Tensorial Minkowski functionals of triply periodic minimal surfaces

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A fundamental understanding of the formation and properties of a complex spatial structure relies on robust quantitative tools to characterize morphology. A systematic approach to the characterization of average properties of anisotropic complex interfacial geometries is provided by integral geometry which furnishes a family of morphological descriptors known as tensorial Minkowski functionals. These functionals are curvature-weighted integrals of tensor products of position vectors and surface normal vectors over the interfacial surface. We here demonstrate their use by application to non-cubic triply periodic minimal surface model geometries, whose Weierstrass parametrizations allow for accurate numerical computation of the Minkowski tensors.

Keywords: morphology; anisotropy; lipid self-assembly; minimal surface; porous material; integral geometry

1. INTRODUCTION

Nature provides impressive examples of network-like labyrinthine geometries based on triply periodic minimal surfaces (TPMS), with the notable example of the cubic srs network or gyroid structure [1] realized, for example, in the wing-scales of several butterfly species where it acts as a photonic crystal [2–5]. Other physical systems that adopt a labyrinthine geometry as their spatial structure include self-assembly processes into bicontinuous mesophases of diblock co-polymers [6,7] and linear terblock co-polymers [8], of lyotropic liquid crystals [9–11] including lipid–water biochemical systems [12–15] and of synthetic surfactants [16], mesoporous inorganic materials synthesized in the presence of amphiphiles [17] and condensed mesoporous inorganics [18], late stage spinodal decomposition in polymer blends [19], biomineralization in crustacean shells [20], and the alveolar surface of a rabbit lung [21]. While the bulk of these labyrinthine phases are of cubic symmetry, anisotropic non-cubic TPMS have also been identified, in linear tri-block polymers [8], tri-continuous hexagonal mesoporous silica systems [22] and in non-cubic deformation modes in lung surfactants of rabbits [21].

These labyrinthine geometries have the defining property that all of the constituent components or phases (i.e. the solid chitin phase and the void phase in the butterfly wing-scales [2–5], or the lipid bilayer and the aqueous channels in lipid self-assembled Q230 phases [23], etc.) are continuous and connected throughout the whole system. Because of this topological property, labyrinthine geometries can be beneficial for the effective design of modern materials. The material properties affected by the labyrinthine topology are, among several others, effective elastic properties [24], heat transport and electrical conduction [25], and photonic properties [26,27], also in the presence of circularly polarized light [28]. Furthermore, several physical processes which take place in labyrinths depend on their shape. Processes that occur inside labyrinths and whose properties depend on their shape include adsorption, catalysis and adhesion [29–32], for instance. Also capillary condensation, i.e. the reduction of the critical point of a fluid in confined pores (for a review, see [33]) and flow phenomena in porous materials [34,35] are crucially influenced by the confining geometry.

The description, analysis and modelling of such processes rely on a thorough understanding of ‘labyrinthine geometry’. The process of developing this understanding consists in two parts: (i) defining labyrinthine model geometries and (ii) defining suitable shape descriptors which correlate with or determine physical properties.

The catalogue of labyrinthine model geometries has grown considerably in the last three decades. Among periodic and ordered labyrinth models are bicontinuous TPMS where the interface is a minimal surface [1,36–43] (figure 1). Out of the large class of TPMS, the three cubic surfaces, Primitive and Diamond [36] and Gyroid [1], have become famous, because of their ubiquity in soft-matter systems. Other labyrinthine model geometries are constant mean curvature surfaces [45], level sets of sums over Fourier modes [46–48], polycrystalline space partitions [49–51] and complements of symmetric packings of convex particles. Models for disordered labyrinths, at least without a long-range order, include...
Gaussian random fields [52, 53]. Further generation techniques for labyrinthine geometries include derivation of both ordered and disordered labyrinth geometries from three-dimensional networks, using network enumeration approaches such as epinet [54].

2. GEOMETRIC DESCRIPTION OF INTERFACES

A quantitative morphological description of labyrinthine geometries, which is relevant to the resulting physical points, is essential for a physically motivated understanding of labyrinthine geometry. One systematic approach is provided by integral geometry which furnishes a suitable family of morphological descriptors, the so-called Minkowski functionals [55]. These shape measures are related geometrically to curvature integrals. Scalar Minkowski functionals have been used to derive thermodynamic relationships and structure–property relations for condensed matter systems (such as a lipid-bilayer self-assembly), for which a curvature-based description by Helfrich functionals [61] is appropriate, the implications are considerable: as curvature fluctuations correspond to energy penalties this means that any labyrinthine mesophase is frustrated. Different candidate geometries with different amount of frustration compete, in contrast to the elliptic and parabolic cases where the uniqueness of spherical micelles and hexagonal cylinder phases are a testimony to the optimality of the sphere and the cylinder.

