Improved models of solid foams based on soap froth

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Abstract

Random Laguerre tessellations are widely used to model the cell systems of solid foams because they enable the reproduction of the cell-volume distributions found in real materials. However, the tessellations have planar cell faces, which over constrain the orientations of cell edges and adversely affect the distribution of edge lengths. The Surface Evolver was used to compute equilibrium microstructures of soap froth by minimizing the total surface area of Laguerre tessellations while preserving their cell-volume distributions. The resulting soap froth structures are more realistic than Laguerre tessellations because the edges of a face do not lie in the same plane and there are significantly fewer short edges. The edge-length distributions of soap froth models are in better agreement with experimental measurements of solid foams with open cells than those with closed cells. We argue that surface tension forces, which control area minimization, are more important during the formation of open-cell foams while viscous forces are more important during the formation of closed-cell foams but are not accounted for in existing models of foam formation. The distributions of other geometric characteristics, such as cell surface area, cell diameter, number of faces per cell and number of edges per face, are not adversely affected by area minimization.

Keywords: edge-length distribution, Laguerre tessellation, model fitting, power Voronoi tessellation, relaxation, stochastic foam model

1. Introduction

Random Laguerre tessellations – a generalization of the well-known Voronoi tessellation – have proven to be practicable and versatile models for the cell structure of solid foams with open and closed cells [16, 27, 29]. While the cells of Voronoi tessellations are generated from random seed points only, the generators of Laguerre tessellations also carry positive weights that can be interpreted as the radii of spheres centered at the seed points. To fit a Laguerre tessellation to a foam sample, the cell generators have to be chosen so that the distributions of foam characteristics are reproduced in the model. The cell system of real foams is usually

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highly regular so the same should be true for the models; consequently, tessellations generated by random
systems of non-overlapping spheres are the most suitable choice. The packings can be simulated by random
sequential adsorption (RSA, [7, p. 132]), dense packing algorithms like the force-biased algorithm [2], or
molecular dynamics [12, 13, 14]. Besides being highly regular, these models have the advantage that each
Laguerre cell completely contains the generating sphere. Consequently, the volume distribution of the cells
is strongly related to the volume distribution of the generating spheres.

The tessellations have to be studied by simulation because their geometric characteristics are not ana-
lytically related to the parameters of the generators. In [19], an automatic fitting procedure was proposed
for a Laguerre tessellation generated by a force-biased system of non-overlapping spheres with the two free
parameters $c$ and $V_r$ – the coefficient of variation of the volume distribution of the spheres and the volume
fraction of the sphere packing, respectively. The best model is found by minimizing a distance function
between the moments of cell characteristics of the real foam sample and the model. More precisely, the first
two moments of volume, surface area, mean width, and number of faces per cell were used in [19]. The
possibility of including dihedral and interior angles in the model fitting is discussed in [27]; however, the
analysis of samples of metallic and polymeric, open- and closed-cell foams shows that including the moments
of the angles does not significantly improve the model fit.

It is known that each normal tessellation (meaning that four cells meet in a vertex as also required in
Plateau’s laws) with convex cells can be represented by a Laguerre tessellation [15]. So if one is interested
in a random tessellation model with convex cells – which is particularly easy from a computational point of
view – Laguerre tessellations are the natural choice. However, planar cell faces – as required by convexity
of the cells – are not typical of real foams. This is best illustrated by the equilibrium structure of soap
froth, which must obey Plateau’s laws to minimize surface area. But no cell face can be a flat polygon with
straight edges and satisfy the Plateau condition that all edges meet at the tetrahedral angle. Planar faces
obviously restrict the shape and orientation of cell edges, but more important, they significantly influence
the distribution of edge lengths [10, 11, 12].

Laguerre tessellations have a lot of short edges, but the edge-length distributions in soap froth are
Gaussian-like and have relatively few short edges. This has also been observed in solid foams with open
cells [17] even though, strictly speaking, they are not subject to Plateau’s laws. Their realistic edge-length
distributions have motivated the use of soap froth models as templates for developing finite-element models
for the mechanics of random open-cell foams [5, 6, 8, 9, 10, 11, 18].

