SAND2017-2075C

Modeling the Effects of Texture on Process-Structure-Property Evolution in Additively Manufactured Metals

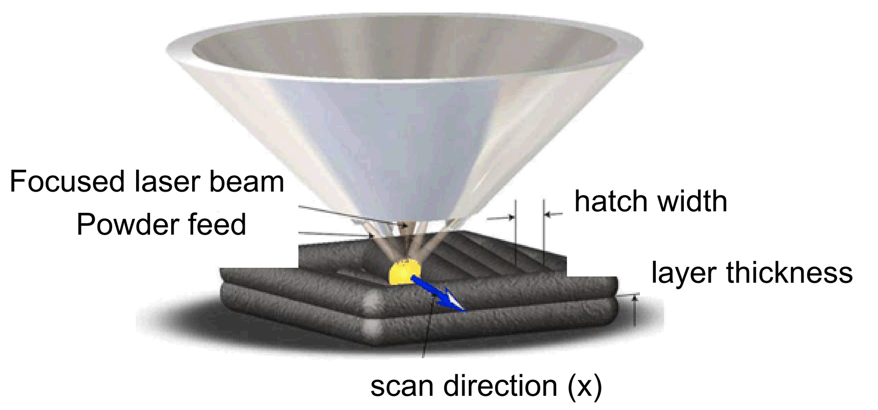
Judith Brown, Joe Bishop, Theron Rodgers
Sandia National Laboratories*, Albuquerque, NM 87185, U.S.A.

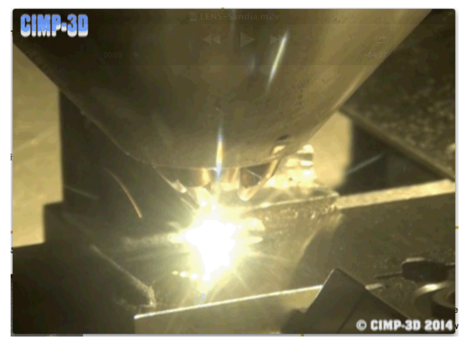
* This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Abstract

A process-structure-property modeling approach was developed to study texture evolution in additively manufactured structures and the resulting effects on mechanical properties. Texture evolution was modeled as a function of thermal gradients and solidification processes in the melt pool, and the macroscale mechanical properties were determined through computational homogenization of the resulting microstructures. The approach is used to investigate the effects of processing parameters such as laser power and scan speed on both microscale and macroscale behavior in FCC metals. The resulting macroscale properties can be used in engineering-scale material models but also include some representation of the microscale features. An a posteriori error-estimation framework is used to quantify modeling errors resulting from the various material model approximations of the material texture. The predictions indicate the resulting mechanical properties can have various degrees of anisotropy related to the solidification textures present.

Additive manufacturing





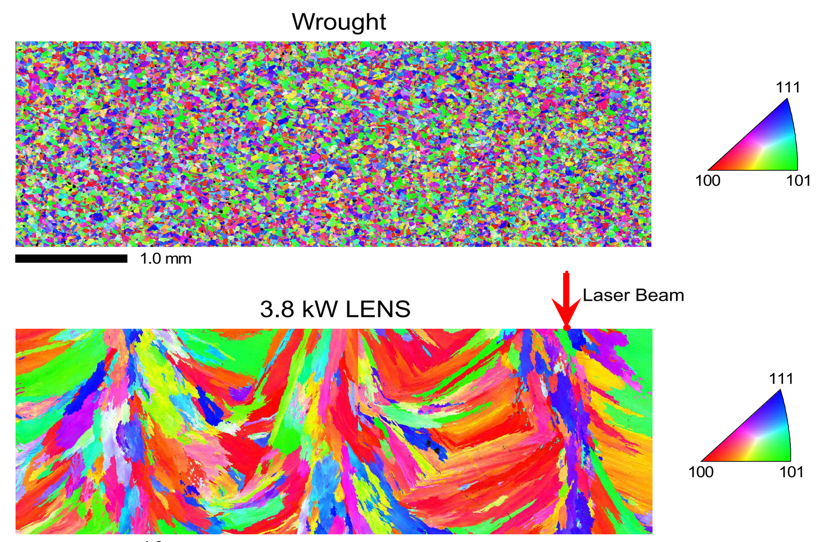
LENS® deposition
(T. Palmer, PSU)

Fundamental questions

1. How can we predict the macroscale mechanical response of AM materials given the microstructural information? (grain morphology, texture)
2. What is the accuracy of homogenization theory for additive materials? (scale separation, anisotropy)
3. How is microscale material variability manifested at the macroscale and what is the relationship with processing parameters?

