Morphological Image Analysis 

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Abstract. We describe a morphological image analysis method to characterize images in terms of geometry and topology. We present a method to compute the morphological properties of the objects building up the image and apply the method to triply periodic minimal surfaces and to images taken from polymer chemistry.

1 Introduction

Image analysis is encountered in many different fields of science and technology. For example the interpretation of (electron microscope or computer simulation) images of materials such as polymer mixtures and ceramics is based on a quantitative characterization of the shape, structure and connectivity of the material constituents. In this paper we describe how to characterize these images in terms of shape (geometry) and connectivity (topology) by means of morphological image analysis (MIA). This involves the calculation of the Minkowski functionals (MF's) known from integral geometry [1,2]. In integral geometry the calculation of the MF's is relatively straightforward and requires little computational effort. The MF's have proven to be very useful to describe the morphology of porous media and complex fluids, the large-scale distribution of matter in the Universe, microemulsions, patterns in reaction diffusion systems, and spinodal decomposition kinetics [3]. In this paper we illustrate the application of MIA to three-dimensional (3D) images of polymers and minimal surfaces.

2 Morphological image analysis

In order to analyze images on a computer we first have to digitize them [4]. The digitization process requires the mapping of the image on a grid and a quantization of the gray level. We will consider 3D images partitioned into cubes. Each cube is centered at a lattice point $\mathbf{x}$ and is called a voxel. In general the range of gray levels is divided into bins and the gray level at any lattice point is required to take on only one of these values. We reduce the gray-scale images to black-and-white pictures by thresholding. If the given

picture $\mathcal{P}(\mathbf{x})$ has gray-level range $[a, b]$, and t is any number between a and b, the result of thresholding $\mathcal{P}(\mathbf{x}, t)$ at t is the two-valued picture $\mathcal{P}(\mathbf{x}, t)$ defined by[4] $\mathcal{P}(\mathbf{x}, t) = 1$ if $\mathcal{P}(\mathbf{x}, t) \geq t$ and $\mathcal{P}(\mathbf{x}, t) = 0$ if $\mathcal{P}(\mathbf{x}, t) < t$. We assign to $\mathcal{P}(\mathbf{x}, t) = 0$ a white voxel (the background) and to $\mathcal{P}(\mathbf{x}, t) = 1$ a black voxel (the object).

According to integral geometry, the morphological properties of the various objects building up the black-and-white picture can be completely described in terms of MF's [1]. In three dimensions the MF's are proportional to the volume V, the surface area A, the integral mean curvature H and the Euler characteristic (EC) χ. The functional χ as defined in integral geometry is the same as the EC defined in algebraic topology [1]: χ is given by the number of connected components minus the number of tunnels plus the number of cavities. The EC is negative for multiply connected structures.

In order to calculate the morphological properties of $\mathcal{P}(\mathbf{x}, t)$ in an efficient way we consider each voxel as the union of the disjoint collection of its interior, faces, open edges and vertices. The values of V, A, H and χ for these single open structures can easily be calculated [5]. By making use of the property of additivity of the MF's and the fact that there is no overlap between open bodies on a lattice, we compute the MF's for the whole pattern $\mathcal{P}(\mathbf{x}, t)$ [5].

3 Triply periodic minimal surfaces

A minimal surface in $\mathbb{R}^3$ is defined as a surface for which the mean curvature is zero at each of its points. We will consider the triply periodic minimal surfaces (TPMS). During the last years TPMS and similar interfaces have been extensively discussed in literature since structures related to TPMS may form spontaneously in physico-chemical and in biological systems [6,7]. MIA allows to study the topology of TPMS without making use of labyrinth graphs or surface tiling [8].

