Generating Synthetic Microstructures w/ DREAM.3D: An Overview Tutorial

Collaborators:
Mike Jackson, Sean Donegan, Somnath Ghosh, Anthony Rollett, Joe Tucker, Marc DeGraef, Patrick Callahan

Dr. Michael A. Groeber
Materials Research Scientist
AFRL/RXCM
• Introduction/Background
  • Goal/Need from Data Flow Perspective
  • What are Synthetic Builders
  • Brief History of Methods and Tools Used

• Synthetic Building Tools in DREAM.3D
  • DREAM.3D’s Synthetic Building Philosophy
  • Statistical Descriptions of “Features”
  • Obtaining Statistics
  • An Example of the Packing Process
  • Highlighting the Current Spectrum of Possibilities

• DREAM.3D – FFT Interaction
  • Simulating Thermal Responses in Thermal Barrier Coatings
  • Other Simulation Packages

• Final Comments
  • Thoughts on Needs for Future
Intro: Goal / Need

Need a path to get to explicit structures from statistics/microstructure attributes

Benefits/Uses:
1) Microstructure Design  
2) Scatter Due to Local Arrangements  
3) Compression
Intro: *What Are Synthetic Microstructure Builders?*

Computational tools capable of creating digital microstructure representations

- Spatial Tessellation Tools
- Physics-based Growth Models
- Geometric Packing Tools
Intro: Brief History of Methods and Tools Used

Spatial Tessellation Tools

**Benefits**
- Directly determined
- Minimal inputs

**Drawbacks**
- Generally ‘non-physical’ planar boundaries
- Inputs not easily tied to goal microstructure statistics
- Size distributions and neighborhood variations limited/biased

Voronoi, Coster 2005

Voronoi, Gibson 2007
**Intro: Brief History of Methods and Tools Used**

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Intro: Brief History of Methods and Tools Used

Physics-based Growth Models

**Benefits**
- ‘Realistic’ curved boundaries
- More ‘tunable’ inputs
- ‘Better’ size distributions and neighborhood variations
- Very complex structures possible

**Drawbacks**
- More computationally involved
- Require material parameters or assumptions

JMAK Model, Coster 2005
Potts Model, Esche 2009
UMatic, Lee 2010
Intro: *Brief History of Methods and Tools Used*

**Geometric Packing Tools**

**Benefits**
- Multiple bases
- Statistics/Empirically guided
- Variable complexity

**Drawbacks**
- More computationally involved
- Possible ‘non-physical’ boundaries
- Dependent on statistics/geometric basis selected
1. Use Geometrical Objects to Represent “Features”
- Eliminates need for “physical” inputs like nucleation rate & interface/boundary mobility
- Statistics necessary become fairly straight-forward metrics feasibly measured at meso- to micro-scale with numerous experimental tools

2. Classify “Features” into “Phase Types”
- Genericizes building tools → makes material agnostic builders
- Sets “necessary statistics” describing “critical” aspects of specific “type” of “feature(s)”

3. Approach Builders as “Fast-Acting”, “Physics-ish” Models
- Exploit constraints of actual physical process to limit statistics & computational “effort”

4. Attempt to Limit Statistics to “Human-Intuitive” Metrics
- Creates limitations, biases and simplifications, but allows more user interaction
Synthetic Building in D3D: Statistical Descriptions

**Primary Phase**
Examples: Grains, Cells, Volume-filling domains
Stats: $V_f$, Size, Shape, Morph. ODF, # of Neighbors, ODF, MDF, GBCD (future)

**Precipitate Phase**
Examples: Non-OR Precipitates, Pores, Fibers, Carbides/Particles
Stats: $V_f$, Boundary Frac., Size, Shape, Morph. ODF, RDF, ODF, Non-Contiguous MDF (future)

**Matrix Phase**
Examples: Composite Matrix, Epoxy, Mean-Field Structure
Stats: $V_f$

**Transformation Phase**
Examples: Twins, $\alpha/\beta$ Colonies, $\gamma'$ Precipitates
Stats: $V_f$, OR, Parent Phase, Size, Shape, Morph. ODF

**Boundary Phase**
Examples: Fiber Coatings, Chemically-Rich/Depleted Layers
Stats: $V_f$, Thickness, Frac. Continuous, Relative Phase Preference

**Others**
Boundary-Transformation Phase (G.B. $\alpha$)
Discontinuous Matrix Phase (Free Si)
1. From Experimental Data
- Straight-forward for microstructures that are single-phase Primary or Matrix-Precipitate...if you have 3D data sets that have adequate resolution (WTM) & are large w.r.t. the “Features”
- Almost all other cases are much more difficult or lacking methods for obtaining them...measuring stats of “snapshots” of structures collected does not measure the “Features” being used in the synthetic process...effectively need analysis/processing tools to run “physics” in reverse.

