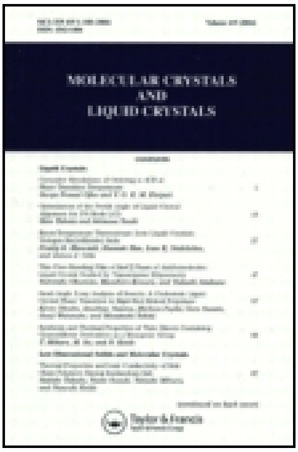

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Tentative Description of Blue Phases with Periodic Surfaces

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TENTATIVE DESCRIPTION OF BLUE PHASES WITH PERIODIC SURFACES

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Abstract: Geometrical models of blue phases usually proposed a description with double twist cylinders. This description was first complemented by introducing minimal surfaces as midway surfaces between the axes of the double twist cylinders. Here we extend the description to any surface. We give the energy expression and its minimization in terms of specific properties of surfaces. We find the tangent director field minimizing the elastic energy for surfaces with constant mean curvature.

Keywords: blue phases, periodic surfaces, models

INTRODUCTION.

Liquid crystal blue phases 1 and 2 are cubic phases with symmetry $I4_132$ and $P4_232$.[1] These phases can be described with use of a uniaxial order parameter **n** such that **n** and -**n** are equivalent.[2][3] Absolute minimization of the free elastic energy leads to a local condition implying a double twist distortion of the director **n**; (in a cholesteric phase, the twist only occurs in one direction of the space). It has been proved that no configuration without defects can rigourously satisfy this condition everywhere.[4] But a cylindrical configuration where tilt of molecules becomes larger when moving away from the cylinder axis mostly fits that condition (the condition is strictly satisfied in the limit $r \to 0$ where r is the cylinder radius). The configurations with quasi double twist can be obtained in confined regions of the space such as cylinders of finite size. Structure of blue phase can then be interpreted[5][6] in terms of arrays of such quasi double twist cylinders associated with arrays of defects (disclinations). But energetical calculations imply the knowledge of the director field in all the space and not only in limited regions such as the double twist cylinders. Recent approaches tend to give a description of the director field filling the gap between the cylinders.(7) (9) In that spirit we focussed our analysis on a geometrical aproach linked to surfaces. We took into account models of cubic phases (5)(6) where double twist cylinders are piled along the edges of the cubes. We showed (9) that in these structures we can exhibit axes of double twist cylinders directed along the core of the labyrinths of some famous cubic infinite periodic minimal surfaces (IPMS), namely the P,F and G surfaces.(8) Core of the IPMS labyrinths or the double twist cylinder axes constitute two different networks.(9) The minimal surface divide the space between the two networks in two parts of equal volume. In that sense the IPMS is a "midway" surface between these two networks. This is not the unique "midway" surface that we could choose but it is a rather good candidate. First it belongs to the good symmetry group. Furthermore the director field on that surface, which minimizes the surface elastic free energy shows singularities(9) (at the flat points of the surface) in the same directions as in the models with piling of double twist cylinders. In that paper we sketch the procedure for the construction of blue phases director field by means of a stratification of the space in terms of surfaces.The idea is to stratify the space with surfaces starting from the IPMS and ending, as a limiting case, with surfaces collapsing along the double twist axes and to find the director field on the surfaces minimizing the elastic free energy. We found in a preceding paper that on the minimal surfaces such director field was directed along the asymptotic lines *i.e.* at a constant angle from the principal directions.(12) Since principal directions play a favoured rôle concerning the double twist condition we shall give in the following the expression of the free energy in terms of a frame directed along the principal directions and the normal to any surface. Then we shall express in those coordinates the general double twist condition and find for some specific surfaces the associated director field.

Elastic free energy.