Beginning with the first studies of mechanical properties of three-dimensional open-cell foams [22, 25],
the short edges in Voronoi tessellations below some threshold length have been removed from the structure,
artificially creating joints with more than four edges. It is argued that this procedure reduces computing
time and has minimal effect on mechanical properties. These trimming processes are essentially unnecessary
when soap-froth models are used as templates to create finite-element models of random foams because short edges are relatively rare \([5, 6, 8, 9, 18]\).

Figure 1 displays the edge-length distributions of several realizations of random Laguerre tessellations generated by force-biased sphere packings with varying parameters. The shape of the curves differs from typical edge-length distributions of real foams as shown, for example, in Figure 4. In particular, a rather large number of short edges occur in all of the curves in Figure 1. This implies that changing model parameters cannot reduce the number of short edges significantly.

Surface Evolver models of random soap froth are the most realistic physics-based models of a real foam available \([12, 13]\). A more complete model of the structure formation process for solid foams would have to consider the expansion of a random suspension of gas bubbles to form the polyhedral cells in low-density foam, and include the viscous flow of the suspending fluid, which eventually solidifies to form the solid phase of the foam. But such models are unavailable. Therefore, to improve the fit of edge-length distributions, we use models of random polydisperse soap froth as templates for solid foams. This involves minimizing the surface area of fitted Laguerre tessellations by using the Surface Evolver \([3]\), an interactive computer program for modeling liquid surfaces shaped by various forces (surface tension) and constraints (cell volumes). The surface evolves toward minimal energy (surface area) by simulating the process of evolution by mean curvature. Our goal is to investigate how the geometry of the models is affected by relaxation and whether the relaxed models better fit the samples.

This paper is organized as follows. First, we review some methods for processing and analyzing tomographic images of foams. We explain how the geometric characteristics estimated from the image data can be used for fitting Laguerre tessellations to the observed foam structures. Finally, the idea of relaxing Laguerre tessellations by using the Surface Evolver is introduced. We apply these techniques to six samples of open- and closed-cell foams. We compare geometric characteristics of the fitted Laguerre tessellations and their relaxed counterparts to investigate the extent to which relaxation improves the model fit.

2. Processing and analysis of tomographic images

The microstructure of the real foam samples is typically imaged by micro computed tomography. In the resulting 3D images, the cells are usually connected, even in ideal closed-cell foams, due to insufficiently resolved cell walls and discretization effects. Therefore, the cells have to be separated in order to measure geometric characteristics of individual cells. This is achieved by using the following well established image processing chain:

1. Binarization yielding the strut system of the foam,
2. Euclidean distance transform on the pore space,
Figure 1: Densities of the edge-length distribution in Laguerre tessellations generated by force-biased sphere packings with $V_V = 30\%, 60\%$ and $c = 0.2, 2.0$. Curves computed from simulations: five realizations with 10 000 cells for each parameter set in a window of $1 \text{mm}^3$ with periodic edge treatment. Left: gamma volume distribution. Right: lognormal volume distribution.

3. inversion, i.e. each voxel gets as new gray value the difference between the maximal gray value and its old value,
4. smoothing to remove superfluous local minima and avoid oversegmentation,
5. watershed transform.

Here, avoiding oversegmentation is the crucial step as the watershed transform assigns a cell to each local minimum in the inverted distance image. Well-proven tools for removing superfluous minima are the h-minima transform, the height adaptive h-minima transform [23, Ch. 6] or a preflooded watershed transform [24]. For details on the choice of the method and its parameters see [20]. Sectional images of the reconstructed cell systems of the foam samples studied in Section 5 are shown in Figure 2.

Based on the reconstructed cell systems, empirical distributions or moments of various cell characteristics can be estimated. Edge effects were taken care of by a minus sampling: a sub-window was chosen such that all cells centered inside it are completely observable. The sample was then restricted to these cells. All image processing and analysis steps described in this section were carried out using the MAVI software package [4].

3. Fitting Laguerre tessellations to foam samples

For fitting a Laguerre tessellation to a foam sample, the foam is assumed to be a realization of a stationary, isotropic random tessellation. That is, the distribution of the cell system is assumed to be invariant with respect to translations and rotations.
This assumption contradicts the experimental observation that most solid foam samples show a certain degree of anisotropy easily detected by comparison of the mean cell diameters in the three coordinate directions. Scaling in coordinate directions to equalize all three mean diameters results in a nearly isotropic image that can be fitted with an isotropic model. Finally, inverse transformation yields a model of the real, anisotropic material.

