Space-Filling Polyhedra as Mechanical Models for Solidified Dry Foams

Thomas Daxner, Robert D. Bitsche and Helmut J. Böhm

Institute of Lightweight Design and Structural Biomechanics, Vienna University of Technology, Gusshausstr. 27-29(317), A-1040 Vienna, Austria

The simulation of the mechanical behavior of idealized cellular structures is important as it gives insight into the principal deformation mechanisms that govern the mechanical behavior of real cellular structures, such as polymer foams or metallic foams, making accessible at least qualitative information about properties that are difficult to determine otherwise, for example the effective strength under hydrostatic loading. For capturing the mechanics of a closed-cell foam material in a meaningful way, three-dimensional models are employed in the context of the Finite Element method. The modeling approach presented in this paper employs generic, periodic unit cell models with the extension of providing physically sound microstructures by basing these models on surfaces of minimal energy calculated with the program Surface Evolver. This program is able to minimize the energy of a surface subject to given constraints, for example a prescribed initial geometry and, where required, periodicity. Accordingly, space-filling polyhedra with cells being separated by walls of minimal total area can be predicted, such as Lord Kelvin’s tetrakaidecahedra or the Weaire-Phelan partition, the latter being energetically more favorable. These physics-based configurations are good representations of solidified (dry) foams. The results obtained by Finite Element stress and deformation analyses comprise the full tensor of elasticity and its dependence on the effective density; the non-planar faces resulting from the surface energy minimization are shown to influence the behavior for very low effective densities. By studying the behavior up to the onset of yielding on the effective, macro-mechanical level including the effects of multi-axial loading conditions, valuable information for the homogenized representation of closed-cell foams is obtained. [doi:10.2320/matertrans.47.2213]

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1. Introduction

Closed-cell cellular structures often exhibit excellent weight-specific mechanical properties, and are, therefore, well suited for application in lightweight design and construction.

If the average size of individual cells is some orders of magnitude smaller than the characteristic size of the cellular component, then the effective mechanical behavior of the aggregate of cells can be described in terms of a homogenized material, which interacts with the rest of the component or structure just as the cellular structure does. The present paper is devoted to the determination of effective mechanical properties for closed-cell cellular materials that fulfill this condition.

Closed-cell cellular structures are very often produced by foaming processes involving a gaseous phase and a liquid phase which is submitted to a phase-change resulting in a foam-like structure with solid cell walls, struts and vertices. A rich body of literature exists on the behavior of liquid foams. The book ‘The Physics of Foams’ by Weaire and Hutzler1 shall be cited here for reference.

The generation and evolution of liquid foams is driven by surface tension and drainage. Usually, a considerable fraction of the liquid is confined in the junction lines between the individual fluid films making up the cell walls. These curved transition regions between adjacent cell walls are called Plateau borders. For dry foams, that is, foams of very low fluid content, these Plateau borders can be replaced by simple junction lines. We consider such dry foams in the following.

From mechanical equilibrium conditions a number of rules can be derived for dry, liquid foams: the law of Laplace states that only a surface of zero mean curvature can separate two cells that have the same internal gas pressure. The laws of Plateau demand that the films can intersect only three at a time and must do so at 120 degrees. Furthermore, no more than four of the intersection lines may meet at the vertices of the foam and those tetrahedral vertices have to be perfectly symmetric, with adjacent edges forming an angle of 109.47 degrees each.

These laws put considerable restrictions on the choice of space-filling cellular structures that are adequate for representing the geometry of dry foams. If, in addition, the structure is sought to be mono-disperse, that is, made up by cells all having the same volume, then the choice is even more restricted.