Essentially addressing this specific fact but motivated by a soft-matter self-assembly, a large body of physics literature has analysed labyrinthine model geometries in terms of their curvature properties. In various disguises, the distribution of curvatures on the surface, or scalar moments of those distributions, are the focus of those studies. Much of this work [11, 41, 62, 63] has looked at TPMS as a specific model system because of their ubiquity in soft-matter physics.

In addition to the local curvature properties of the interface, the geometry of a labyrinth is also characterized by global or off-surface properties. Scalar descriptors of global embedding are \( V/A \) ratios, scale-invariant homogeneity indices [64] or topology indices [65]. Domain width and channel radius variations, conveniently quantified by the distance from TPMS to a centred medial surface [66–69] or to a centred skeletal graph [70, 71] or by the so-called covering radius transform [24], represent a further way to quantify off-surface properties.

Integral geometry provides an alternative way of quantifying both the on- and off-surface geometric properties of labyrinthine surfaces: instead of analysing distributions of curvatures or channel diameters, integrated measures of parallel bodies are considered. The parallel body (or dilation) of a labyrinth surface with thickness \( \varepsilon \) is defined as the sub-volume of one of the labyrinthine domains composed of all points with a distance less than \( \varepsilon \) from the original interface. The Minkowski functionals are then defined as the volume.
the area, the integrated mean curvature and the Euler index of the parallel body, and are considered as functions of ε [72]. For small ε (i.e., smaller than both the inverse of the maximal principal curvature and the minimal medial surface distance [66]) these functions relate to curvature integrals of the original interface with ε = 0 (Steiner formula); for larger ε, for which the topology and smoothness of the parallel body may differ from that of the original surface, these functions capture global properties of the embedding of the surface as well as local aspects. Various systems have been analysed with this approach, including porous materials [35], reaction–diffusion systems [73] and dewetting of thin films [74]. However, several of the aspects relating integral geometry to labyrinthine geometries and the relationship to the curvature and distance distributions are still not fully explored.

2.1. Minkowski functionals and tensors

Minkowski functionals constitute a family of measures which discriminate spatial patterns according to size, shape and connectivity. These scalar descriptors can be generalized by tensor-valued curvature measures, which provide additional morphological information on orientation and anisotropy. These scalar functionals as well as their vector-valued counterparts have been investigated for a long time in mathematics [75,76] as well as in physics [77]. Their higher-rank tensorial generalizations have only recently become used in the context of physics and material science [57–59,78–81] (see [57,78] for an overview).

Scalar Minkowski functionals are (the only linear-independent) motion-invariant and convex-continuous functionals of equation (2.4) are of the above-defined Minkowski tensors are linearly independent, in addition to trivially tensorial functionals obtained by multiplying scalar Minkowski functionals with the rank-2 unit tensor E [82] (see also the discussion in the study of Schroeder-Turk et al. [57]). Out of these six tensorial functionals, the two translation-invariant (but rotation-covariant) tensors W_{1}^{0,2} and W_{2}^{0,2} are of particular importance for the characterization of infinite structure. For d = 3, the definitions of equation (2.4) are

\[ W_{0}(K) = \int_{K} \text{d}x, \quad (2.1) \]

with \( \text{d}x \) being the d-dimensional volume element and d further measures, which are located on the bounding surface \( \partial K \) of \( K \); for the special case of a smooth surface, these can be written as surface integrals

\[ W_{v}(K) = \frac{1}{v} \int_{\partial K} \text{d}A d^{d-1}(\kappa_{1}, \ldots, \kappa_{d-1}) \quad (2.2) \]

for \( v = 1, \ldots, d \). Here, \( d^{d-1} \) denotes the \( (d-1) \)-dimensional surface element (specifically for \( d = 3 \), we henceforth use the abbreviation \( \text{d}A = \text{d}A^{2} \)) and \( \kappa_{i} \) with \( i = 1, \ldots, (d-1) \) the principal curvatures. The Minkowski functionals therefore quantify curvature. The elementary symmetric functions \( s_{\kappa}^{(d-1)} \) are defined implicitly by the relationship

\[ \prod_{\mu=1}^{d-1} (x_{\mu} + \varepsilon) = \sum_{v=0}^{d-1} \varepsilon^{s_{\kappa}^{(d-1)}(x_{1}, \ldots, x_{d-1})} (2.3) \]

for arbitrary numbers \( x_{\mu} \in \mathbb{R} \) for \( \mu = 1, \ldots, d-1 \). Specifically for \( d = 3 \) and with \( x_{1} = k_{1} \) and \( x_{2} = k_{2} \) the principal curvatures, the elementary symmetric functions are \( s_{\kappa}^{(2)}(k_{1}, k_{2}) = 0 \), \( s_{\kappa}^{(2)}(k_{1}, k_{2}) = k_{1} + k_{2} = 2H \) (with the mean curvature \( H \)) and \( s_{\kappa}^{(2)}(k_{1}, k_{2}) = k_{1}k_{2} = G \) (with the Gauss curvature \( G \)).