Periodic surfaces can be divided into equivalent regions bounded by a unit cell of space. We give our data for the crystallographic cell [9], simply called the unit cell from now on, and assume that the bicontinuous structure of total volume L^3 is composed of several unit cells of typical length scale L_0. Then the EC χ of the whole system is given by $\chi = \overline{X}(L/L_0)^3 \equiv \overline{\chi}N$, where N denotes the number of unit cells. The volume, area and integral mean curvature of the whole system may be written as $V = \overline{V}L_0^3N$, $S = \overline{S}L_0^2N$, $B = \overline{B}L_0N$. The quantities $\overline{V}$, $\overline{S}$, $\overline{B}$ and $\overline{\chi}$ characterize the structure within one elementary unit cell. We compute the MF's for the P (primitive) [10] the D (diamond) [10] and the G (gyroid) [11] surfaces, which may be approximated by periodic nodal surfaces [12–14]. In Fig. 1 we show the P, D and G surfaces, in their unit cell. The geometrical properties for the thresholded oriented P, D and G surfaces ($t = 0.5$) for one unit cell and $L_0 = 128$ can be summarized as follows

$$P : \overline{V} = 0.5(0.5); \quad \overline{A} = 3.68(2.35); \quad \overline{H} = 0(0); \quad \overline{\chi} = -2(-2)$$

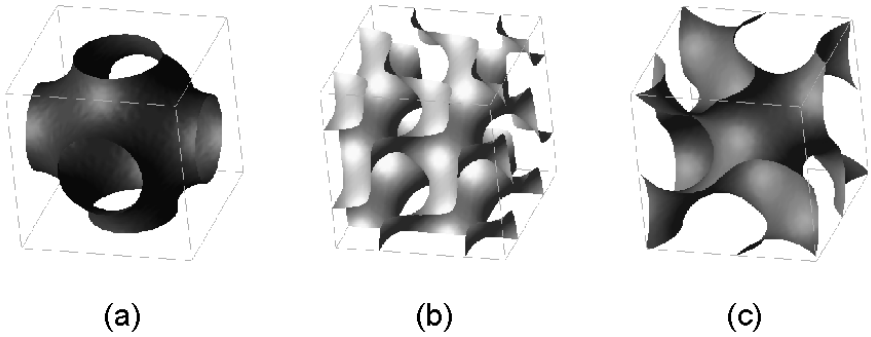

Fig. 1. Unit cube for the primitive P surface (a), the double diamond D surface (b) and the gyroid G surface (c).

$$\begin{aligned} D &: \overline{V} = 0.5(0.5); \quad \overline{A} = 6.00(3.84); \quad \overline{H} = 0(0); \quad \overline{\chi} = -8(-8) \\ G &: \overline{V} = 0.5(0.5); \quad \overline{A} = 4.85(2.09); \quad \overline{H} = 0(0); \quad \overline{\chi} = -4(-4). \end{aligned} \tag{1}$$

The numbers in brackets are the values found in the literature [9,15,16]. The values for the geometrical properties, calculated using integral geometry based MIA, are in good agreement with the numbers quoted in literature [9,15,16]. The numbers for the area are about a factor of 1.6 larger than the numbers quoted in literature. This systematic error is due to the thresholding of the picture. This operation transforms the smooth surface to a more stepwise surface which enlarges the covered area. A method to reduce this error is described elsewhere [5].

Examples of TPMS may be found in block copolymers [17]. Block copolymers are materials that are capable of forming mesoscale structures whose morphology can be tailored by controlled synthesis. Identification and quantification of the morphology of these mesoscale structures may be rather difficult. In this section we consider an example for which conventional crystallographic techniques, such as calculating the structure factor, do not work and for which MIA proves to be very valuable.

We perform a MIA on computer-simulation data of an A/B binary polymer blend containing $A-B$ type block copolymer. Fig.2 shows the 3D domain structures, obtained by the self-consistent field (SCF) dynamic density functional method ((a) and (c)) and the Ginzburg-Landau (GL) method ((b) and (d)), of an A_{10}/B_{10} polymer blend containing 20% volume fraction of A_n-B_{20-n} block copolymer [18,19]. A quantitative comparison between the SCF method and the GL method has shown the validity and efficiency of the GL approach [18,19]. The data for the SCF method and the GL method are taken at different moments in time. The segment interaction parameter (so-called χ-interaction parameter) is set to 0.5. The simulation box is a cube of edge length 32 with periodic bounadries.