A well-investigated candidate structure is Kelvin’s tetrakaidecahedron, which can be envisaged as an octahedron, the corners of which have been truncated, leaving a base cell with 6 quadrilateral faces and 8 hexagonal faces, see Fig. 1. One of the earliest papers using Finite Element models based on equilateral tetrakaidecahedra structures was published by Simone and Gibson2 who investigated the effects of the distribution of material between the cell walls and the Plateau borders on the stiffness and strength of 2D-honeycombs and 3D-Kelvin foams. To the best of our knowledge no other author has since modelled the geometry of Plateau borders with continuum Finite Elements in three dimensions.

Equilateral tetrakaidecahedral structures were one out of several regular cellular structures for which the effective elastic behavior was determined by Grenestedt.3) Grenestedt and Tanaka4 extended this work by randomly disturbing the regularity of the tetrakaidecahedra cell aggregate and by observing the resulting changes of the effective stiffness. A different kind of imperfection was introduced by Grenestedt and Bassine5 by randomly changing the thickness of individual faces in an equilateral tetrakaidecahedra structure. Roberts and Garboczi6 included equilateral tetrakaidecahedral structures as reference structures in their paper on the elastic moduli of random closed-cell cellular solids. They employed a voxel-to-element approach obtaining a continuum Finite Element model.
As a matter of simplification, all of the beforementioned studies treat the hexagonal faces of the tetrakaidecahedra structure as being flat, which is not strictly the case when considering the geometry of a dry Kelvin foam, as we try to emphasize in Fig. 1, where the corrugation of one of those faces is magnified. The influence of arbitrary face curvature and corrugations on the stiffness and strength of equilateral tetrakaidecahedral structures was investigated by Simone and Gibson.7)

Perhaps less well known is the Weaire-Phelan structure, which was presented8) as an example for a space-filling, periodic, monodisperse dry foam structure that has lower surface energy than the Kelvin structure. The Weaire-Phelan structure consists of pentagonal dodecahedra with non-planar faces and tetrakaidecahedra with two flat hexagonal faces and twelve non-planar pentagonal faces,9) compare Fig. 2. Albeit being more representative of real foam than Kelvin’s structure, the Weaire-Phelan structure has received no particular attention from the solid mechanics point of view, and is, consequently, chosen as the focus of the present paper.

Furthermore, the implications of the slight curvature of the cell walls, which is a consequence of the laws of Plateau being fulfilled in the dry foam prior to solidification, will be addressed.

2. Method

The effective mechanical properties of space-filling Kelvin and Weaire-Phelan structures are determined by discretizing periodically repeating unit-cells by means of the Finite Element (FE) method and deducing the effective relationships between stresses and strains from the displacements and the nodal forces of master FE nodes, which are coupled to the rest of the structure by appropriate constraint equations.

Representing a cellular material by a representative, periodically space-filling unit-cell is a well-introduced method in micro-mechanics of materials, often referred to as the unit-cell method or a periodic micro-field approach. The unit cell in Fig. 1 and the respective unit cell for the Weaire-Phelan structure (not shown) are chosen sufficiently large to allow for periodic deformation patterns, which is essential for simulating shear deformations. The Finite Element code ABAQUS10) was used, and a discretization with bi-linear, triangular shell elements with a sufficiently high mesh refinement was chosen.

The apparent density $\rho^*$ was used in connection with the density $\rho_S$ of the solid (cell wall) material to define the relative apparent density $\rho_{rel} = \rho^*/\rho_S$ and, thus, the fraction of solid material in the unit cell. This volume fraction was used directly for calibrating the shell thickness. It has to be noted that overlapping of the cell walls as a consequence of the intersection of shell elements at the cell face junction lines is not specifically accounted for, and no corresponding correction of the apparent density was performed.

The mesh geometry, that is, the position of the FE nodes, was obtained by means of the program Surface Evolver by K. Brakke,11) which is capable of calculating the shape of membranes of minimal surface energy under periodicity constraints by means of a triangular discretization. This program is well-suited for predicting the geometries of dry, liquid foams, which are chosen as the base geometries for the shell FE models in this paper.