Tensorial Minkowski functionals, also called ‘Minkowski tensors’, are obtained as a generalization of the surface integrals in equation (2.2). Minkowski tensors are motion-covariant functionals

\[ W_{v}(x) = \int_{\partial K} \text{d}A^{d-1}(\kappa_{1}, \ldots, \kappa_{d-1}) \quad (2.4) \]

for \( v = 1, \ldots, d \) and \( r, s = 0, 1, \ldots \), where \( x \) is the position vector, \( n \) the surface normal vector, and the product of tensors and vectors defined by the fully symmetric tensor product \( \otimes \); for example, for two vectors \( a \) and \( b \) the product is a rank-2 tensor with components \( (a \otimes b)_{ij} = (a_{i}b_{j} + a_{j}b_{i})/2 \), and \( a^{\otimes 2} := a \otimes a \). The rank of the tensor \( W_{v}^{r,s} \) is \( r + s \). The set of Minkowski tensors is complemented by a generalization of the volume integral of equations (2.1) to

\[ W_{0}(K) = \int_{\partial K} \text{d}x. \quad (2.5) \]

Formally, we set \( W_{v}^{r,s} = 0 \) for \( v > d \); for \( v, s, r < 0 \); and for \( s > 0 \) if \( v = 0 \).

Specifically for bodies in three-dimensional space, six of the above-defined Minkowski tensors are linearly independent, in addition to trivially tensorial functionals obtained by multiplying scalar Minkowski functionals with the rank-2 unit tensor \( E \) [82] (see also the discussion in the study of Schroeder-Turk et al. [57]). Out of these six tensorial functionals, the two translation-invariant (but rotation-covariant) tensors \( W_{1}^{0,2} \) and \( W_{2}^{0,2} \) are of particular importance for the characterization of infinite structure. For \( d = 3 \), the definitions of equation (2.4) are

\[ W_{1}^{0,2}(K) := \frac{1}{3} \int_{\partial K} n \otimes n \text{d}A \quad (2.6) \]

and

\[ W_{2}^{0,2}(K) := \frac{1}{3} \int_{\partial K} H(x) n \otimes n \text{d}A, \quad (2.7) \]

with \( H(x) \) being the point-wise mean curvature of \( \partial K \) at point \( x \). Note the close relationship of \( W_{1}^{0,2} \) to the Doi–Ono interface tensor, defined in the earlier studies [83,84].

Algorithms are available to calculate Minkowski tensors in two and three dimensions and up to rank 2 based on triangulations of the bounding surface (see [80,81] and www.theorie1.physik.uni-erlangen.de/karambola). The sensitivity of the technique has been studied in Arns et al. [85]. With these algorithms, we discovered an intrinsic local anisotropy in granular bead packs [58], in fluids [86] and porous solid foams [57], and (by an analysis of higher-rank tensors) onset of crystallization in jammed spherical bead packs [87]. Minkowski functionals have been used to derive a density functional theory for fluids of non-spherical particles [88,89], possibly applicable to nematic fluids confined in pores.
Here, we focus on the shape of TPMS and the characterization of their degree of anisotropy by use of Minkowski tensors of rank 2.

2.2. Anisotropy measures

Based on eigenvalue ratios of Minkowski tensors \( W_{1,2}^{0,2}(K) \) robust measures of intrinsic anisotropy can be defined that are sufficiently sensitive to capture subtle anisotropy effects and that are applicable to almost arbitrary microstructure. Essentially, the anisotropy indices \( \beta_{1}^{0,2} \) and \( \beta_{2}^{0,2} \) are defined as the minimal-to-maximal eigenvalue ratio of the Minkowski tensors \( W_{1,2}^{0,2} \) and \( W_{2}^{0,2} \). These measures characterize the intrinsic anisotropy, i.e. their value does not depend on the size, aspect ratio or position of the observation window (provided the spatial structure is homogeneous on length scales greater than the size of the observation window).

It is useful to express the anisotropy measure \( \beta_{1}^{0,2} \) in relation to the distribution of normal vectors \( w_{1}(n') = \int dA \delta(n - n')dA \) where \( \delta \) is the Dirac delta distribution. The function \( w_{0}(n') \) gives the total surface area of all (infinitesimal) patches with surface normal vector \( n \). The Minkowski tensor \( W_{1,2}^{0,2} \) can be expressed for an arbitrary body \( K \) as

\[
W_{1,2}^{0,2}(K) = \frac{1}{3} \int dA \, w_{1}(n) \, n \times n
\]

with the unit sphere \( S^{2} \). Therefore, \( W_{1,2}^{0,2}(K) \) can be interpreted as an integral (and hence robust) measure of the distribution of the normals on the bounding surface of \( K \). A convenient scalar characteristic of this tensorial quantity is the eigenvalue ratio

\[
\beta_{1}^{0,2} = \frac{\mu_{\text{min}}}{\mu_{\text{max}}},
\]

where \( \mu_{\text{max}} \) and \( \mu_{\text{min}} \) are the maximal and the minimal eigenvalues of the corresponding Minkowski tensor \( W_{1,2}^{0,2} \).

