Sheet-like chiro-optical material designs : C(Y) surfaces

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ABSTRACT

A spatial structure for which mirror reflection cannot be represented by rotations and translations is chiral. For photonic crystals and metamaterials, chirality implies the possibility of circular dichroism, that is, that the propagation of left-circularly polarized light may differ from that of right-circularly polarized light. Here we draw attention to chiral sheet- or surface-like geometries based on chiral triply-periodic minimal surfaces. Specifically we analyse two photonic crystal designs based on the C(Y) minimal surface, by band structure analysis and by scattering matrix calculations of the reflection coefficient, for high-dielectric contrasts.

Keywords: Gyroid Photonics, chiral optics, circular polarisation, biophotonics, minimal surfaces

1. INTRODUCTION

Nature disposes of several chiral geometries, including the helical structure of DNA on the small scale and the curvature of snails on the large scale. This article is concerned with chiral structures at length scales commensurate with the wavelengths of visible light. Of particular relevance in this context, are the helical wood-pile structures known as Bouligand structures in plants and in insects (see\textsuperscript{1,2} for recent reviews), as well as the chiral bicontinuous gyroid structure\textsuperscript{3} found in butterflies and likely in other arthropods (see\textsuperscript{4} for a recent review).

This article addresses sheet-like structures related to bicontinuous triply-periodic minimal surfaces (TPMS\textsuperscript{5-7}). These surfaces divide space into two domains, with the minimal surface as their joint and only interface. The gyroid (or ‘I4\textsubscript{1}32 single gyroid’ or 1-srs) is an ordered structure consisting of a single network-like solid component embedded in a single-component air matrix. It is related to the Gyroid minimal surface, which is the interface between two intergrown srs nets, one of right-handed (RH) and one of left-handed (LH) chirality.

Because of the presence of both a RH and a LH component, the gyroid surface or the double gyroid (where both networks represent the same material type) are not chiral. A material difference between the two networks is required to break the symmetry (e.g. in the butterfly structure, the fact that one channel is hollow and the other solid). For the same reason, a ’sheet’ of solid material that is symmetrically draped over the Gyroid minimal surface (occupying a volume within ±L/2 around the gyroid minimal surface, for the sheet thickness L) is not chiral. However, other bicontinuous surfaces exist that are chiral even as a sheet structure.

2. THE CHIRAL TRIPLY-PERIODIC C(Y) MINIMAL SURFACE

The C(Y) surface, described by Fischer & Koch,\textsuperscript{8} is balanced, that is, rotations exist that map the infinite surface onto itself and that exchange the two labyrinthine domains. As an oriented surface (that is, for example if its two sides are colored differently) it has simple cubic symmetry P\textsubscript{4}3\textsubscript{2} (Fig. 1, top). As an non-oriented surface (that is uncolored and without point normals or other features that distinguish inside and outside) it has body-centered cubic symmetry I\textsubscript{4}3\textsubscript{2}. This is the space group of the thickened surface sheet and of the double-graphs in Fig. 1 (bottom). The non-oriented and the oriented surface are both chiral.

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Based on the C(Y) minimal surface a number of photonic crystal designs can be derived: Space can be partitioned, with symmetry $P4_332$, into two congruent like-handed domains on either side of the minimal surface of different dielectric constant, see Fig. 1 (top). For brevity, we will refer to one of the domains as solid and the other as void. Structures obtained by inflating a single C(Y) graph to a solid tubular network also have symmetry $P4_332$; the tubular radius $r$ determines the solid volume fraction. Similarly, a solid/void partition of space on either side of a constant mean curvature companion surface to the C(Y) minimal surface result by minimizing interface area while maintaining fixed volume and topology.\(^9\)

Geometries with the symmetry $I4_132$ of the non-oriented C(Y) minimal surface and that of two C(Y) graphs are: The C(Y) minimal surface is inflated to a solid sheet of constant thickness (bounded by two parallel surfaces at distance $\pm r$), leaving two unconnected network-like void domains (Fig. 3). The geometric shape of the interface may again be altered, to be either given by CMC surfaces (in which case the thickness of the sheet is no longer constant) or by tubular representations of the skeletal network.

The different local chiral elements of these geometries are demonstrated in Fig. 1. For the $I4_132$ C(Y) geometries there are two symmetrically distinct four-fold screw axes along the [100] directions, one left-handed (LH) and one right-handed (RH). However, their local geometry is different hence breaking the symmetry between the two hands. While the LH screw corresponds locally to a continuous helicoid-like surface patch along the rotation axes (also evidenced by the double helix shape of the two skeletal graphs), the RH screw axis locally maps surface patches perpendicular to the rotation axes and is topologically discontinuous (corresponding to the dog-bone stacking of the corresponding skeletal graph elements). For the $P4_332$ geometry, a single LH $4_3$ screw axis exist, corresponding to a single-helix structure around the rotation axis. The axis corresponding to the RH dog-bone $4_1$ screw of the $I4_132$ geometry is an achiral $2_1$ screw axis for the $P4_332$ geometry, neither LH nor RH.