The deviation of a model from the real foam data is measured by using the relative distance measure

$$\rho(\hat{c}, c) = \sqrt{\sum_{i=1}^{n} \left( \frac{c_i - \hat{c}_i}{\hat{c}_i} \right)^2},$$

where the entries of $\hat{c} = (\hat{c}_1, \ldots, \hat{c}_n)$ and $c = (c_1, \ldots, c_n)$ are geometric characteristics of the cells of the original foam and the model, respectively. In our case, these characteristics are the means and standard deviations of the volume $V$, surface area $S$, number of faces $N_{32}$, and diameter (mean width) $\bar{b}$ of the cells. See [19] for a detailed explanation of the choice of the features.

In practice, typically a parametric tessellation model is chosen by fixing the generating process and a parametric distribution for the sphere volumes. Then the value of $\rho(\hat{c}, c)$ in (1) is minimized on the parameter space of the model by repeated simulation of the model. An approach avoiding the time-consuming simulation was presented in [19] for Laguerre tessellations of dense packings of spheres with lognormal and gamma
distributed volumes. These models are of particular interest for the modeling of foam structures due to their regularity. Furthermore, the volume distribution in cellular materials is often assumed to be a lognormal or a gamma distribution. Hence, model realizations for various packing fractions $V_T$ and coefficients of variation $c$ of the volume distribution were generated. Subsequently, polynomials in $c$ were fitted to the estimated geometric characteristics for each value of $V_T$. Using these results, the minimization of the value of $\rho(\hat{c}, c)$ in (1) reduces to the minimization of a polynomial, which allows for a quick and easy model fit.

4. Relaxation of random tessellations with the Surface Evolver

The fitted Laguerre models are relaxed with the Surface Evolver [3], the standard software package for computing the cell-level structure of soap froth, a foam with minimal surface area.

The faces of the tessellation cells are interpreted as the thin liquid films that separate gas bubbles in soap froth. Relaxation simulates the process of evolution by mean curvature to form an equilibrium soap froth, which satisfies Plateau’s laws and minimizes surface area [28]. The minimization is constrained by preserving cell volumes. As a consequence of the angle conditions in Plateau’s laws, the cell faces in the relaxed structure are curved, and in general, the vertices of a face do not lie in a plane, neither of which is true of Laguerre tessellations.

Short edges are particularly unfavorable for surface-area minimization. During relaxation with the Surface Evolver, a significant fraction of the short edges shrink to zero length, which violates the Plateau condition requiring four edges to meet at each cell vertex. Local stability is restored by, so-called, T1 topological transitions, which are modifications of the structure and topology of the local cell neighborhood to produce vertices with four edges. Detailed descriptions of the computational algorithms can be found in [12, 13]; a brief summary is given here.

A T1 is performed when an edge is removed because its length is less than $p\%$ of the average edge length in the foam. The simulation parameter $p$ is normally between 1 and 10%, with 5% being typical. The iteration process is terminated when edges no longer shrink and provoke topology changes. Regardless of the exact value of $p$, relaxation typically produces Gaussian-like edge-length distributions.

Further reductions in surface area can be achieved by performing annealing cycles, in which the foam is subjected to large extension and compression deformations, followed by relaxation, along all three axes of the reference system. Annealing provokes additional topological transitions.

Computation time depends on the number of cells and the geometry of the triangular mesh that represents the curved surfaces. Relaxing large systems with 1728 cells typically requires over a day of computer time; annealing takes more than a week. This makes a repetition of the study in [19] for relaxed structures impractical. As a compromise, we fit a Laguerre tessellation to the foam structure using the method in [19] and then relax the resulting structure. In this way, we hope to improve the fit of the edge-length distribution.
without affecting the geometric characteristics used to fit the model. The extent to which this is achieved was studied for several real foam samples in the following.

5. Application to solid foam samples

To cover a wide range of foam microstructures, we study both open- and closed-cell foams made from either metal or polymer. The microstructure of the cell systems is analyzed using μCT images of the materials. The following list summarizes the available samples and image data.