For example, if \( K \) is a sphere, then \( w_{1}(n) \) is constant and \( \beta_{1}^{0,2} = 1 \) as expected. For the rectangular box \([0,a] \times [0,b] \times [0,c] \), the function \( w_{1}(n) = 0 \) for all \( n \), except for \((+e_{1}) = cd \delta(n \pm e_{1})\), and analogous for \( e_{y} \) and \( e_{z} \), quantifying the total surface area with a given normal direction. The resulting anisotropy measure is \( \beta_{1}^{0,2} = bc/ab \) for \( a \geq b \geq c \).

Similar to \( W_{1,2}^{0,2} \), it is instructive to express the second scalar characteristic of Minkowski tensor \( W_{2}^{0,2} \) by a distribution of normals and curvatures. The function

\[
w_{2}(n',H') = \int dA \delta(n - n') \delta(H - H')
\]

is the surface integral of the normal direction \( n' \) and the mean curvature \( H' \), which yields

\[
W_{2}^{0,2}(K) = \frac{1}{3} \int dH \, H \int_{S^{2}} dA \, w_{2}(n',H',n) \times n
\]

If the function \( w_{2} \) can be written as a product \( w_{2}(n, H) = w_{2}^{0}(H)w_{2}(n) \), then the anisotropy characteristics \( \beta_{1}^{0,2} \) and \( \beta_{2}^{0,2} \) defined as the ratios of the largest to the smallest eigenvalue of \( W_{1,2}^{0,2} \) and \( W_{2}^{0,2} \) are identical. In this sense, \( \beta_{2}^{0,2} \) provides a higher-order anisotropy measure that quantifies anisotropy of the curvature distribution.

A more detailed discussion of these anisotropy indices can be found in Schröder-Turk et al. [81]. Note also that related scalar anisotropy indices can be derived from the interface tensor [83,84,90]. In the following, we demonstrate the use of these anisotropy measures for labyrinthine bodies bounded by TPMS.

3. NON-CUBIC TRIPLY PERIODIC MINIMAL SURFACES

TPMS are oriented surfaces in \( \mathbb{E}^{3} \) that have constant vanishing mean curvature \( H = 0 \) and that are periodic with three linearly independent lattice vectors [1,36,39,41,91]. Any TPMS \( S \) divides \( \mathbb{E}^{3} \) into two domains \( K \) and \( K := \mathbb{E}^{3} \setminus K \) in positive and negative normal direction from \( S \), respectively. Both domains are continuous (i.e. connected), hence the term bicontinuous.

In general, \( K \) and \( K \) may not be congruent, although for the specific examples considered in this article they are.

The symmetry group of a TPMS is not necessarily cubic. While the ubiquity of the cubic (G)yroid [1], (D)iamond [36] and (P)rimitive [36] surfaces in soft-matter systems hints at their special significance, non-cubic TPMS are known [36,41,43,91–94] and have been analysed with respect to their relevance for soft-matter self-assembly [41,59,68,95].

We here analyse lower-symmetry distortions of the cubic P, D and G surfaces that are of particular relevance as transition pathways between these cubic cases, e.g. for the pressure-induced transitions between the corresponding lipid mesophases [96]. The surfaces are one-parameter families of TPMS with a free parameter that alters their shape and in particular also the lattice parameters of their symmetry groups; nevertheless these surfaces are bicontinuous, non-self-intersecting and minimal for all values of this free parameter. Specifically, we analyse the one-parameter TPMS-families \( tP \), \( tD \) and \( tG \) of tetragonal, \( rG \) and \( rPD \) of rhombohedral and \( H \) of hexagonal symmetry [41], also discussed in Schröder-Turk et al. [68]. See figure 2 for a parameter map to these surfaces highlighting the common shared members. Triangulations of almost arbitrary vertex coordinate precision can be obtained from the Weierstrass representation for minimal surfaces. We use the notation that \( r_{0} \) is the free parameter of \( tP \), \( tD \), \( rPD \) and \( H \) surfaces, and \( \phi_{0} \) the free parameter of the \( tG \) and \( rG \) families. For certain values of the free parameters, the rhombohedral and tetragonal TPMS family members correspond to cubic TPMS.