3. CIRCULAR-POLARIZATION EFFECTS IN C(Y) PHOTONIC CRYSTALS

Photonic band structures and transmission coefficients are computed on voxelized binary data sets.\(^*\) These are obtained from triangulations of the C(Y) minimal and constant mean curvature surfaces computed by conjugate

\(^*\)128\(^3\) voxels per cubic unit cell for scattering matrix calculations; 512\(^3\) voxels per primitive unit cell along with a discrete Fourier grid of size 64\(^3\) for MPB
Circular dichroism as a function of frequency is characterized by reflectance rates computed by a scattering matrix approach and by analyzing the degree of circular polarization of the magnetic eigenfields of a band structure for infinite crystals. In this latter approach (described in detail in, see also), coupling amplitudes of an incident circularly-polarized plane wave with the crystal Bloch modes are computed in the crystal cut-off plane perpendicular to the wave-vector of the incoming wave. A circular dichroism index \( \beta \) is derived that measures the dichroism strength, with \( \beta = 0 \) corresponding to no dichroism and \( \beta = \pm 1 \) to maximal dichroism. A mode with \( \beta > 0.5 \) and \( \beta < -0.5 \) is called right-circularly-polarized (RCP) and left-circularly-polarized (LCP), respectively. Further, a coupling index \( \beta \in [0, 1] \) measures the degree to which an incident plane wave of arbitrary polarization to couple with a crystal mode. A mode is called low coupling if \( \beta < 0.1 \). This article uses the exact definitions of ref. This method is a coarse approximation of a more rigorously defined scattering method; see reference for details of the scattering method and for a numeric implementation.

Figures 2 and 3 show the circular-dichroism optical response of a double network structure (Fig. 2) and a sheet-like structure (Fig. 3), respectively. In both figures, the y-axes represent the frequency in dimensionless units (with the lattice constant \( a \), the vacuum speed of light \( c \) and the angular frequency \( \omega \). The x-axis are: A The circular dichroism index \( \beta \), B the absolute value of the corresponding wave vector \( k \) in [100]-direction from \( \Gamma \)-point to the Brillouin-zone border, C the coupling index \( \beta \) and D the reflectance rate \( R \). Modes with \( |C| > 0.5 \) are called circular-polarized and modes with \( \beta < 0.1 \) are called low coupling. Red [blue] color is for right [left] circular polarization. A-C The color represents the value of \( C \), point size the value of \( \beta \).

For the double-network structure (composed of two equal-handed networks, we find a substantial degree of circular dichroism and a strong photonic response (Fig. 2): For \( k \) along [100] a partial band gap is observed between \( [\omega_1, \omega_2] := \{\omega|\omega_1 < \omega/a/(2\pi c) < \omega_2\} \), that is a frequency range without any bands regardless of polarization (this is in a high-dielectric contrast material with \( \epsilon \) corresponding to silicon). This observation agrees with the observed full reflectance (\( R \approx 1 \)). Further, a RCP circular dichroism band gap of relative width \( \Delta \approx 9\% \) is observed for \( [\omega_3, \omega_4] \), this is a frequency band for which only a LCP band (with sufficiently high coupling coefficient \( \beta \)) exists but no RCP band; this explains the almost complete reflection of RCP incident light (\( R \approx 1 \)) and the low reflectance of LCP light (\( R \approx 0 \)). A less clearly resolved feature of the photonic band structure is the existence of another circular dichroism band gap of opposite polarization, LCP, for \( [\omega_5, \omega_6] \). While the presence of CP bands of opposite polarisation would be a fascinating feature for 'circular polarisation switches', the feature is ambiguous within our analysis.

For the sheet-like structure (Fig. 3), the principal result of this analysis is that neither the band structure nor the reflectance rates show any substantial amount of circular dichroism even though the spatial structure is chiral with clearly handed local spiral elements. This results is valid for other filling fractions as well. The
partial band gap in the frequency regions $[\omega_1, \omega_2]$, $[\omega_3, \omega_4]$ and above $\omega_5$, where only low coupling modes exist, correspond to high reflectivity $R$. In some regions, strong circular dichroism $C$ of opposite handedness for a pair of bands is found, e.g. below $\omega_1$. However, the modes of these two bands are almost degenerate, explaining why no circular dichroism is observed in the reflectance spectrum. There is no single polarization sense, which couples significantly better to the chiral crystal structure than the opposite sense.

4. CONCLUSIONS
This article represents a first attempt at using chiral sheet-like triply-periodic minimal surface geometries as blue-prints for photonic materials, rather than the now wide-spread network-like chiral gyroid-like structures. We find that the geometric structure analysed here, Fischer-Koch’s C(Y), does not display particularly strong circular dichroic photonic properties, even when realised in materials with high dielectric contrast. However, this lack of strong response should not deter from the investigation of other sheet-like structures as possible interesting photonic chiral materials. Further minimal surfaces of cubic symmetry that are chiral in their uncolored and their colored space groups are include the “C(Y)b”,” the “D2c” and the “Yb” surfaces." In particular when cross-property material properties are important, sheet-like structures may be of interest, due to their higher surface-to-volume ratios and due to their enhanced mechanical stiffness.16

We acknowledge the support of the Deutsche Forschungsgemeinschaft through the Cluster of Excellence ‘Engineering of Advanced Materials’. We thank Klaus Mecke for support, advice, comments and discussions.

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