- **Rohacell®** polymethacrylimide (PMI) closed-cell foam (WIND-F RC100), voxel size 2.72 μm, image size 1200 × 1100 × 1300 voxels,
- **Rohacell®** polymethacrylimide (PMI) closed-cell foam (RIST RC71), voxel size 2.7 μm, image size 1200 × 1440 × 1400 voxels,
- **Airex** polyvinyl-chloride (PVC) closed-cell foam (Airex T92-100), voxel size 7.26 μm, image size 700³ voxels,
- open-cell polymer foam, voxel size 70.88 μm, image size 670 × 670 × 270 voxels,
- open-cell aluminum foam (Al), voxel size 64.57 μm, image size 820 × 820 × 278 voxels,
- **Duocel®** open-cell copper foam (Cu), voxel size 38.15 μm, two images, image sizes 625 × 625 × 625 voxels and 635 × 630 × 640 voxels.

A complete analysis of the open-cell aluminum and polymer foams can be found in [19] and [27]. The open-cell copper foam is analyzed and modeled in [16]. The anisotropy of all three open-cell foams has been corrected as described in Section 3. The closed-cell PMI samples are also modeled in [27]. The closed-cell foams can be considered isotropic so the models are fitted directly to the unscaled images of microstructures. The results presented below are for the isotropic versions of the foams.

In Table 1, the moments of the characteristics of the samples and the parameters of the best fitting models are summarized. Models are fitted with the procedure outlined in [19] with respect to mean value and standard deviation of volume $V$, surface area $S$, mean width $b$, and number of faces per cell $N_{32}$.

For each sample, we simulate three realizations of random Laguerre tessellations generated by a force-biased sphere packings with the estimated parameters. Each realization contains 1000 cells and is relaxed with the Surface Evolver. In Figure 3, the original Laguerre tessellations and the corresponding relaxed structures for two different foams are shown. The high polydispersity of the Airex sample can be recognized by the occurrence of some very large cells, whereas the model of the aluminum foam is essentially monodisperse. Comparing the visualizations, one can see that the geometry of the cells is modified only locally and that
Table 1: Characteristics of the foams and parameters of the best-fitting models. Size features in mm.

<table>
<thead>
<tr>
<th>Foam Type</th>
<th>V</th>
<th>σ(V)</th>
<th>S</th>
<th>σ(S)</th>
<th>b̄</th>
<th>σ(b̄)</th>
<th>N_{32}</th>
<th>σ(N_{32})</th>
<th>(V_V,c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WIND-F</td>
<td>0.021</td>
<td>0.011</td>
<td>0.413</td>
<td>0.154</td>
<td>0.383</td>
<td>0.078</td>
<td>14.34</td>
<td>3.78</td>
<td>(60%,0.798)</td>
</tr>
<tr>
<td>RIST</td>
<td>0.021</td>
<td>0.013</td>
<td>0.395</td>
<td>0.151</td>
<td>0.364</td>
<td>0.067</td>
<td>13.78</td>
<td>3.68</td>
<td>(60%,0.853)</td>
</tr>
<tr>
<td>Airex</td>
<td>0.019</td>
<td>0.024</td>
<td>0.363</td>
<td>0.301</td>
<td>0.348</td>
<td>0.154</td>
<td>13.35</td>
<td>5.97</td>
<td>(60%,1.742)</td>
</tr>
<tr>
<td>Open poly</td>
<td>60.565</td>
<td>11.363</td>
<td>86.855</td>
<td>10.826</td>
<td>5.689</td>
<td>0.384</td>
<td>13.65</td>
<td>1.90</td>
<td>(30%,1.311)</td>
</tr>
<tr>
<td>Al foam</td>
<td>21.437</td>
<td>2.855</td>
<td>43.720</td>
<td>3.859</td>
<td>3.807</td>
<td>0.171</td>
<td>13.83</td>
<td>1.21</td>
<td>(60%,0.166)</td>
</tr>
<tr>
<td>Cu foam</td>
<td>49.234</td>
<td>9.591</td>
<td>79.777</td>
<td>10.286</td>
<td>5.083</td>
<td>0.322</td>
<td>13.91</td>
<td>1.48</td>
<td>(60%,0.286)</td>
</tr>
</tbody>
</table>

The relaxed models appear to be more regular because there are fewer short edges and the faces have fewer small angles.

Figure 3: Visualizations of the Laguerre and corresponding relaxed models for the samples of Airex (left) and aluminum foam (right). Model parameters: (V_V,c) = (60%,1.742) for Airex, (V_V,c) = (60%,0.166) for aluminum. Visualizations with Surface Evolver.

