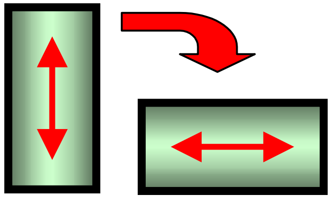
Cubic to Tetragonal Phase Transformation



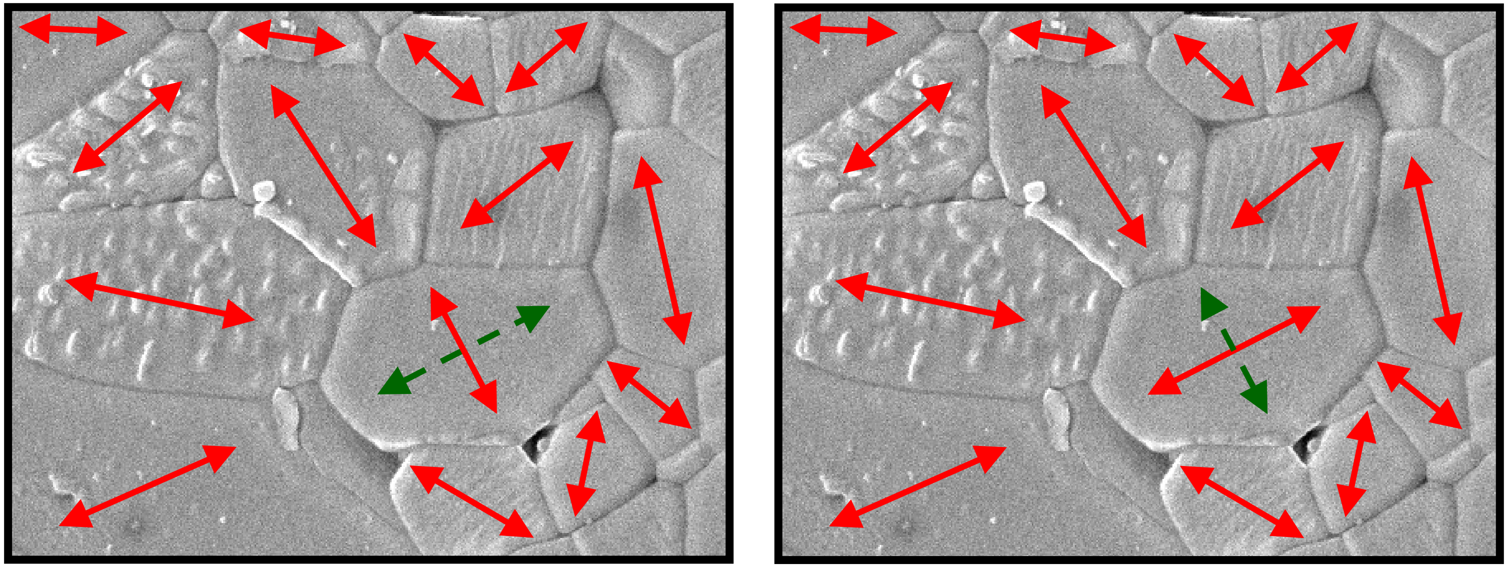
Mechanically-Induced Switching

Principles and Applications of Ferroelectrics and Related Materials, M. E. Lines and A. M. Glass (Clarendon Press, Oxford, 1977), p. 14.