Unique Microstructures

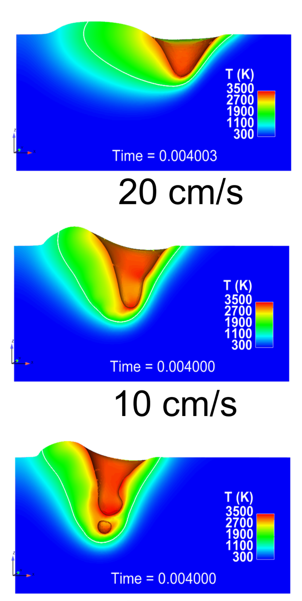
- Highly process-dependent:
  - Local thermal history
  - Parent material system
  - Scanning pattern, velocity
- Resulting microstructure:
  - Grain morphology and texture
  - Variability along the scan length



(D. Adams, SNL)

Process-Microstructure-Property Modeling Approach

Thermal/Fluid Melt Pool Model | Microstructure Generation—Potts KMC | Computational Homogenization | Effective Elastic Properties



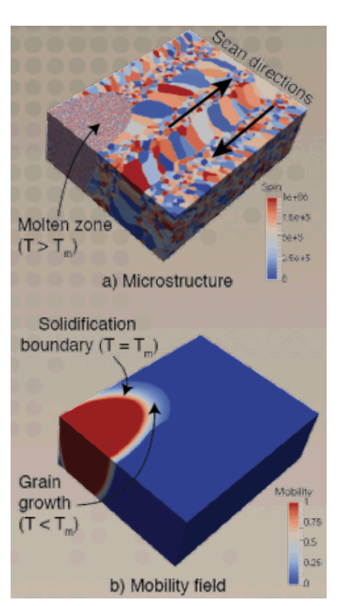
20 cm/s

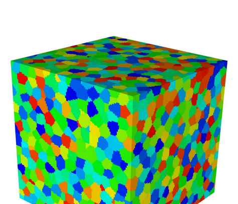
10 cm/s

5 cm/s

(M. Martinez, SNL)

$\nabla T, \vec{V}_n$





Representative Volume Element (RVE) including grain morphology, orientations

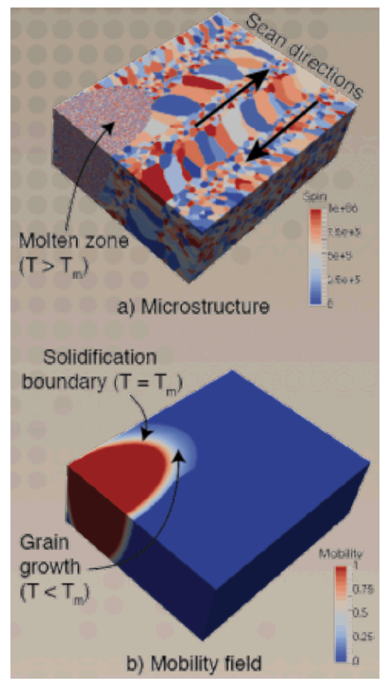
E_{11}, E_{22}, E_{33}, ν_{12}, ν_{23}, ν_{13}, G_{12}, G_{23}, G_{13}

Microstructure generation using Potts Kinetic Monte Carlo (KMC)

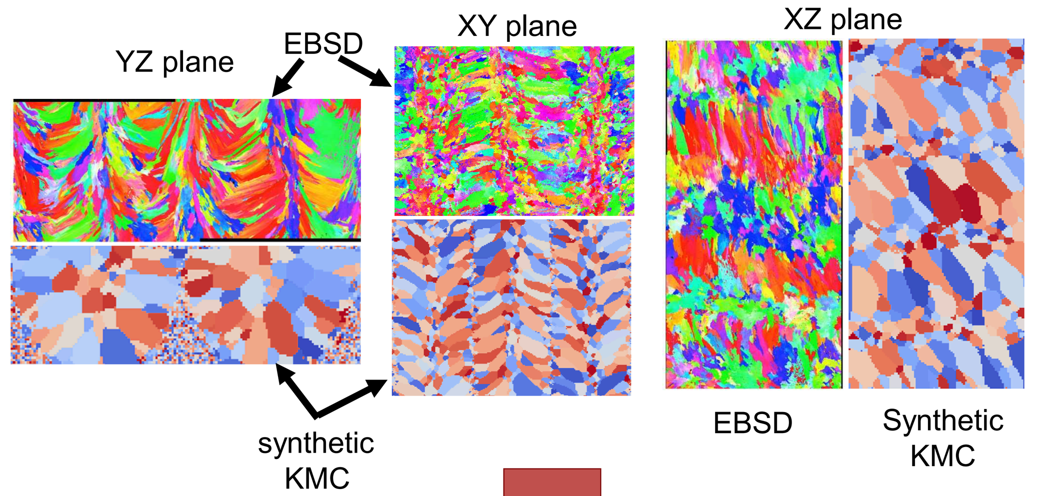
(http://spparks.sandia.gov)
(T. Rodgers, et al., JOM, 2016, 68(5): 1419-1426)