The edge-length distributions of the samples and models are shown in Figure 4. The edge lengths in the real foams were computed from the CT images using the algorithm presented in [27]. This algorithm is used to reconstruct the vertices of the foam cells, from which the edge-length distribution is easily calculated. We also investigate the distributions of surface area and diameter of the cells, the number of faces per cell, and the number N_{21} of edges per face, which are shown in Figures 5 to 8. With the exception of cell volume, these include all characteristics used for fitting the Laguerre tessellations. The volume distributions are not shown because relaxation preserves cell volumes so the distributions for the Laguerre and relaxed models coincide.

In all samples, the distributions of surface area (Figure 5) and number of faces per cell (Figure 7) are similar in both models. Typically, the difference between the two models is smaller than the difference between either of them and the real structure. The distributions of cell diameter (Figure 6) show similar behavior for the open-cell foams. A slight improvement following relaxation is evident in the distribution of
the number of faces per cell for the open-cell foams and in the diameter distribution for Airex. In contrast, the
fit of the diameter distribution is slightly reduced by relaxation for the two other closed-cell foams. In total,
we conclude that the goodness-of-fit obtained by estimating the parameters of the Laguerre tessellation is
not degraded by relaxation. However, a clear change in the edge-length distribution (Figure 4) is observed.
As expected, the number of short edges is reduced by relaxation, but the goodness-of-fit of edge-length
distributions appears to depend on whether the cells are open or closed.

The three samples of open-cell foam behave similarly. The edge-length distributions show high peaks
and fewer short edges. Consequently, they are fitted much better by relaxed models than by Laguerre
tessellations.

The two PMI foams show different behavior: the edge-length distributions are wider and have a lower
peak and more short edges than the open-cell foams. Consequently, relaxation removes too many short
edges, and produces edge-length distributions that are too narrow.

The sample of Airex shows a hybrid behavior. The edge-length distribution has a high peak, but the
shape of the distribution is different from the relaxed models and leans towards short edges. Hence, it is not
clear which model is a better fit to this material.

The open-cell foams are significantly less polydisperse than the closed-cell foams that were analyzed in
this study. The open-cell foams have coefficients of variation of cell volumes ranging between 0.13 and 0.20,
while the closed polymer foams show a higher polydispersity with coefficients of variation of 0.52 (WIND),
0.62 (RIST) and 1.26 (Airex). The standard deviation of $N_{32}$ is also much higher for the closed-cell foams
than the open-cell foams. This is consistent with Surface Evolver simulations [13], which indicate that $\sigma(N_{32})$
increases as polydispersity increases, as exemplified by Airex.

6. Discussion

Random tessellation models are capable of reproducing many significant features of the distributions
of cell characteristics in real foams; however, they fail to reproduce realistic edge-length distributions. To
overcome this problem, the model fitting procedure in [19] was supplemented by relaxing the resulting
tessellations with the Surface Evolver. The examples presented in this paper indicate that the distributions
of geometric characteristics used to fit the model are not strongly influenced by the additional relaxation
step. Hence, the goodness-of-fit of the tessellation model is not degraded by relaxation.

The results indicate that relaxation significantly improves the edge-length distribution of the open-cell
foams, which are nearly monodisperse. The benefit of relaxation on the edge-length distribution of the closed-
cell foams, which are highly polydisperse, is more difficult to judge. More realistic models of closed-cell foams
probably require the development of accurate simulations of bubble growth that account for viscous flow. It
is impossible to distinguish between open cells or low polydispersity as the key characteristic, therefore, it
would be very useful to extend this analysis to high-polydispersity open-cell foams and low-polydispersity closed-cell foams.

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References


Figure 4: Edge-length distribution estimated from the samples compared with the edge length distribution in the fitted Laguerre tessellations and in the relaxed models.
Figure 5: Cell surface area distribution estimated from the samples compared with the cell surface area distribution in the fitted Laguerre tessellations and in the relaxed models.
Figure 6: Cell diameter distribution estimated from the samples compared with the cell diameter distribution in the fitted Laguerre tessellations and in the relaxed models.
Figure 7: Distribution of the number of faces per cell estimated from the samples compared with the number of faces per cell in the fitted Laguerre tessellations and in the relaxed models.
Figure 8: Distribution of the number of edges per face estimated from the samples compared with the number of edges per face in the fitted Laguerre tessellations and in the relaxed models.