Details on the practice of applying effective (far field) stresses and strains to a given unit cell via concentrated nodal forces or prescribed displacements at the master nodes can be found in a paper by Michel et al.,12) where the term ‘method of macroscopic degrees of freedom’ is introduced.

The bulk material of the structure is modeled as an isotropic elasto-plastic solid governed by $J_2$-plasticity with isotropic hardening. The bulk material parameters were selected in order to represent those of a generic aluminum foam; the Young’s modulus and Poisson’s ratio of the solid material are chosen as $E_S = 70$ GPa and $\nu_S = 0.3$, respectively. Above the yield limit, the hardening behavior is calibrated such that the relationship between the true uniaxial stress $\sigma_S$ and the uniaxial logarithmic strain $\varepsilon_S$ obeys the

![Fig. 1 Unit cell of the Kelvin foam structure. The corrugation of one hexagonal face is displayed with a magnification factor of 10.](image1)

![Fig. 2 A cluster of unit cells building up the Weaire-Phelan foam structure.](image2)
power function $\sigma = K(\varepsilon)^n$, with the exponent being chosen as $n = 0.1$ and the coefficient $K$ set to $K = 486.96$ MPa giving an ultimate engineering stress of $\sigma_{ult} = 350$ MPa in a hypothetical tension test of this material.

For obtaining the effective tensor of elasticity a general procedure involving the prediction of the linear elastic deformations of the unit cell under six linearly independent load cases was followed. For each load case ($m = 1 \ldots 6$) the respective engineering strain and stress tensors, $\varepsilon_{ij}^{(m)}$ and $\sigma_{ij}^{(m)}$, were determined, and Hooke’s Law:

$$
\sigma_{ij}^{(m)} = E_{ijkl}^{(m)}\varepsilon_{kl}^{(m)}
$$

... was formulated, which, in combination with considering the symmetry of the involved tensors, gave enough equations for determining the components $E_{ijkl}$ of the effective tensor of elasticity $E$. The considered six load cases comprised the application of uniaxial, tensile unit stresses in the directions of all three axes of the reference coordinate system as well as loading by unit shear stresses in the three planes mutually spanned by those axes, respectively. Note, that the cubic structural symmetry was not exploited in this context.

Regarding the effective non-linear behavior the simulations were extended to the domain of geometrical and material non-linearity with the objective of identifying initial yield surfaces. The onset of macroscopic yielding was defined (arbitrarily) by those loading states, for which-after elastic unloading-the root-mean-square of the components of the tensor of macroscopic residual (plastic) strain starts to exceed an equivalent value of $\varepsilon_{pl} = 0.2\%$. Under the assumption of an additive split of the total macroscopic strain tensor $\varepsilon_{ij}$ into an elastic and a plastic part, the plastic strain components can be found by:

$$
\varepsilon_{ij}^{(pl)} = \varepsilon_{ij} - C_{ijkl}\sigma_{kl},
$$

where the components $C_{ijkl}$ are associated with the compliance tensor $C = 1/E$.

It was soon established that the elastic unloading procedure did not show any noticeable non-linearity in the FE simulations. Therefore, the effective, plastic residual strains were calculated directly by subtracting the elastic part of the strain tensor from the total strain tensor according to eq. (2).

3. Results and Discussion

The effective elastic properties of a micro-structural material possessing cubic structural symmetry can be described by an effective elastic modulus $E^*$, an effective Poisson’s ratio $\nu^*$ and an effective shear modulus $G^*$ with respect to a coordinate system that is spanned by the intersection lines ($x$, $y$, $z$) of the three symmetry planes. As opposed to isotropic elastic behavior these three parameters are independent of each other for a material with cubic symmetry. In this context we also use the notation ‘[100]’ and ‘[111]’ of Miller for describing the directions along the $x$-axis and along the space diagonal of the unit cell, respectively.