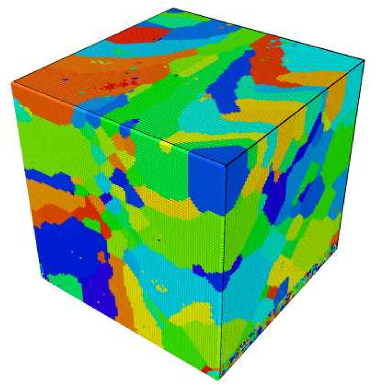
- Predicts solidification considering melt pool velocity, shape of the hot-zone trailing the melt pool's path
- When a voxel solidifies, its orientation is selected from one of the neighboring grains based on the misorientation between the grain's {100} plane normals, $\vec{n}$, and the direction of the maximum temperature gradient, $\vec{T}$:

$$P = \begin{cases} p_o(\theta) M(T) \exp\left(\frac{-\Delta E}{k_B T_s}\right), & if\ \Delta E > 0 \\ p_o(\theta) M(T), & if\ \Delta E \leq 0 \end{cases}, \qquad P = 1 - \vec{n} \cdot \vec{T}$$



Comparison with LENS 3.8 kW EBSD results





Generate Representative Volume Elements (RVE) including solidification texture

Computational Homogenization

Single crystal elastic constants (304L, austenite)

$C_{11} = 204.6$ GPa
$C_{12} = 137.7$ GPa
$C_{44} = 126.2$ GPa

anisotropy ratio

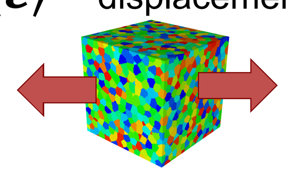
$$A = \frac{2C_{44}}{C_{11} - C_{12}} = 3.77$$

Uniaxial and Shear Boundary Value Problems to Populate Stiffness Tensor

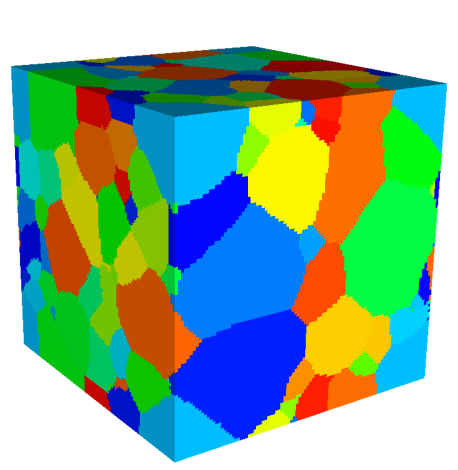
$$\langle \boldsymbol{\sigma} \rangle = \mathbb{C} \langle \boldsymbol{\varepsilon} \rangle$$

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{\Omega_V} \int_{\Omega_V} \boldsymbol{\sigma}(x) d\Omega$$

