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Modelling polycrystalline microstructures by tessellations

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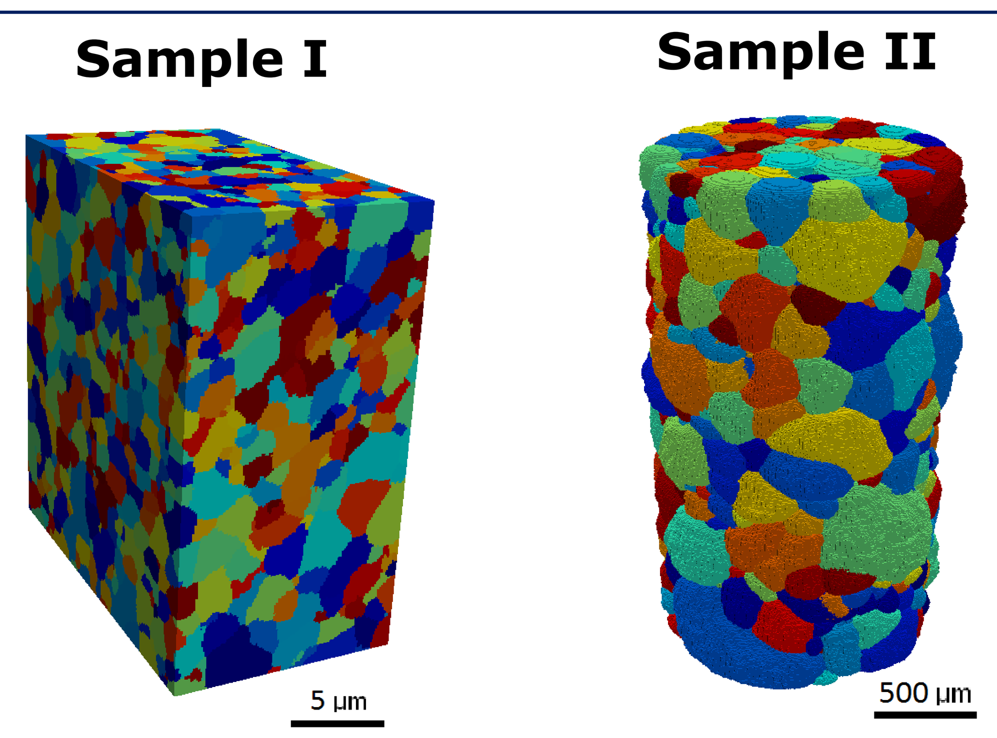
Description of the problem

Representation of the 3D microstructures by parametric tessellation models allows an efficient **conversion of voxel-based data to vector-based data**.

Advantages

- significant **data reduction**
- **avoids processing steps** related to smoothing of grain boundaries
- **consistent estimation** of size and shape characteristics
- allows for generation of **virtual microstructures**



Visualization of grains in the 3D microstructure of Al-3wt.%Mg-0.2wt.%Sc (Sample I) and Al-1wt.%Mg (Sample II).

Model fitting

- A **tessellation** is a division of $\mathbb{R}^k$ into a countable collection of non-overlapping sets called *cells* or *grains*.
- We use **parametric tessellation models** generated by a marked point pattern $\boldsymbol{P} = \{(\boldsymbol{x}_i, \boldsymbol{\theta}_i)\colon \boldsymbol{x}_i \in \mathbb{R}^k, \boldsymbol{\theta}_i \in \Theta\}$, where Θ is a parametric space.
- The **cells** of a tessellation $\boldsymbol{P}$ are defined by

$$C_i = \{\boldsymbol{x} \in \mathbb{R}^k\colon d(\boldsymbol{x}, (\boldsymbol{x}_i, \boldsymbol{\theta}_i)) \leq d(\boldsymbol{x}, (\boldsymbol{x}_j, \boldsymbol{\theta}_j)),\ \ \forall j \neq i\}$$

  with certain distance measure d.
- We focus on **generalized balanced power diagrams** (GBPD) defined by $d(\boldsymbol{x}, (\boldsymbol{x}_i, M_i, r_i)) = (\boldsymbol{x} - \boldsymbol{x}_i)^{\mathrm{T}} M_i (\boldsymbol{x} - \boldsymbol{x}_i) - r_i$,
  $r_i \in \mathbb{R}, M_i \in \mathbb{R}^{3x3}$ a symmetric positive definite matrix

For fitting a tessellation to empirical image data I, we use a stochastic optimization method known as **simulated annealing**.

Algorithm

1) Initialization. Identify initial parameters $\{\boldsymbol{x}_i, M_i, r_i\}$. Set $n = 1$.

