Random tessellations for modelling of sintered structures



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The sinter process

Initial state

powdered or granular material is compressed in a die

Intermediate states

material is heated to a temperature close to but below the melting point

=> particles stick together resulting in a porous material

Final state

space completely filled by the material





Modelling of sintered structures

Project

MAVO MMM-Tools (multiscale materials modelling)



Fraunhofer internal project (9 institutes)

Focus

development of a method for the characterization of materials on all scales of temporal and spatial resolution





Modelling of sintered structures

Our task	geometric modelling of sintered materials in all stages of the sintering process
	=> development of a structure generator for sintered materials
Problems	 samples from the same material may look quite different depending on conditions during sintering
	 find a geometric model for arbitrary states without simulation of the physical process (too complicated)
	 modelling of rare events e.g. defects



Examples

Different structures of Alumina crystals

Defect





Examples

Fracture surfaces and cuts of sinter ceramics



Al2O3 vom ISC (Dr. Springer)







Models for the sinter process

Initial state => (dense) packing of particles

Intermediate states => incomplete tessellation

Final state

=> (random) tessellation



The initial state – Packing of particles

Desired

(dense) packing of particles

Possible solutions

Force biased algorithm (used at the moment)

- Volume density of approximately 64%
- No analytic description

Marked hard core point field

• Not yet clear which model to use



The final state - Tessellations

Voronoi tessellation



Given: $\mathcal{P} = \{p_i \mid i \in I\} \subset \mathbb{R}^d$ set of points

Cells:
$$C(p_i) = \left\{ x \in \mathbb{R}^d \, | \, d(x, p_i) \le d(x, p_j) \, \forall p_j \in \mathcal{P} \right\}$$

<u>Problem</u>: size of cells does not correspond to size of particles

Johnson-Mehl tessellation



Given: $\mathcal{P} = \{(p_i, r_i) \mid i \in I\} \subset \mathbb{R}^d \times \mathbb{R}$ set of weighted points

Cells: $C(p_i, r_i) = \left\{ x \in \mathbb{R}^d \, | \, d(x, p_i) - r_i \leq d(x, p_j) - r_j \, \forall (p_j, r_j) \in \mathcal{P} \right\}$

Problem: complicated shape of cells



The final state - Tessellations

Laguerre tessellation



Given: $\mathcal{P} = \{(p_i, r_i) \mid i \in I\} \subset \mathbb{R}^d \times \mathbb{R}^+$ set of weighted points

Cells: $C(p_i, r_i) = \left\{ x \in \mathbb{R}^d \, | \, d(x, p_i)^2 - r_i^2 \le d(x, p_j)^2 - r_j^2 \, \forall (p_j, r_j) \in \mathcal{P} \right\}$

- d=3: Every simple convex cellular structure is a Laguerre tessellation. (Davis 1959)
- realistic in shape and size of cells
- used in many applications, but not yet treated analytically



Applications of Laguerre tessellations

Modelling of

- polycrystalline materials
- foams
- biological tissues
- molecular surfaces (proteins)

Algorithms for

- construction
- motion of points
- elementary topological transformations (disappearance of cells, change of neighbours)



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Model for different states

Initial state: 200 balls in a cube with 200 pixels side length created by force biased algorithm





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Initial state: 200 balls in a cube with 200 pixels side length created by force biased algorithm





Interesting questions

adequate model for initial state

replace force biased algorithm with marked (Gibbs) point process

properties of random Laguerre tessellations

cell characteristics

probability for empty cells

=> easiest case: marked Poisson point process, interesting for applications: Hard core point process

limits of the Laguerre model in applications

more general particles (platelets, polyhedra, ...)