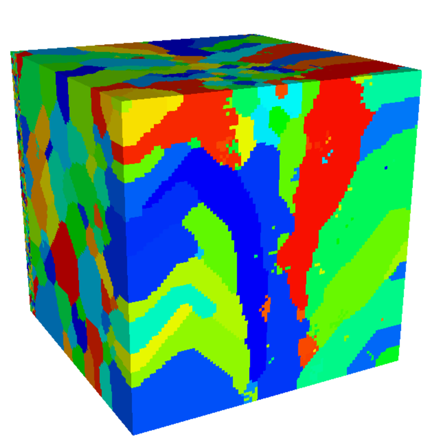
Applied displacement



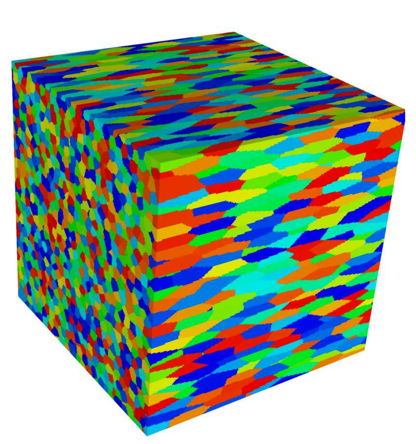
KMC-Equiaxed Growth



KMC-Additive Microstructure



Pure Fiber Texture <100>



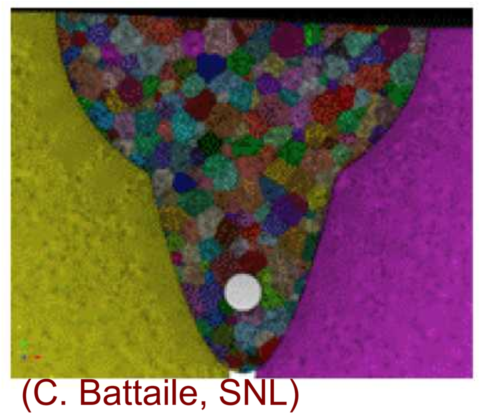
Effective Elastic Properties (GPa)

	E_{11}	E_{22}	E_{33}	ν_{12}	ν_{23}	ν_{13}	G_{12}	G_{23}	G_{13}
Pure Fiber Texture	143	143	90.9	0.114	0.615	0.615	58	126	126
KMC-Additive Microstructure	189	188	186	0.296	0.313	0.303	70	71	70
KMC-Equiaxed Growth	200	198	176	0.229	0.358	0.313	61	73	73

Error Estimation: Material Model Error

- What is error introduced by using an approximate material model?

High Fidelity Representation at Local Scale

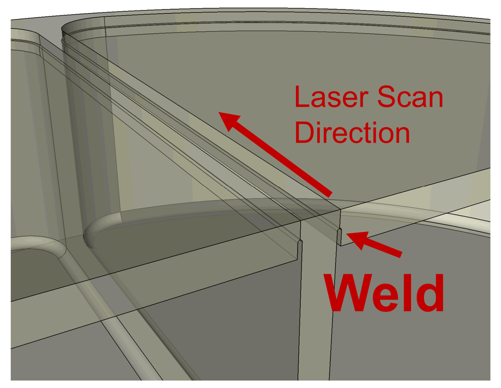


(C. Battaile, SNL)

Reduce Material Model Complexity

Material Model Form Errors Introduced

Simplified Representation at Engineering Scale



Upper Bound for Energy Norm of Displacement Error:

$$||\mathbf{u} - \mathbf{u}^0||_E^2 \leq \int_\Omega (\boldsymbol{\varepsilon}^0 - \bar{\boldsymbol{\varepsilon}}) : (\bar{\boldsymbol{\sigma}} - \boldsymbol{\sigma}^0)\, d\Omega \approx \sum_{i=1}^{N} V_e\, \eta_i^2$$

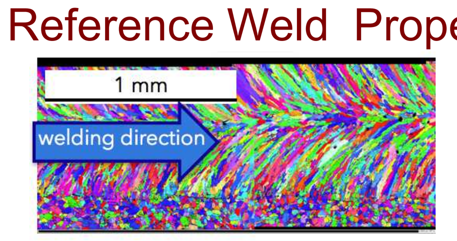
(Zohdi, Oden, Rodin, 1996, "Hierarchical modeling of heterogeneous bodies", CMAME)

$$\eta_i^2 \approx \left(\boldsymbol{\epsilon}^0 - \bar{\boldsymbol{\epsilon}}\right) : \left(\bar{\boldsymbol{\sigma}} - \boldsymbol{\sigma}^0\right) = \left(\mathbb{I} - \mathbb{C}^{-1}\mathbb{C}^0\right)\boldsymbol{\epsilon}^0 : \left(\mathbb{C} - \mathbb{C}^0\right)\boldsymbol{\epsilon}^0$$

- **Approximate Model**—contains known simplifications/lower fidelity representation
  - Example: Homogeneous Isotropic Properties
- **Reference Model** – Best representation of true material behavior
  - Examples: Effective properties from RVE, Direct Numerical Simulation of microstructure

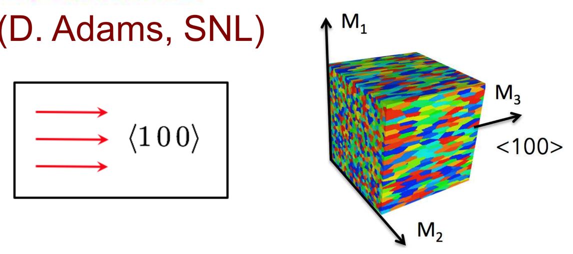
Welded Structure: Error Estimation Example