Out of these material parameters we first take a look at the effective elastic modulus $E_{[100]}^*$ along the axes of the symmetry coordinate system. Figure 3 shows the dependence of this material stiffness on the apparent relative density of the material. This relationship is almost linear indicating that cell wall stretching is the dominant mode of deformation for the considered closed-cell structures. For intermediate and high relative densities the modulus $E_{[100]}^*$ of the Weaire-Phelan structure is about 10% larger than the one for the Kelvin structure. This trend is reversed for very small densities, where the Kelvin structure becomes stiffer than the Weaire-Phelan structure in the [100]-direction.

As far as the effective shear modulus $G^*$ is concerned, Figure 3 shows this parameter being approximately 10% larger for the Kelvin structure compared to the Weaire-Phelan structure at intermediate to high relative densities. For very low densities the roles reverse once more and the Weaire-Phelan structure becomes stiffer with respect to shear than the Kelvin structure.

The effect of the relative apparent density on the transverse behavior of the cellular structures is described by plots of the effective Poisson’s ratios in Fig. 4. In this figure dashed lines indicate the results for reference structures with flat cell walls, whereas the solid lines give the density dependence of the structures based on the dry foams’ geometries. Values for $\nu^*$ reported by Grenestedt for flat-celled tetrakaidecahedra structures are given for comparison. They fit very well with the values found for the respective structures in the present investigation. For very low apparent densities the Poisson’s ratio of the flat Kelvin and Weaire-Phelan structures are 0.328 and 0.32, respectively. For higher apparent densities these values decrease slightly with 0.32 being a good average value.

A markedly non-linear dependence of the Poisson’s ratio of the structures with corrugated cell walls on the relative apparent density can be observed for relative apparent densities below 5%. By means of analogy, namely in the form of the stiffness of a curved beam, it can be shown that this strong deviation for low densities can indeed be explained by the relationship of the cell wall thickness and the amplitude of the corrugations, which was the same for all the considered models.

Another important aspect of the linear elastic behavior of the structures under investigation is the direction dependence of the elastic properties, which is a consequence of their inherent cubic anisotropy. In the following we focus on the direction dependence of the effective elastic modulus $E^*$.
For calculating the effective Young’s modulus for arbitrary uniaxial loading direction some basics of elasticity and tensor algebra have to be recalled.

The tensor of compliance $C$ is defined as the inverse $C = E^{-1}$ of the tensor of elasticity $E$. The inverse of the projection $C_n$ of the tensor of compliance along a given normalized direction vector $n$ is equivalent to the effective elastic modulus $E_n$ that can be observed when the structure is loaded unidirectionally in the direction $n$:

$$E_n = (n \otimes n) : \left( C_{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l \right): (n \otimes n)^{-1}$$  \hspace{1cm} (3)

In eq. (3) the symbols ‘$\otimes$’ and ‘$:$’ denote the dyadic product and the double contraction of two tensors, respectively. Eq. (3) gives the sought relationship between the loading direction vector $n$ and the effective elastic modulus along this direction.

In Fig. 3 this was exploited for predicting the modulus $E_{[111]}^*$ along the space diagonal of the cellular structures. Cubic symmetry dictates that the extrema of the elastic moduli must coincide with the [100] and the [111] directions. Considering the Kelvin structure, it shows that the modulus $E_{[111]}^*$ tends to be up to 15% larger than the modulus $E_{[100]}^*$. For the Weaire-Phelan structure the modulus $E_{[111]}^*$ is up to 3% smaller at high apparent densities. In other words the anisotropy of the structures with respect to the elastic modulus is much more pronounced for the Kelvin structure than for the Weaire-Phelan structure. This is indicated by the hashed areas between the bounding $E_{[100]}^*$ and $E_{[111]}^*$ curves for the effective moduli in Fig. 3. One consequence of this relationship is that the average effective Young’s modulus is effectively the same for both structures with the relative difference being below 1% for intermediate and high relative densities. Again, the relationships are more complicated for small apparent densities owing to the strong relative influence of the cell wall corrugations for these cases.

