Laguerre tessellations: fitting a model to rigid closed-cell polymer foams

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Geometric models allow to investigate how physical properties are influenced by material’s microstructure. We deal with polymethacrylimide (PMI) foams, which are rigid closed-cell foams imaged by µCT. Random Laguerre tessellations are a suitable model for these structures. In this work, we will introduce the characteristics of the model, outline the fitting procedure and discuss methods to automate the model choice.

Introduction

Polymethacrylimide (PMI) foams are rigid closed-cell foams featuring both high stiffness and very low specific weight. These highly desirable properties are definitely due to their specific cellular microstructure. However, it is not yet understood exactly how the microstructure influences the materials’ physical properties. Geometric models of the microstructure and numerical simulations of materials’ properties can be exploited to allow a better understanding of this link. We start with the geometric characteristics of the foams gained by quantitative analysis of reconstructed µCT images as explained in the contribution of R. Schlimper et al., CellMat 2012. Given the measured features, we fit a stochastic model to the microstructure. A well-suited class of models are random Laguerre tessellations, i.e. a generalization of the well-known Voronoi diagram such that each point is assigned a weight. Thanks to its flexibility, this model is suitable to embed the materials’ geometric properties. In fact, a good model matches the main geometric features observed in the microstructures. To comply with this principle, the model’s parameters are chosen to minimize a certain distance measure of several geometric characteristics of the model’s and material’s typical cell. In order to speed up the fitting procedure, we need to investigate how the parameters influence the geometric properties of the model. In the general case, there are no analytical formula expressing this relation. Nevertheless, if the Laguerre tessellation is generated by a system of non-overlapping spheres, its properties are strongly related to those of the underlying process. For example, the cell size distribution is highly influenced by the volume distribution of the packed spheres. Moreover, there is a polynomial dependency of the model characteristics on the parameters of the sphere packing. Based on these observations, parameters of the model best fitting the data can be found without further numerical simulations.

Laguerre tessellations

The easiest tessellation generated by a (random) point process is the Voronoi tessellation. Given a point process \( S = \{ x_i, i=1,2,\ldots \} \) the Voronoi cell of the tessellation generated by \( S \) is defined by

\[
C_V (x, S) = \{ y \in \mathbb{R}^d : \|y - x\|^2 \leq \|y - x'\|^2, \forall x' \in S \}, \quad x \in S.
\]

In other words, space is tessellated by a minimum distance map defined on the points in the set \( S \). The benefit is a model with a few number of parameters and, with further assumptions, analytical formulations of the geometric properties depending on the parameters. However, the flexibility of Voronoi tessellations is limited.

Generalizations are Laguerre tessellations, which are generated by a marked point process, that is a point process in which to each point a random mark is assigned. Thus, the tessellation can be seen as generated by a system of spheres \( S = \{ s(x, r), r > 0, i=1,2,\ldots \} \). The Laguerre cell of the tessellation generated by \( S \) is

\[
C_L (s(x, r), S) = \{ y \in \mathbb{R}^d : \|y - x\|^2 - r^2 \leq \|y - x'\|^2 - r'^2, \forall s(x', r') \in S \}, \quad s(x, r) \in S.
\]

For system of spheres with constant fixed radius, the Laguerre tessellation is a Voronoi.

In general, the cells of the tessellation are full dimensional convex polytopes. For \( k < d \), we call \( k \)-face of the tessellation the \( k \)-dimensional intersection of adjacent cells. In 3D, the \( k \)-faces for \( k=0,\ldots,3 \) are nodes, edges, facets and cells, respectively. Laguerre tessellations are face-to-face, i.e. the faces of the tessellations are faces of the cells, and normal, i.e. every \( k \)-face belongs almost surely to \( d-k+1 \) cells. Moreover, in 3D or higher dimension, all tessellations which are face-to-face and normal can be seen as Laguerre tessellation [LauZuy08]. Since these properties are also observed in the real materials, modeling with Laguerre tessellation is not restrictive.

From now on, we restrict to the 3D case. The typical cell is a random cell with the same distribution as a uniformly randomly chosen cell of the given tessellation. Tessellations can be described by the mean values of \( k \)-faces per unit volume or by geometric characteristics of the typical cell: mean volume, mean surface area, mean total edge length, mean mean width of a cell, mean area of a facet, mean perimeter of a facet, mean edge length, mean number of \( j \)-faces adjacent to \( k \)-faces \( N_{ij} \).

Model fitting

The properties of the Laguerre tessellation strongly depend on the underlying sphere packing. However, there are no analytical
formulations linking parameters and properties of the model in the general case, cf. results in [Lau08].

Considering systems of non-overlapping spheres brings multiple advantages. Each sphere is completely contained in the cell it generates, cf. Fig.1, thus the minimal cell is larger than the smallest ball. Moreover, the size distribution of the tessellation is closely related to that of the spheres. The higher the volume covered by the sphere system, the better the control on the tessellation. Therefore, we are interested in producing high density sphere packings. A method is by a force biased algorithm [Bar01]. Initially, spheres are randomly inserted in an observation window and overlapping is allowed. Through a collective rearrangement, spheres are shifted and shrunken to reduce, and eventually avoid, intersections. At the same time, the initial size distribution is preserved, up to a scaling factor. The free parameters of the algorithm are: the number of spheres (i.e. the intensity of the process), the size distribution, the desired volume fraction $V_V$ and the coefficient of variation $c$ of the volume distribution. Typically cell size distribution in real foams follow a gamma or a log-normal distribution [Fan04].