Reference Weld Properties:



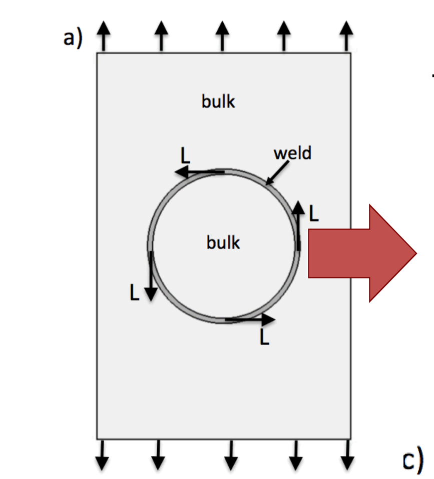
Weld EBSD

(D. Adams, SNL)

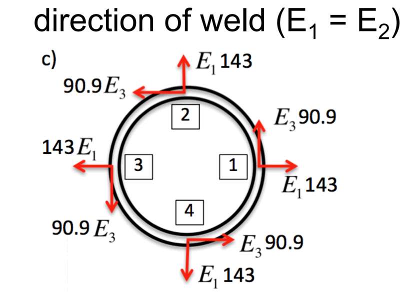


Assume fiber texture in <100> directions and homogenize

Boundary Value Problem

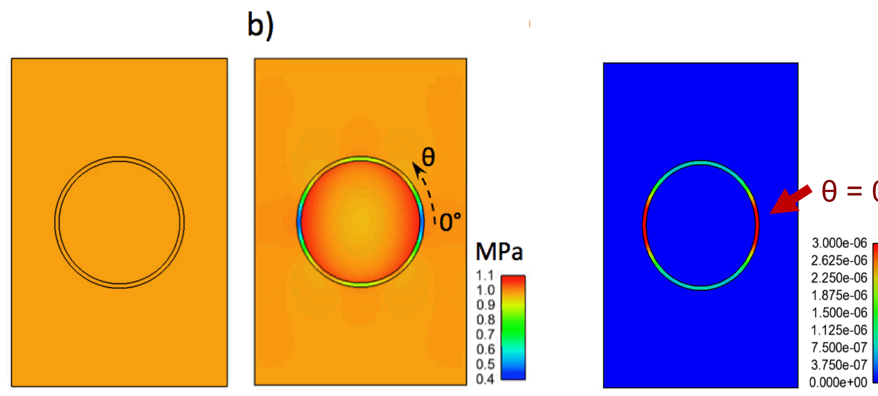


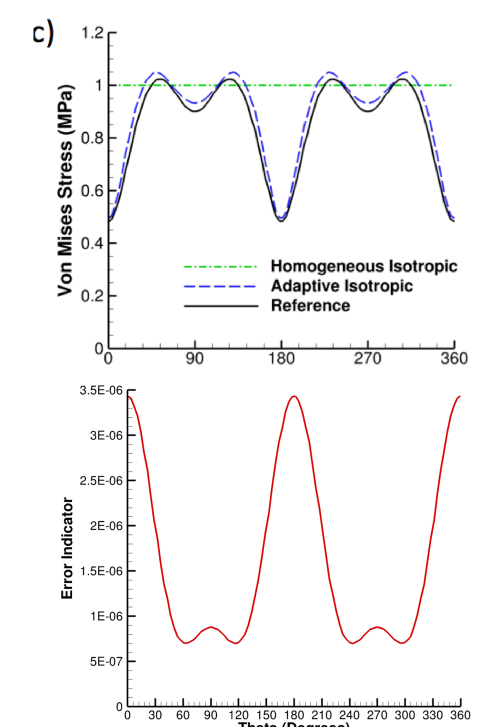
Transversely isotropic along L direction of weld ($E_1 = E_2$)



von Mises Stress Fields

Approximate Model: Homogeneous Isotropic | Reference Model: Transversely Isotropic | Error Indicator





Ongoing and future work

1. Comparison with experimental efforts: part build history, microstructure characterization, mechanical testing
2. Explore effects of various processing parameters (eg., laser scan speed, laser power, scan pattern) on microstructure and mechanical properties
3. Microscale variability: what is range of local mechanical properties in a single build?
4. Extend error-estimation framework to study plastic regime and other quantities of interest