The symmetry groups of these minimal surfaces imply that the eigendirections correspond to lattice directions (we use the orientation and lattice axes as specified in the International Tables of Crystallography [97] for the symmetry groups given in table 1). In particular, for the cases studied here, the tensor \( W_{1,2}^{0,2} \) has an eigendirection corresponding to the \( z \)-axis and a degenerate eigenspace corresponding to the \( xy \)-plane. Instead of the ratio of smallest to largest eigenvalue, the anisotropy of these structures is even...
Table 1. Details of the TPMS families: conventional name of the free parameter, Weierstrass function \(R(a)\), limits \(\varphi_2\) and \(\varphi_1\) of the integration domain \(r\) \(\text{exp}(i\varphi)\) with \(0 \leq r \leq 1\) and \(\varphi_i \leq \varphi \leq \varphi_i + \pi\) and symmetry group of the oriented TPMS (i.e. of the solid body that results from filling one of the two labyrinthine domains with a solid). For the relationship between \(\omega_0 = \omega_0(\phi_0)\) and the Bonnet angle \(\theta(\phi_0)\) for the tG and the rG family, we refer to the original reference where these surfaces were parametrized [41].

<table>
<thead>
<tr>
<th>free parameter</th>
<th>(R(a, \omega_0))</th>
<th>(\omega_0)</th>
<th>(\theta)</th>
<th>([\varphi_2, \varphi_1])</th>
<th>coloured space group</th>
</tr>
</thead>
<tbody>
<tr>
<td>tG</td>
<td>(\phi_0 \in [-\pi/2, 0])</td>
<td>1 (/(w^2 - w_0^2)^{(w^2 - w_0^2)})</td>
<td>(\omega_0 = \omega_0(\phi_0))</td>
<td>(\theta(\phi_0))</td>
<td>([\phi_0, \phi_0 + \pi])</td>
</tr>
<tr>
<td>tP</td>
<td>(r_0 \in [0, 1])</td>
<td>1 (/(w^2 - w_0^2)^{(w^2 - w_0^2)})</td>
<td>(\omega_0 = r_0)</td>
<td>(\pi/2)</td>
<td>([-\pi/2, 0])</td>
</tr>
<tr>
<td>tD</td>
<td>(r_0 \in [0, 1])</td>
<td>0 (/(w^2 - w_0^2)^{(w^2 - w_0^2)})</td>
<td>(\omega_0 = r_0)</td>
<td>0</td>
<td>([-\pi/2, 0])</td>
</tr>
<tr>
<td>rPD</td>
<td>(r_0 \in [0, \pi])</td>
<td>1 (/(w^2 - w_0^2)^{(w^2 - w_0^2)})</td>
<td>(\omega_0 = r_0)</td>
<td>(-\pi/2)</td>
<td>([0, 2\pi/3])</td>
</tr>
<tr>
<td>rG</td>
<td>(\phi_0 \in [-\pi/2, 0])</td>
<td>0 (/(w^2 - w_0^2)^{(w^2 - w_0^2)})</td>
<td>(\omega_0 = \omega_0(\phi_0))</td>
<td>(\theta(\phi_0))</td>
<td>([\phi_0, \phi_0 + 4\pi/3])</td>
</tr>
<tr>
<td>H</td>
<td>(r_0 \in [0, 1])</td>
<td>0 (/(w^2 - (r_0^2 + r_1^2)^{(w^2 + 1)})</td>
<td>(\omega_0 = \omega_0(\phi_0))</td>
<td>(\theta(\phi_0))</td>
<td>([\phi_0, \phi_0 + 4\pi/3])</td>
</tr>
</tbody>
</table>

The difference between the curves \(\sigma_1^{0,2}\) and \(c/a\) in figure 3 highlights the fact that anisotropy is a multi-faceted geometric property, with different measures quantifying different aspects. As explained above, the Minkowski measure \(\sigma_1^{0,2}\) captures the degree to which the surface area is isotropically distributed over all possible surface normal directions. The ratio \(c/a\) of the crystallographic lattice parameters \(a\) and \(c\) characterizes the anisotropy with respect to periodic repetition. For instance, the \(\sigma_1^{0,2}\) data for the tP surface family indicate that the TP surface continuously transforms from a structure dominated by approximately perpendicular surface patches (i.e. with surface normal in the \(xy\)-plane) and large \(\sigma_1^{0,2}\) at large \(r_0\) to a structure dominated by approximately horizontal patches (i.e. with surface normal in the \(z\)-direction) and small \(\sigma_1^{0,2}\) for small \(r_0\) (see figure 4). For the member with cubic symmetry, at \(r_0 = 0.5\), the contributions are balanced and \(\sigma_1^{0,2} = 1\). The \(c/a\) ratio does not show a signature of this behaviour. This suggests that for porous materials, ordered or random, the ratios of eigenvalues of \(W_1^{0,2}\) are a sensitive measure of anisotropy (with respect to surface orientation) that is also easy to compute if a three-dimensional real-space representation is available.