90° Domain Switching in a Polycrystalline Ceramic



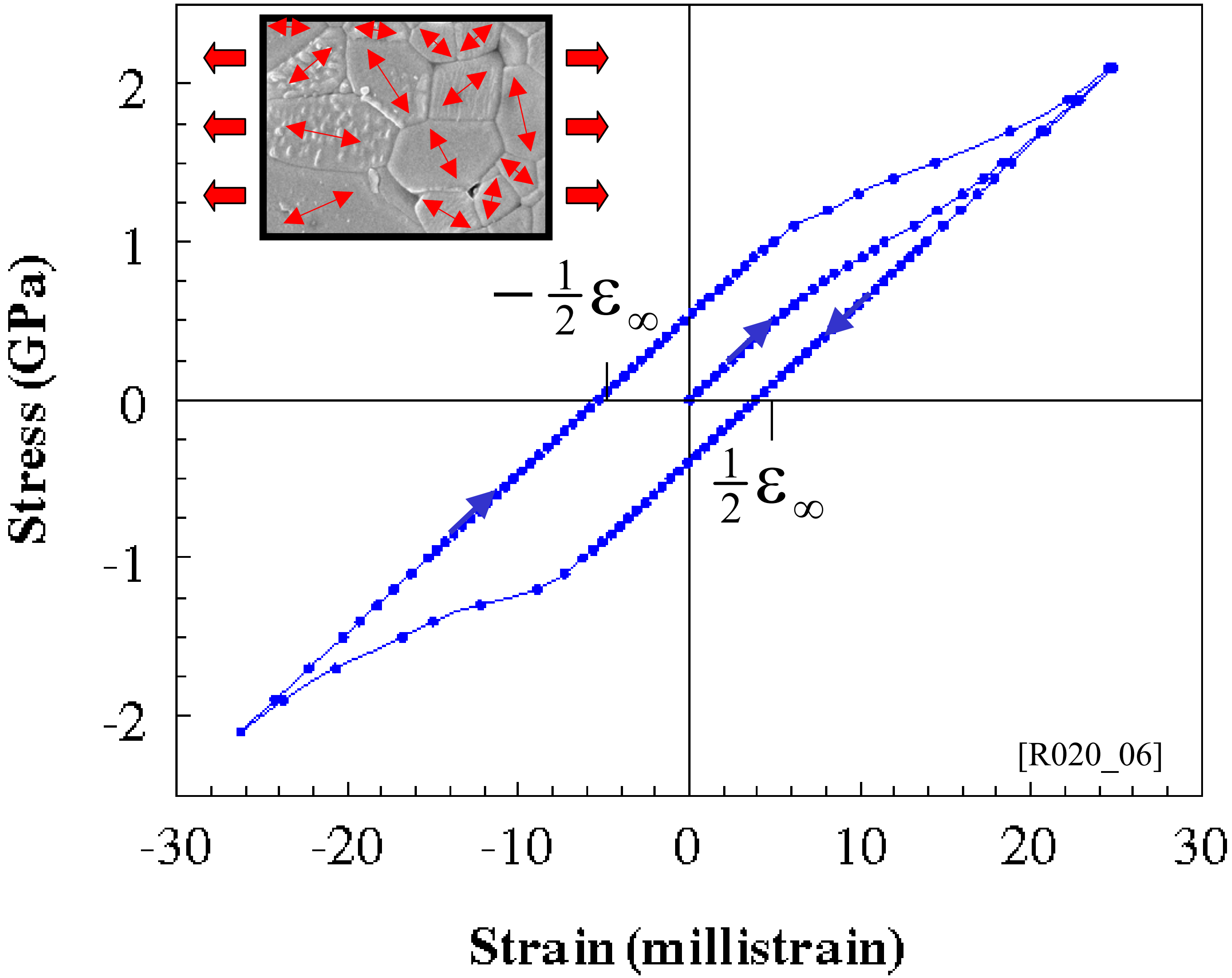
State 1 **State 2**



c-axis

Possible states for N domains:
3^N for 3-D and 2^N for 2-D

Macroscopic Stress-Strain Curve



Predicting Physical Properties From Microstructures

SUMMARY:

- A suite of object-oriented finite element (*OOF*) tools are being developed for simulating physical properties and nonlinear behavior of *heterogeneous, stochastic* microstructures
- Computer simulations of physical properties and nonlinear behavior provide a new paradigm for *empirical* materials research on complex materials
- These tools are being used to elucidate microstructural influences on CTE, elasticity, thermal conductivity, residual stresses, damage behavior, ferroelectric behavior, chemical diffusivity, etc. of complex systems

Abstract

Predicting Physical Properties From Microstructures

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Point-to-point knowledge of the physical and mechanical properties of multifunctional materials is crucial in the design and reliability of components using these materials. However, such property measurements generally are time consuming and require special expertise. Furthermore, many measurements are typically required to qualify new materials. Accordingly, the development cycle for new materials and processes has not kept pace with the component development cycle. Computational tools provide a stratagem for shortening the material and process development time. Such a computational tool, called OOF, is being developed at NIST. OOF, which stands for Object Oriented Finite element analysis, is a computational tool that allows material scientists to simulate physical properties of complex microstructures from an image of that microstructure. Examples will be presented of applications of OOF to elucidate influences of stochastic microstructural features, such as, porosity and microcracks, on thermal and mechanical behavior, of thermal expansion anisotropies on residual-stress distributions and microcrack-damage evolution, and of ferroelastic transitions on domain switching behavior.