For examining this point further we define the degree of anisotropy $a$ of a structure showing cubic symmetry by the ratio of the effective elastic modulus $E_{[111]}^*$ in the [111] direction and the modulus $E_{[100]}^*$ in the [100] direction:

$$a = \frac{E_{[111]}^*}{E_{[100]}^*}$$ \hspace{1cm} (4)

Plotting this measure for the anisotropy of the structures we come up with the diagram shown in Fig. 5. Above 5% of relative density the ratio between the highest and the lowest elastic modulus for a given structure and density is not strongly dependent on the relative density itself. The fact that the curve for the Weaire-Phelan structure runs very close to the horizontal line for $a = 1$ indicates that the direction dependence of the elastic modulus and, hence, the anisotropy is not very pronounced.

Below 5% relative apparent density the anisotropy measure $a$ becomes strongly dependent of the relative density. Furthermore, the maxima and minima of the elastic moduli switch from the [100] to the [111] direction (and vice versa) below a certain threshold density, for which the moduli $E_{[100]}^*$ and $E_{[111]}^*$ are identical ($a = 1$) and for which the structure behaves isotropically. The dashed lines in Fig. 5 do not intersect the $a = 1$ line indicating that direction-independent elastic moduli can be obtained only for the structures with corrugated cell walls.

The anisotropy of the elastic modulus can also be visualized in the form of 3D plots as is demonstrated in Fig. 6. Here, a surface is defined by a set of vectors, the direction of which coincides with a given loading direction, and the length of which corresponds to the elastic modulus experienced in this loading direction. To further the three-dimensional impression the relative value of the elastic modulus is coded by shades of grey on the surfaces, with light values indicating large moduli and dark values indicating small moduli. The degree of anisotropy can be judged visually by the degree of deviation of these ‘anisotropy surfaces’ from the shape of an ideal sphere. In Fig. 6 the Kelvin and the Weaire-Phelan structures are each considered at a very low ($\rho^*/\rho_S = 0.1\%$) and a very high density ($\rho^*/\rho_S = 25\%$). The direction-dependence of the elastic modulus of the Kelvin structures is represented in Fig. 6(a) for a relative density of $\rho^*/\rho_S = 0.1\%$ and in Fig. 6(c) for a relative density of $\rho^*/\rho_S = 25\%$. The same results are presented in Fig. 6(b) for the Weaire-Phelan structure with a relative density of $\rho^*/\rho_S = 0.1\%$ and in Fig. 6(d) for the same structure with a relative density of $\rho^*/\rho_S = 25\%$.

The low-density structures represent a pretty extreme end of the density scale, and exhibit, in accordance with Fig. 5, comparatively high degrees of anisotropy caused by the
corrugated cell walls. The shapes of the corresponding ‘surfaces of anisotropy’ resemble rather octahedra or cubes than sphere-shaped objects. The opposite is true for high relative apparent densities, where, especially for the case of the Weaire-Phelan structure, the ‘surface of anisotropy’ can hardly be distinguished from a sphere that would represent perfect isotropy.

Beside the effective elastic properties of the two structures the limit of linear elastic behavior was a subject of this investigation. This limit was defined by a threshold value of a chosen norm of the plastic macroscopic strain tensor, which was produced during the considered multi-axial loading scenarios; details of this procedure can be found in Section 2. By performing non-linear simulations for different linear loading paths in the space of macroscopic normal stresses, it was possible to probe the macroscopic yield surfaces of the structures.

Figure 7 shows visualizations of such yield surfaces in the three-dimensional space spanned by the normal stress components \(\sigma_{xx}, \sigma_{yy}, \sigma_{zz}\), which are identical to the principal stress components in the considered three-axial loading scenarios. The yield surfaces are determined for a Kelvin unit-cell model and a Weaire-Phelan unit-cell model with a relative density of 10% each.