An interesting question with physical relevance for bicontinuous lipid phases that arises from this analysis has been discussed in detail in Schröder-Turk et al. [59]: The member of the hexagonal H surface for which the ratios \(\beta_1^{0,2}\) or \(\sigma_1^{0,2}\) of eigenvalues of \(W_1^{0,2}\) are unity (this is the member with \(r_0 \approx 0.679\) and \(c/a = 0.832\) may be a candidate for an isotropic hexagonal bicontinuous lipid mesophase, somewhat similar to the ubiquitous cubic P, D and G surfaces. We note that this isotropic H surface (i) is very close to the members of the H surface family that have minimal packing and bending frustration [68], (ii) has a powder scattering pattern in simulations of small angle X-ray experiments that closely resembles that of the \(P^{229}\) phase based on the cubic Primitive surface, (iii) has an isotropic response to shear, at least in a linear-elastic approximation of the bilayer, and (iv) is possibly optically isotropic. These similarities raise the possibility of experimental misidentification of this hexagonal lipid phase as a cubic phase based on the \(P\) (primitive) surface.

Figure 2. Schematic of the three cubic TPMS and the pathways of the one-parameter families between them. Arrows indicate the direction in which the free parameters chosen to parametrize the surfaces increase. Adapted from Schroeder-Turk et al. [68], which is slightly different from the original figure in Fogden & Hyde [41].

better elucidated by the anisotropy index

\[
\sigma_1^{0,2} = \frac{\mu_x}{\mu_z} \tag{3.1}
\]

with \(\mu_x\) and \(\mu_z\) being the eigenvalues of \(W_1^{0,2}\) corresponding to the \(z\)-axis and the \(xy\)-plane, respectively. For an isotropic normal distribution (note that this includes cubic symmetry), one obtains \(\sigma_1^{0,2} = 1\). This definition can be extended to any other rank-2 Minkowski tensors to obtain \(\sigma_1^{0,2}\) and \(\sigma_1^{0,2}\).

For minimal surfaces, the space of translation-invariant valuations of rank 2 reduces to \(W_1^{0,2}\) and \(W_4\) since \(W_2^{0,2} = 0\) as the mean curvature vanishes for minimal surfaces. Figure 3 shows the dependence of eigenvalue ratios of \(W_1^{0,2}\) of the free parameter for the surface families listed above, as well as the ratio of lattice parameters \(c/a\) of the symmetry groups of the respective surfaces [68]. The diagrams also contain exact representations of the Minkowski anisotropy indices measures derived from the Weierstrass representation, which are calculated in §4.
translational unit cell is a smallest possible translational unit. For general TPMS, the number of sheets of the Riemann surface is equal to \( n = g - 1 \), where \( g \) is the genus of the surface in the primitive translational unit cell. The Weierstrass map

\[
S : \mathbb{C}^* \rightarrow \mathbb{E}^3
\]

is specified by an analytic non-vanishing function \( R(\omega) \) which is called the Weierstrass function and the Bonnet angle \( \theta \), both specific to the parametrized surface (Re is the real part). The Weierstrass functions for the surfaces discussed here are given in table 1. The Weierstrass parametrization is the inversion of the Gauss map composed with the stereographic projection (see [99,100] and figure 5). The Gaussian curvature of \( S \) at point \( p = p(\omega) \) is

\[
G(\omega) = -4(1 + |\omega|^2)^{-1}|R(\omega)|^2,
\]

the area element is

\[
dA = d^2\omega (1 + |\omega|^2)^2 |R(\omega)|^2
\]

and, as the inverse of the stereographic projection, the normal vector \( n(\omega) \) is

\[
n(\omega) = \left( \frac{2 \text{Re}(\omega)}{|\omega|^2 + 1}, \frac{2 \text{Im}(\omega)}{|\omega|^2 + 1}, 1 - \frac{2}{|\omega|^2 + 1} \right)^T.
\]

For the translation-invariant tensor \( W^{0,2}_1 \) this yields

\[
W^{0,2}_1(S_{\text{TUC}}) = \frac{1}{3} \int_{\mathbb{C}^*} dA |n(\omega)|^{\text{G}}^2
\]

for a fraction \( S_{\text{TUC}} \) of the surface that corresponds to the primitive translational unit cell (note that we have relaxed notation and use the bounding surface \( S_{\text{TUC}} \) rather than the body, as the argument of \( W^{0,2}_1 \)). The translational unit cells considered above are not necessarily the primitive unit cells (but rather the cubic unit cells). The ratio of eigenvalues of translation-invariant tensors is independent on the fraction of the surface on which it is evaluated as long as the portion is a translational unit cell.

