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Title: Towards Random Generation of Microstructures of Spatially Varying Materials from Orthogonal Sections

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Towards Random Generation of Microstructures of Spatially Varying Materials from Orthogonal Sections

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Problem Motivation



- Aims of research:
- New manufacturing techniques produce materials which show spatial variation in the microstructure.
 - Given only orthogonal slices from such materials, simulate microstructures so that orthogonal slices from simulations match slices from samples

Figure 1: EBSD image from additively manufactured 304L stainless steel by LENS. How would you simulate a microstructure that has orthogonal slices like this?

Ellipsoid Growth Model

- Current methods, as in Dream3D, remove spatial structure by optimal packing of ellipsoids
- Idea: Grow ellipsoids in place from nucleation site
- Each grain has parameters: Nucleation site (x_j, y_j, z_j) , growth velocities along axes v_1, v_2, v_3 , and orientation matrix $O_j \in SO_3$
- Grains grow as ellipsoids until they interfere.
- Every spatial point x is assigned to the closest grain, as determined by travel times:

$$T(x \rightarrow X_j) = \left[(x - X_j)^T O_j^T (\text{diag } v_j^{-2}) O_j (x - X_j) \right]^{1/2}$$

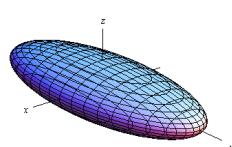


Figure 2: Each grain is represented by an ellipsoid. Each ellipsoid requires a nucleation site, growth velocities along each axis, and an orientation. Ellipsoids are grown until interference with each other.

Simulation of Microstructures

Parameters are simulated using hyperparameters:

- Nucleation sites (x_j, y_j, z_j) follow a Matérn hard-core process.
- Velocities follow gamma distribution with mean aspect ratios k_1, k_2 and concentration κ_v
- Orientations follow UARS distribution with orientation $S = (\phi_1, \Phi, \phi_2)$ and concentration κ_s

Microstructure simulation procedure:

- Choose hyperparameters $k_1, k_2, \kappa_v, S, \kappa_s$
- Randomly generate N nucleation sites (x_j, y_j, z_j)
- Use hyperparameters to simulate parameters v_1, v_2, v_3 and O_j for each grain and grow in space

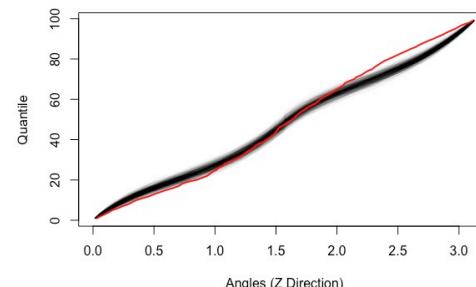


Figure 3: Observed (Red) and Simulated (Black) area-weighted densities of aspect ratio in the Y direction. Shading of black line represents simulation variance. By matching these lines, hyperparameters can be estimated.

Comparing Microstructures

- Each grain in slice treated as an ellipse to calculate area, aspect ratio, and angle of rotation
- Area-weighted cumulative distribution function used to summarize distributions of quantities

$$G(a) = \frac{\sum_g A_g * I(a_g < a)}{\sum_g A_g}$$

- Best fit hyperparameters are those which produce close $G(a)$ matches between simulated and real EBSD slices

Results

- Data: Sample of Tantalum Starck – eight EBSD images in A direction, six EBSD images in TT direction (only two directions)
- Sample shows variation in the morphology.

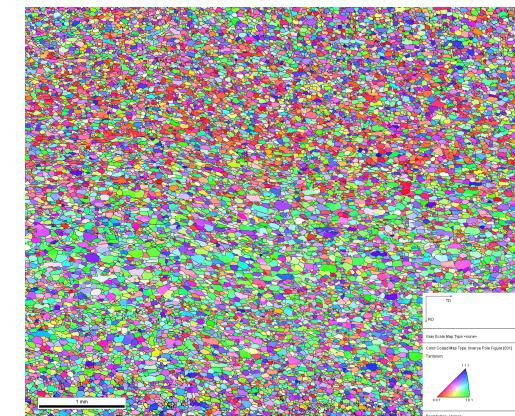


Figure 4: A large slice taken from the sample of Tantalum Starck, showing spatial variation in the morphology of the grain size distribution caused by the particular manufacturing process.

- Three directions (A = B, TT), three quantities (area, aspect ratio, angle) compared for nine $G(a)$ distributions.
- Able to identify preferential grain growth direction, but still lack of fit in elliptical growth model, most noticeable in areas.

k_1	k_2	κ_v	κ_s	ϕ_1	Φ	ϕ_2
1.00	0.61	10	10	5.353	0.200	0.797
0.94	0.61	100	10	1.910	2.880	0.000
1.00	0.61	100	10	5.353	0.200	0.797
1.00	0.61	10	5	5.353	0.200	0.797
1.00	0.61	100	5	5.353	0.200	0.797

Table 1: Five best-fit hyperparameter sets for the Tantalum Starck sample found by minimizing the avg. max distance of area weighted CDFs in Figure 3.