2) Modification. Modify a single parameter of a random cell.

3) Updating. Evaluate the current discrepancy $D^{(n)}(I, \boldsymbol{P})$, counting incorrectly assigned voxels, and the new discrepancy $D^{(new)}(I, \boldsymbol{P})$. Accept the new state (i.e. set $D^{(n+1)}(I, \boldsymbol{P}) = D^{(new)}(I, \boldsymbol{P})$) with probability

$$\alpha = \begin{cases} 1 & \text{if } D^{(new)}(I, \boldsymbol{P}) \leq D^{(n)}(I, \boldsymbol{P}) \\ \exp\left\{\dfrac{D^{(n)}(I, \boldsymbol{P}) - D^{(new)}(I, \boldsymbol{P})}{T}\right\} & \text{otherwise} \end{cases}$$

4) Iteration. If a predefined stopping condition is met, stop. Otherwise set $n = n + 1$ and repeat from step 2.

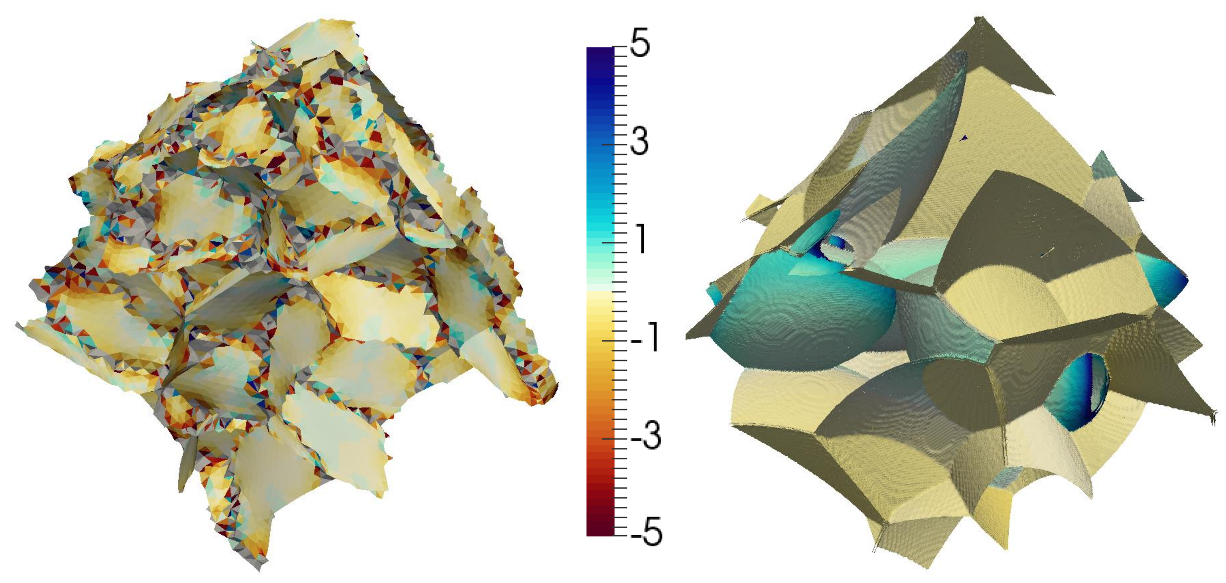
Results (comparison of GBPD with some other common models)

		Sample I	Sample II
Voronoi tessellation	$d(\boldsymbol{x}, \boldsymbol{x}_i) = \Vert\boldsymbol{x} - \boldsymbol{x}_i\Vert$	57.5	58.6
Laguerre tessellation	$d(\boldsymbol{x}, (\boldsymbol{x}_i, r_i)) = \Vert\boldsymbol{x} - \boldsymbol{x}_i\Vert^2 - r_i$	79.4	85.4
spherical grain growth model	$d(\boldsymbol{x}, (\boldsymbol{x}_i, r_i)) = \Vert\boldsymbol{x} - \boldsymbol{x}_i\Vert / r_i$	83.1	86.6
GBPD	$d(\boldsymbol{x}, (\boldsymbol{x}_i, M_i, r_i)) = (\boldsymbol{x} - \boldsymbol{x}_i)^{\mathrm{T}} M_i (\boldsymbol{x} - \boldsymbol{x}_i) - r_i$	92.0	95.0

percentage of correctly assigned voxels

Estimation of geometric characteristics

Grain boundaries in the GBPD model are parts of **quadric surfaces**. Thus, **size and shape characteristics** can be computed from analytical formulas.