The shape of both yield surfaces is that of an ellipsoid which is aligned with the axis of purely hydrostatic stress states. This shape is very similar to the cigar-shaped yield surfaces described by quadratic macroscopic failure criteria for metallic foams such as, for example, the Deshpande-Fleck yield criterion.\(^\text{13}\) Yield surfaces of this shape can also be found in experiments on metallic foams which are able to achieve multi-axial loading conditions.\(^\text{13}\)

The length of the ellipsoid is approximately four times as large as its equatorial radius. This indicates that the effective hydrostatic strength is well above the effective uniaxial strength of the respective materials. The hydrostatic yield strength of the Kelvin and the Weaire-Phelan structures under tension is almost the same, namely 19.51 and 19.42 MPa, respectively, for 10% relative apparent density. This makes the Kelvin structure slightly (by 0.46%) more resistant against hydrostatic tensile loads than the Weaire-Phelan structure.

The yield stress under hydrostatic compression is approximately the same as the one under hydrostatic tension. Unfortunately, though, the respective simulation protocols indicate that instability points were crossed during the loading process, and, thus, great caution has to be taken when interpreting these results. Vertices on the yield surfaces for which the occurrence of instabilities cannot be excluded are marked by a darker shade of gray in Fig. 7. It has to be assumed that the equilibrium paths that were followed for the determination of these points on the yield surfaces are unstable ones, and therefore, the respective vertices have no actual physical relevance. The gray zone of unstable macroscopic stress states forms a cap on the yield surface around the ‘pole’ corresponding to yielding under purely hydrostatic pressure loading.

The yield strength under uniaxial loading shows a maximum scatter of ±5% around a mean value of 11.2 MPa for the Kelvin structure of 10% relative density. For the Weaire-Phelan structure these data are 12.6 MPa ±2.8%. These results indicate a 12.5% larger uniaxial yield strength for the Weaire-Phelan structure as compared to the Kelvin structure. Furthermore, the uniaxial yield strength depends
that is equivalent to the one of dry, liquid foams, this paper presented two candidate unit cells for space-filling, monodisperse foam structures, namely the Kelvin structure and the Weaire-Phelan structure. The effective mechanical properties of materials, which are built up by filling their respective macroscopic domain by repeating those base structures periodically, are expressed in terms of their effective tensors of elasticity and their effective yield surfaces.

Both structures possess cubic symmetry. The Kelvin structures show a larger degree of anisotropy, and, therefore, a larger direction-dependence of the effective elastic modulus than the Weaire-Phelan structures. The average effective elastic modulus, though, is approximately the same for both structures provided they have the same apparent density.

For the relative density range up to 25%, the relationship between effective average modulus and apparent relative density can be described well by a more or less linear function. The fact that some of the cell walls are non-planar in order to fulfill the laws of Plateau for dry, liquid foams affects the mechanical behavior of the solid structures derived from these foams, and must not be disregarded for low-density models (apparent relative density below 5%).

With respect to the onset of yielding under multi-axial loading conditions, no significant differences could be found between Kelvin and Weaire-Phelan structures. Both types of cellular structures give the same characteristic ellipsoidal shape of the yield surface in the three-dimensional space of normal stress components that has been observed in multi-axial experiments. The quantitative differences are in the range of a few percent.

The properties of the Kelvin structures show, again, a higher degree of direction-dependence than the Weaire-Phelan structures. The major conclusions that can be drawn from this work are (a) the average effective mechanical properties of Kelvin and Weaire-Phelan structures are the same to within a few percent, (b) the Weaire-Phelan structure exhibits less anisotropy than the Kelvin structure, and (c) the influence of cell wall curvature must not be neglected for foams of very low apparent density. Considering that the Weaire-Phelan structure is a closer representation of the topology of actual foam cells its use can be recommended for further studies.

REFERENCES