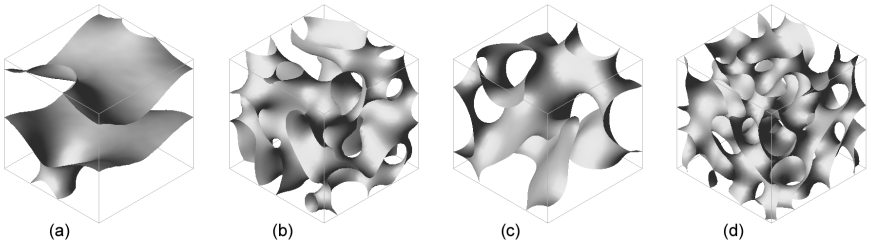

Fig. 2. Three-dimensional domain structures of an A_{10}/B_{10} polymer blend containing 20% volume fraction of A_nB_{20-n} block copolymer. (a): A_4-B_{16}, ($f = 0.2$), SCF method; (b): A_4-B_{16}, ($f = 0.2$), GL method; (c): A_{10}-B_{10}, ($f = 0.5$), SCF method; (d): A_{10}-B_{10}, ($f = 0.5$), GL method.

In Figs.2(a),(b) ((c),(d)) a block copolymer with block ratio $f = 0.2$ ($f = 0.5$) is added, the block ratio being defined as the ratio between the length of block A to the total chain length of the block copolymer. In all cases interconnected bicontinuous domain structures are observed [19]. In order to study the morphology of the domain structures in more detail we compute their MF's. The results can be summarized as follows

$$\begin{aligned}
&(a) : N = 1; \quad \overline{V} = 0.47; \quad \overline{A} = 3.29; \quad \overline{H} = 0.56; \quad \overline{\chi} = -1 \\
&(b) : N = 8; \quad \overline{V} = 0.47; \quad \overline{A} = 3.65; \quad \overline{H} = 0.55; \quad \overline{\chi} = -1.88 \\
&(c) : N = 1; \quad \overline{V} = 0.50; \quad \overline{A} = 5.31; \quad \overline{H} = -0.69; \quad \overline{\chi} = -5 \\
&(d) : N = 8; \quad \overline{V} = 0.50; \quad \overline{A} = 4.55; \quad \overline{H} = 0.047; \quad \overline{\chi} = -3.75. \qquad (2)
\end{aligned}$$

The MF's for thresholded oriented P and G surfaces ($t = 0.5$) for one unit cell and $L_0 = 32$ are

$$\begin{aligned}
&P : \overline{V} = 0.50; \quad \overline{A} = 3.71; \quad \overline{H} = 0; \quad \overline{\chi} = -2 \\
&G : \overline{V} = 0.50; \quad \overline{A} = 4.90; \quad \overline{H} = 0; \quad \overline{\chi} = -4 \qquad (3)
\end{aligned}$$

From (2) and (3) it follows that the surfaces in Figs.2(a),(b) resemble a P-surface and the ones in Figs.2(c),(d) a G-surface. Since computer simulations for these polymer systems can only be performed for relatively small system sizes it is rather difficult to draw a similar conclusion from the structure factor.

4 Summary

We have described a morphological image analysis (MIA) method to characterize black-and-white images in terms of shape (geometry) and connectivity (topology). Integral-geometry-based MIA allows a straightforward calculation of the morphological quantities and requires little computational effort. The approach has been illustrated by computation of the morphological measures of triply periodic minimal surfaces as obtained from nodal surfaces and

computer simulations of polymer systems. In the latter case MIA provides information about the domain structures that is hard to obtain by other methods.

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