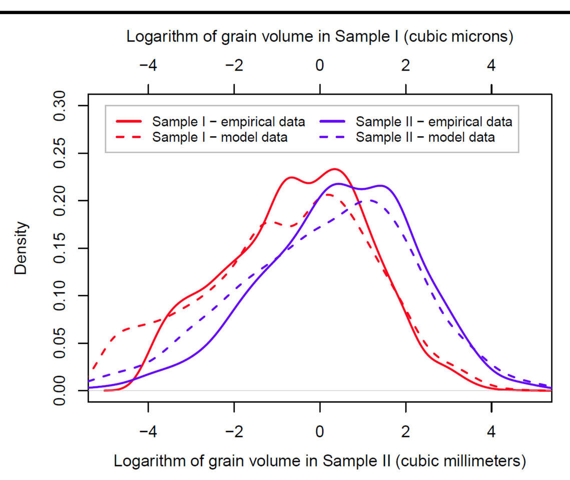
Cutout of grain boundary network fitted by triangular surface mesh (left) and the GBPD model (right), coloured with respect to Gaussian curvature.

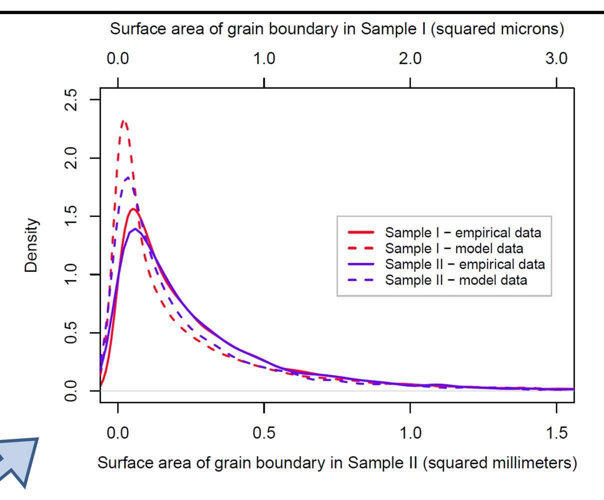
Size characteristics

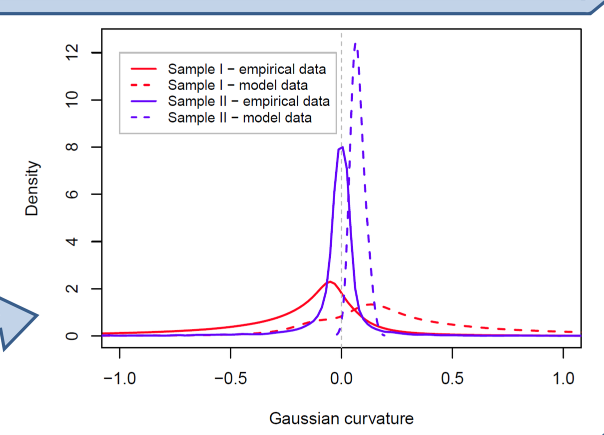
1) **Volume** of grains
2) **Surface area** of grain boundaries
3) **Length** of triple junctions

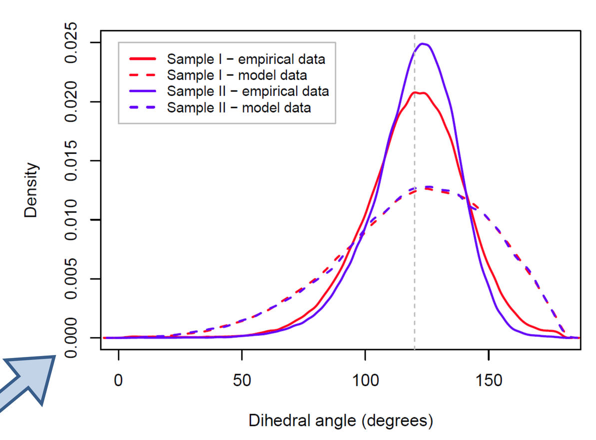
Local shape characteristics

1) **Curvature** at grain boundaries
2) **Dihedral angle** at triple junctions









References

[1] O. Šedivý, T. Brereton, D. Westhoff, L. Polívka, V. Beneš, V. Schmidt and A. Jäger. 3D reconstruction of grains in polycrystalline materials using a tessellation model with curved grain boundaries. *Philosophical Magazine* 96:18 (2016), 1926-49.

[2] O. Šedivý, J.M. Dake, C.E. Krill III, V. Schmidt and A. Jäger. Description of the 3D morphology of grain boundaries in aluminum alloys using tessellation models generated by ellipsoids. *Image Analysis & Stereology* 36 (2017), 5-13.