Predicting Physical Properties From Microstructures

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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

- Bimodal Si₃N₄
- ZrO₂
- NiO
- Fe₂TiO₅

Air-Plasma-Sprayed Thermal Barrier Coating
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

Materials Science & Engineering Laboratory
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.

Virtual Test

δT

Visualize and Quantify

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

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

- 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

\[ E = (1-\alpha)E_{\text{shape}} + \alpha E_{\text{homogeneity}} \]

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

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

\[ a_i = \text{fractional area of pixel type } i \]

\[ N = \text{number of pixel types} \]

\[ E_{\text{hom.}} > 0 \]

\[ E_{\text{hom.}} = 0 \]
Adaptive Meshing by Components: refine elements and move nodes via Monte Carlo annealing to reduce $E = (1-\alpha)E_{\text{shape}} + \alpha E_{\text{homogeneity}}$
Adaptive Meshing by Components

Generate a finite-element mesh following the material boundaries.
OOF Tool

Virtual Experiments:
Temperature Gradient

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

To $+\delta T$

To $-\delta T$
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
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Elastic Modulus and CTE of Double Cemented Carbides

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

Coefficient of Thermal Expansion, $10^{-6} \text{K}^{-1}$

- OOF - DC 1, 2, & 3
- OOF - DC 6
- Dilatometer - DC 1, 2, & 3
- Dilatometer - DC 6

$\Delta T = \sim 1000$

Rosen-Hashin Bounds
Elastic Modulus
Resonance Ultrasound Spectroscopy & OOF

![Graph showing the relationship between Young's Modulus (GPa) and Volume % Co in Matrix. The graph includes data points for RUS - DC 1, 2, & 3, RUS - DC 6, OOF - DC 1, 2, & 3, and OOF - DC 6. The Hashin-Shtrikman Bounds are also indicated on the graph.](image-url)
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

$k_{eff} / k_{solid}$ vs $k_{gas} / k_{solid}$

- ▼ refined adapted mesh
- ▲ annealed simple mesh
Thermal Conductivity Simulations

Anneal Temperature

0.35 Tm
0.39 Tm
0.43 Tm
0.48 Tm

$k_{\text{gas}} / k_{\text{solid}}$

$k_{\text{eff}} / k_{\text{solid}}$

Anneal Temperature, $T / T_m$

Sample 103
Sample 210

$k_{\text{gas}} / k_{\text{solid}} = 0.00001$
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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

Cooling from strain-free temperature

< Microstresses are independent of grain size >
Alumina Microstructure via OIM

Untextured (MRD=2)

Textured (MRD=90)

Grain Normals

Residual Stress Distribution in Untextured Alumina ($\Delta T = -1500^\circ C$)

- 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

32.3 ± 1.9 kJ/m³

23.7 ± 2.4 kJ/m³

high-angle GB's

35.3 ± 1.0 kJ/m³

David M. Saylor, NIST & Thomas Weiß, Universität Göttingen,
Residual Stresses in Alumina

Untextured (MRD=2)

Textured (MRD=90)

Stress Invariant \((\sigma_{11} + \sigma_{22})\) for \(\Delta T = -1500 \degree C\)

plane stress with free boundary conditions

total number of elements = 117,612
Residual Stress Distributions

Total: 117,612

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

Random = 2563 ($\approx 2.2\%$)

Textured = 221 ($\approx 0.2\%$)
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

A1  B1  C1
A40  B40  C40
A100  B100  C100

crystallographic → morphologic

Stress (MPa)
Nonlinear Simulations

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

Microcrack Formation in Alumina

grain-boundary microcracks

decreasing temperature

Damage versus Misfit Strain

Normalized Misfit Strain, $\varepsilon \sqrt{\langle G \rangle} B/R$

Damage Fraction
(# of fractured elements)

Threshold at 4.22

$\langle G_c \rangle \approx 192 \, \mu m$

mean

std. dev.

(\# of grain boundary elements)
Thermal Degradation of Marbles

Thomas Weiß and Siegfried Siegesmund, Universität Göttingen, Germany
Texture Effects

Different randomly generated textures produce ...

...different CTE's and fracture patterns

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

90° Domain Switching in a Polycrystalline Ceramic

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

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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.