For convenience (in particular to avoid the cumbersome treatment of branch cuts of \( \mathbb{C}^* \)), we use the Weierstrass formalism only for the domain \( C \subseteq \mathbb{C}^* \) that corresponds to an asymmetric patch of the symmetric surface. We then apply all symmetry group operations (listed in table 1) to obtain the tensor for the whole translational unit cell. If \( W^{0,2}_0 = W^{0,2}_0(S_{\text{surf}}) \) is the Minkowski tensor of a single asymmetric patch \( S_{\text{surf}} \) and \( G \) the symmetry group of the body bounded by the periodic surface, the tensor of the translational unit cell is given by

\[
W^{0,2}_\nu(S_{\text{TUC}}) = \sum_{\varphi \in G} w_\nu W^{0,2}_\nu.
\]

The symmetry group is that of the body \( K \) bounded by the TPMS, i.e. the same as that of the oriented bounding surface with a specified normal orientation and that is

\[\text{Figure 3. Ratio } \sigma_i^{\alpha^2} = \mu_i/\mu_\alpha \text{ as a function of the free parameter } (\rho_0 \text{ or } \phi_0) \text{ of the } TPMS \text{ families (x-axis as in Schröder-Turk et al. [68]). These quantities are scale-invariant and independent of the system-size, provided it is composed of an integer multiple of a single primitive translational unit cell. For the tP, tD, tG, rPD and rG family, the parameter values for which } \sigma_i^{\alpha^2} = 1 \text{ are expectantly the cubic } P, D \text{ and } G \text{ minimal surfaces (see, [41,68] for the corresponding values of the free parameter); for the H surface, the member with } \rho_0 \approx 0.679 \text{ has } \sigma_i^{\alpha^2} = 1 \text{ and is hence an 'isotropic hexagonal' TPMS; its properties have been discussed in depth in Schröder-Turk et al. [59]. Shown is data obtained from triangulations of the translational unit cell (+), and the result of the analytic expressions obtained in §4 (solid lines). Also shown (in dashed lines) is the axis ratio } c/a \text{ of the crystallographic lattice parameters in the space groups given in table 1.} \]
called the symmetry group of the oriented (i.e. coloured) surface, and not that of the unoriented (or uncoloured) bounding surface. If the two domains are congruent, then the latter contains operations that map the bounding surface onto itself with reversed normals, i.e. a reversal of inside and outside. Note, however, that for the TPMS discussed here the operations of the unoriented symmetry group that reverses the normal field are either twofold rotations or site inversion $C_{22}$, the application of which corresponds to a multiplication by 2 for the translation-invariant tensor $W_{0}; 2$. Hence, for the analysis presented here the unoriented group can be used instead of the symmetry group of the oriented TPMS.

For the TPMS discussed here, the asymmetric unit patch corresponds to a wedge of the complex plane given by the points $r \exp(i \varphi)$ with $r \in [0, 1]$ and $\varphi \in [\varphi_a, \varphi_b]$. The values of $\varphi_a$ and $\varphi_b$ and the range of permissible values for the single free parameter of these surface families, denoted $\eta_0$ or $\phi_0$, are given in table 1. The expression for $W_{10}^2$ is then given by integrals of the type

$$W_{10}^2(S_{w_{\text{toy}}}) = \int_{\varphi_a}^{\varphi_b} \int_0^1 r(1 + r^2)|R(\omega)|^2|\mathbf{n}(\omega)|^{10} \, d\varphi \, dr$$

(4.7)
with \( \omega = r \exp(i\phi) \). The curves in figure 3 are plots of the solutions of equations (4.6) and (4.7) obtained by numerical integration and numerical determination of eigenvalues. The Weierstrass functions and symmetry groups for all surfaces discussed in figure 3 are shown in table 1. Note that the expressions cannot be given in a closed form, but numerical integration yields values with high accuracy.

In principle, equation (4.6) can be further simplified as the symmetric structure of all TPMS imposes constraints on the Minkowski tensors. General principles valid for all rank-2 tensors, detailed e.g. in the study of Bhagavantam & Suryanarayana [101], lead to the following relationship of the eigenvalues and eigenvectors: if a structure has an \( n \)-fold symmetry axis with \( n = 3, 4, 6 \), two of the eigenvalues become degenerate (identical) and the corresponding eigenspace is the plane normal to the rotation axis; the third eigenvector is by definition parallel to the rotation axis. If a body has two or more \( n \)-fold rotation axis with \( n = 3, 4, 6 \) that are not parallel, then all eigenvalues are identical and the structure is called isotropic; this is specifically the case for all structures with cubic symmetry. This requirement implies that triclinic, monoclinic and rhombic systems have up to three distinct eigenvalues, tetragonal, hexagonal and rhombohedral structures up to two and cubic structures only a single distinct eigenvalue. Specifically for the translation-invariant tensors \( W_{0,2}^0 \) and \( W_{0,2}^2 \), the duplication of a body by application of a twofold rotation axis is equivalent to a multiplication of these tensors by a factor of 2.