The Delaunay tessellation corresponding to the sphere packing is determined by constructing a 4-dimensional convex hull, which depends on centers and radii of the spheres, and by projecting it back on the 3D space [Sug00]. By duality, the Laguerre tessellation generated by the sphere packing is found. Notice that the whole process is completely determined by the sphere packing.

In order to choose the best fitting model, we minimize the distance function between material's and model's characteristics, defined as

$$d(\hat{m}, m) = \sqrt{\sum_{i=1}^{n} \left( \frac{\hat{m}_i - m_i}{\hat{m}_i} \right)^2}$$

where $\hat{m}$ hat is the vector of features estimated from the material's images and $m$ the corresponding characteristics of the model. Following [Lau08], we consider the following set of characteristics: volume, surface area, mean width and number of facets per cell. Mean values do not carry enough information about the variability of these features in the sample, hence standard deviations are considered as well. From now on, we will use this set of eight characteristics for model fitting.

Typically, the model with the best fitting characteristics had to be found by simulations. In the work presented in [Red09], some empirical relations between the characteristics and the parameters of the model are determined. The number of cells in the observation window is fixed. Laguerre tessellations are simulated varying desired volume fraction and coefficient of variation, for each size distribution (gamma and log-normal). One can see a regular behavior in the plots of each characteristic depending on the coefficient of variation $c$, for each volume fraction $V_V$ and size distribution. Polynomials of 3rd degree well fit to these curves. Thus we can write $m_i = p_{V,V}(c)$, $i=1,...,8$ and substitute them in the distance function. The characteristics are estimated from the image data via integral geometry methods [OhSc09] with a suitable edge treatment.

By minimizing the distance function with respect to the coefficient of variation, the model parameters which best fit the data are found. This can be fulfilled automatically, without further simulations nor need of expert knowledge on stochastic models. In the following section, we show this method on PMI hard foams.

Figure 1: Example of Laguerre tessellation generated by a system of non-overlapping spheres
Application example

We now consider images of PMI foams taken and segmented with the techniques outlined in [Sch12]. We will present the procedure on a sample of ROHACELL® WIND-F 100 RC. Two-dimensional sections of the computed tomography images and the corresponding reconstructed cells are displayed in Fig. 2a, 2b. A volume rendering of the reconstructed wall system is shown in Fig. 3a.

In order to compare the characteristics with those of the tessellation, which is space-filling, the wall system must be removed. This is achieved by morphological dilation, Fig. 2c. The characteristics are computed from the image with the software MAVI and MAVIIlib [MAVI05]. These can be fed to the distance function and by minimization, one has the parameters of the sphere packing. For this sample, the minimum of the distance function occurs for gamma size distribution, desired volume fraction $V_f = 60\%$ and coefficient of variation $0.77$. A realization of the Laguerre tessellation is represented in Fig. 2d in a two dimensional section and in Fig. 3b with a volume rendering of the edge system.

Mean values and standard deviations of the features used in model fitting are shown in Table 1. The values for the Laguerre tessellation are computed on a set of five independent realizations, for a total of 2450 cells. The mean values are matching better than the standard deviations, which show a higher variability in the models. For model validation, we look at the whole distribution of the volumes of the cells. From the histograms represented in Fig. 4, the distributions do not match well for small cells.

Moreover, we can compare the shapes of the cell, for example by considering the sphericity of cells, i. e. the first isoperimetric shape factor [OhSc09]. The distribution of this shape factor is represented in Fig. 5. It seems that there is a set of cells in the model that well match the shapes of the real cells. However, additional to these, there is a considerable amount of cells with small shape factor, which does not match the cells in the foam.

![Figure 2: 2D sections of the sample of WIND-F 100 RC foam and model. From left to right, (a) µCT, pixel size = 2.73 µm, (b) reconstructed cells, (c) dilated cells, (d) Laguerre tessellation, respectively](image1)

![Figure 3: PMI foam and Laguerre tessellation generated by a force-biased sphere packing with best fitting parameters](image2)
Discussion

We showed that it is possible to model foam structures by random Laguerre tessellations generated by a force-biased system of non-overlapping spheres completely automatically. The parameters found by minimizing the distance function define the model in this class which fits best to the data. This method proved successful in [Red09] for open aluminum foam and an open polymer foams. Nevertheless, the PMI foams are rigid and closed cells with different geometric characteristics, hence this class of models might not be the best for these materials.

The question we will investigate in future research is how to change the model to better match size and shape distribution of the cells. For example, instead of force-biased algorithm for the sphere packing, random sequential adsorption (RSA) can be used to generate systems of non-overlapping spheres. Again, the relation of the parameters and the desired model characteristics is not analytical, nevertheless, it is possible to proceed analogously to [Red09]. By simulations, an approximation of how the characteristics depend on the model parameters can be found, thus allowing again automatic model fitting.
Table 1: Comparison of the first and second moment of volume, surface area, mean width and number of facets of a cell. Values in m.

<table>
<thead>
<tr>
<th></th>
<th>mean(V)</th>
<th>sd(V)</th>
<th>mean(S)</th>
<th>sd(S)</th>
<th>mean(B)</th>
<th>sd(B)</th>
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<td>PMI</td>
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References