2. Stats Generator / Other “Design” Tool
- Very easy to establish statistics → input anything you want
- Much more difficult to create “realistic” or even “possible” statistics
  · no sanity-check to statistics entered (within SG)
  · often statistics are not independent, but may not be intuitively linked
Grain Descriptions (Geometric Shapes)

Grains/Features defined by size, shape and orientation (morphological)
-Shape and orientation can be correlated to size
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Grain Descriptions (Geometric Shapes)

**Ellipsoids**
- Curved boundary
- No inherent # of neighbors
- Only aspect ratios needed

**Super-Ellipsoids**
- Curved+faceted boundaries
- 6, 8 or no inherent # of neighbors
- $\Omega_3$ linked to exponent, $n$

**Cube-Octahedra**
- Faceted boundaries
- 6, 8 or 14 neighbors
- $\Omega_3$ linked to clipping depth, $\gamma$

*Shape is difficult to describe and in the limit requires infinite details*
- Shape classes or bases allow for lower order descriptors to fully define shapes
Geometric features are placed and moved in a Monte Carlo fashion while attempting to optimize space filling and local feature arrangement (neighborhoods).

- During packing care must be taken to limit biases.
Similar to feature packing, orientation placement and rearrangement follows a Monte Carlo process while attempting to match both the ODF and MDF. GBCDs have only been matched for random structures with a coherent $\Sigma 3$ twin peak.
Synthetic Building in D3D: Current Possibilities

Equiaxed Grains

Rolled Grains

Precipitates
Synthetic Building in D3D: *Current Possibilities*

- Fiber Composites
- Carbides/Nano-particles/Porosity
- Bimodal Features/ALA Grains/MTRs
Synthetic Building in D3D: *Current Possibilities*

Far-Field HEDM  
(Data informed synthetic)

Polycrystalline Atomistics  
Structure
DREAM.3D – FFT Interaction: TBC Structure
DREAM.3D – FFT Interaction: TBC Structure

EB-PVD TBC

Top Coat

TGO

Bond Coat
DREAM.3D – FFT Interaction: TBC Structure
DREAM.3D – FFT Interaction: Synthetic TBCs

- TC
- TGO
- BC
- substrate
DREAM.3D – FFT Interaction: Synthetic TBCs

TGO: no texture

TGO: texture
DREAM.3D – FFT Interaction: Synthetic TBCs

phase maps

 localized Potts model
High resolution structures consisting of $315^3$ Fourier grids (~31 million Fourier points). Variation in top coat morphology, TGO texture, bond coat material, and interface roughness.
## DREAM.3D – FFT Interaction: Stress Analysis

<table>
<thead>
<tr>
<th>Interface Type</th>
<th>BC Material</th>
<th>TGO Texture</th>
<th>Maximum EED (kJ/m³)</th>
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<tr>
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<td>NiCoCrAlY</td>
<td>random</td>
<td>10113.101</td>
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<tr>
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</tbody>
</table>

Majority of EED contained in the TGO. Structures with rumpled interfaces display systematically larger peak stresses.
DREAM.3D – FFT Interaction: Hot Spot Correlation

contour map

z-smooth EED

POT
quantify hot spots
DREAM.3D – FFT Interaction: Hot Spot Correlation

columnar top coat, textured TGO, (Ni,Pt)Al bond coat

Hot spots at the BC/TGO interface generally lie in regions of low elevation (i.e., troughs)

splat top coat, textured TGO, (Ni,Pt)Al bond coat
Hot spots at the TGO/TC interface do not display a consistent trend with elevation, though the largest lie in regions of high elevation (i.e., ridges).
columnar top coat, textured TGO, (Ni,Pt)Al bond coat

splat top coat, textured TGO, (Ni,Pt)Al bond coat
DREAM.3D – FFT Interaction: Hot Spot Correlation

columnar top coat, textured TGO, (Ni,Pt)Al bond coat

splat top coat, textured TGO, (Ni,Pt)Al bond coat
Final Comments: Thoughts and Future Needs

**Thoughts**

- Synthetic structures are a powerful tool for obtaining many, many instances of a microstructure and may be critical in determining what aspects of the microstructure are important for a given property.
- Synthetic structures can also serve as “phantoms” for testing and understanding our workflows and analysis/processing tools.

**Future Needs**

- We need a lot of development in our tools with respect to transformation and boundary phases.
- We need a lot of work/thought on defining the appropriate “set” of attributes that define the “local state.”
- We could benefit from coupling the current tools with “real physics-based” tools for “healing” our best efforts.