We note that \( W_{1,2}^0(K) = W_{1,2}^0(K') \) holds for any two bodies whose bounding surfaces \( \partial K \) and \( \partial K' \) are isometric (see Gray [100] for the definition). This is, for example, the case for the cubic Primitive, Diamond and Gyroid surfaces with the length scale that results from equation (4.1), which are related by the so-called Bonnet transformation [100,102,103]; in equation (4.1), this transformation corresponds to adjusting the Bonnet angle \( \theta \). This is evidenced by the fact that \( \theta \) does not occur in equations (4.4) and (4.3). However, rescaling the length scale, e.g. to yield constant surface-to-volume ratio, lifts that degeneracy.

The same formalism can also be used to compute the scalar motion-invariant Minkowski functionals, and in principle also the translation-covariant Minkowski tensor valuations. A problem with the latter is that the domain \( C \) that corresponds to the translational unit cells used in §3 is not readily known (and the translation-covariant tensors depend on the precise form of the translational unit cell, in contrast to the translation-invariant tensors).

5. CONCLUSION AND OUTLOOK

Knowledge of the fundamental geometric properties of a complex spatial structure is often essential for gaining an understanding of the physical mechanisms involved in the formation of that structure; a perfect example for this is the intimate relationship between curvature properties of TPMS and their spontaneous formation in lipid mesophases. One of the most basic requirements of the geometric analysis of complex structure clearly is an ability to describe structure and structural properties, through shape measure that describes shape both qualitatively and quantitatively on all length scales. In material science, where enhanced material properties often result from improvement in the control over material microstructure, such shape measures are of paramount importance when deriving structure-property relationships between geometry and structure on the one hand, and physical properties on the other. Faced with an ever-growing repertoire of increasingly complex structure detected in both natural and man-made materials, the development of fundamental, yet applicable geometric analysis tools remains a very current research topic.

Here, we have described a new approach for quantitative shape and anisotropy analysis based on integral geometry and Minkowski tensors. These tensorial shape indices are suitable for the quantitative characterization of scale- and orientation-dependent properties of complex spatial structure, especially of labyrinthine geometries with saddle-shaped interfaces. The set of Minkowski tensors includes some tensorial shape measures that have already been usefully applied in soft-matter systems, such as close relatives to the Doi–Ohta interface tensor (well-known in immiscible liquid mixtures and equilibrium foams) and of the tensor of inertia. Based on theorems developed in the mathematical discipline of integral geometry, Minkowski tensors provide an encompassing framework for (additive) tensorial shape measures and suggest further, as yet unexplored, tensorial descriptors of anisotropic structure.

Importantly, Minkowski tensors are generalizations of the scalar Minkowski functionals that have proven to be well suited for the development of structure-property relationships for cellular materials, particularly for thermodynamic properties [29,56]. Inasmuch as Minkowski tensors will prove useful for similar purposes, the Minkowski tensor algorithms described in the earlier studies [80,81,57] are useful tools for such developments.

More theoretically, the study of integrated curvature properties of a surface in the framework of Minkowski functionals and tensors provides a new perspective for the analysis of soft-matter interfaces. While individual Minkowski tensors have previously been studied in this context, in particular the interface tensor [83,84], it is useful to view these in the broader framework of all Minkowski tensors and of the theory of additive valuations developed by integral geometry. One example for this is the degree to which the curvature may be distributed anisotropically on a surface: as illustrated here, the surface integral \( W_{1,2}^0(K) \propto \int_S n \odot n \, dA \) (where \( S \) is the translational unit cell of a periodic surface that bounds a continuous periodic body \( K \), see equation (2.6)) can be anisotropic in the sense that this tensor need not be proportional to the unit tensor \( E \), equivalent to an eigenvalue ratio \( \beta_{1,2}^1 \neq 1 \) and an anisotropic distribution of the surface area with different spatial directions. The tensor \( W_{0,2}^2 \propto \int_S Hn \odot n \, dA \) (which quantifies the orientational distribution of mean curvature and which vanishes for minimal surfaces with \( H = 0 \), see equation (2.7)) can also be anisotropic for general surfaces. However, the curvature tensor \( W_{0,2}^2(K) \propto \int_K G n \odot n \, dA \).
(with the Gaussian curvature $G$) is always isotropic for all surfaces $S$ that bound a convex object $K$ (or a poly-convex object $K$, i.e. a union of a finite number of convex objects), in the sense of $W_3^{(2)}(K) \propto xE$ with $x$ being the Euler index; this is guaranteed by a set of linear dependencies for Minkowski tensors identified in equation (2.1) of Hug et al. [82]. The validity of this linear-dependency is less clear if $K$ is the translational unit cell of a continuous periodic body, such as the domains bounded by TPMS. However, Weierstrass calculations indicate that for all of the TPMS studied here the linear relationship is fulfilled and the tensor $W_3^{(2)}$ is isotropic.

The analysis of this article points towards the usefulness of using Minkowski tensors as shape and anisotropy measures for labyrinthine spatial structure, with negative average Gaussian curvature. The discussion of the non-cubic TPMS in this article provides an important reference system which benefits from the accurate solutions afforded by the Weierstrass parametrizations.

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