The expression $\mathcal{E}$ of the elastic energy of blue phases results from the classical Frank energy.[10] Surface terms usually omitted for configurations with fixed boundary conditions on the director are to be retained since in blue phases many defects are present.

$$\mathcal{E} = \int \mathcal{F} vol$$

where the energy density $\mathcal{F}$ is:

$$\begin{aligned} 2\mathcal{F} =& (div\mathbf{n})^2 + K_{22}(\mathbf{n}.\mathbf{curl}\ \mathbf{n} + q_o)^2 + K_{33}(\mathbf{n} \wedge \mathbf{curl}\ \mathbf{n})^2 \\ & (K_{22} + K_{24}) div(\mathbf{n}.\mathbf{curl}\ \mathbf{n} + \mathbf{n} div\mathbf{n}) \end{aligned} \tag{1}$$

q_o is the pitch defining the natural twist.
In the one elastic approximation $K_{11} = K_{33}$ and limit $K_{24} = 0$, this energy reduces to [10]:

$$\mathcal{E} = \int \sum_{i,j} (\partial_i n^j + q_o \epsilon^j_{ik} n^k)^2 vol$$

where (i, j, k) is an orthonormal frame. In this frame, the minimization of the energy leads to the double twist condition[4] [5]:

$$\nabla^{DB}_i n^j = \partial_i n^j + q_o \delta^{jl} \epsilon_{ilp} n^p. \tag{2}$$

We now want to express this condition using coordinates related to some reference frame specific to the surface. At any point of the surface one can define the normal $\mathbf{N}$ and the curvature tensor in terms of the second and first fondamental forms.[11] The two eigenvectors $\mathbf{e_1}$ and $\mathbf{e_2}$ correspond to the two directions with extreme curvature. k_1 and k_2 are the eigenvalues or principal curvatures associated to the two principle directions $\mathbf{e_1}$ and $\mathbf{e_2}$. Then in the following we shall use the orthonormal frame $(\mathbf{e_1}, \mathbf{e_2}, \mathbf{N})$ as a reference frame associated to the surface (fig. 1).

If $k_1 = k_2$ this frame is no longer defined; all tangent vectors on the surface are equivalent. At the vicinity of the surface we can express the director field $\mathbf{n}$ as:

$$\mathbf{n} = X^1\mathbf{e_1} + X^2\mathbf{e_2} + X^3\mathbf{N}$$

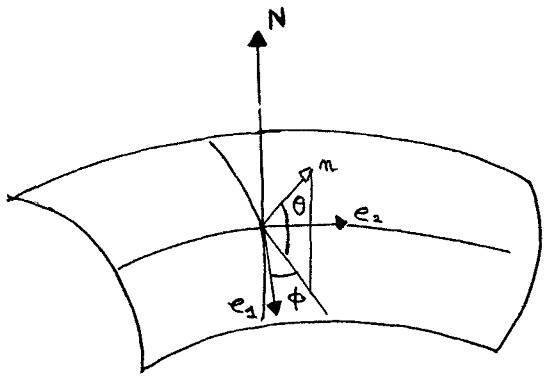

FIGURE 1 Frame($\mathbf{e_1}, \mathbf{e_2}, \mathbf{N}$). $\mathbf{e_1}$ et $\mathbf{e_2}$ are the principal directions (extrema of curvature), $\mathbf{N}$ is the normal to the surface.

In order to express the free energy (eq. 1) in this frame of coordinates one has to take into account the variations of the frame ($\mathbf{e_1}$,$\mathbf{e_2}$,$\mathbf{N}$) on the surface related to the principal curvatures and their variations:

$$
\begin{aligned}
\nabla_1 \mathbf{e}_1 &= \begin{pmatrix} 0 \\ \frac{\nabla_2(k_1)}{k_1-k_2} \\ k_1 \end{pmatrix} \\
\nabla_2 \mathbf{e}_1 &= \begin{pmatrix} 0 \\ \frac{\nabla_1(k_2)}{k_1-k_2} \\ 0 \end{pmatrix} \\
\nabla_1 \mathbf{e}_2 &= \begin{pmatrix} -\frac{\nabla_2(k_1)}{k_1-k_2} \\ 0 \\ 0 \end{pmatrix} \\
\nabla_2 \mathbf{e}_2 &= \begin{pmatrix} -\frac{\nabla_1(k_2)}{k_1-k_2} \\ 0 \\ k_2 \end{pmatrix} \\
\nabla_1 \mathbf{N} &= \begin{pmatrix} -k_1 \\ 0 \\ 0 \end{pmatrix} \\
\nabla_2 \mathbf{N} &= \begin{pmatrix} 0 \\ -k_2 \\ 0 \end{pmatrix}
\end{aligned}
\tag{3}
$$

Since we are looking for twisting director field we introduce *ab initio* some twist q in the normal direction to the surface and take:

$$
\begin{aligned}
\nabla_3 \mathbf{N} &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \\
\nabla_3 \mathbf{e}_1 &= \begin{pmatrix} 0 \\ -q \\ 0 \end{pmatrix} \\
\nabla_3 \mathbf{e}_2 &= \begin{pmatrix} q \\ 0 \\ 0 \end{pmatrix}
\end{aligned}
\tag{4}
$$

The Frank energy is expressed in the frame associated to the surface as:

$$
\begin{aligned}
\mathcal{F} = & \sum_{i,j}(\nabla_i X^j)^2 + \\
& + 2\frac{\nabla_2(k_1)}{k_1 - k_2}(X^1\nabla_1 X^2 - X^2\nabla_1 X^1) \\
& + 2\frac{\nabla_1(k_2)}{k_1 - k_2}(X^1\nabla_2 X^2 - X^2\nabla_2 X^1) \\
& + 2k_1(X^1\nabla_1 X^3 - X^3\nabla_1 X^1) \\
& + 2k_2(X^2\nabla_2 X^3 - X^3\nabla_2 X^2) \\
& - 2q_o(X^2\nabla_1 X^3 - X^3\nabla_1 X^2) \\
& - 2q_o(X^3\nabla_2 X^1 - X^1\nabla_2 X^3) \\
& + 2(-q + q_o)(X^2\nabla_3 X^1 - X^1\nabla_3 X^2) \\
& - 2q_o(k_1 - k_2)X^1 X^2 \\
& + 2(-k_2\frac{\nabla_1(k_2)}{k_1 - k_2} - q_o\frac{\nabla_2(k_1)}{k_1 - k_2})X^1 X^3 \\
& + 2(k_1\frac{\nabla_2(k_1)}{k_1 - k_2} - q_o\frac{\nabla_1(k_2)}{k_1 - k_2})X^2 X^3 \\
& + (X^1)^2(\left(\frac{\nabla_2(k_1)}{k_1 - k_2}\right)^2 + \left(\frac{\nabla_1(k_2)}{k_1 - k_2}\right)^2 + k_1^2 + q_o^2 + (q - q_o)^2) \\
& + (X^2)^2(\left(\frac{\nabla_2(k_1)}{k_1 - k_2}\right)^2 + \left(\frac{\nabla_1(k_2)}{k_1 - k_2}\right)^2 + k_2^2 + q_o^2 + (q - q_o)^2) \\
& + (X^3)^2(2q_o^2 + k_1^2 + k_2^2)
\end{aligned}
\tag{5}
$$

Since we are looking for a unitary director field one can define the angles θ and ϕ (fig. 1) as:

$$
\begin{aligned}
X^1 &= cos(\theta)cos(\phi) \\
X^2 &= cos(\theta)sin(\phi) \\
X^3 &= sin(\theta)
\end{aligned}
$$

and write the associated expression for the energy density:

$$
\begin{aligned}
\mathcal{F} = \sum_i & ((\nabla_i\theta)^2 + cos^2\theta(\nabla_i\phi)^2 \\
& + 2\nabla_1\theta(k_1 cos\phi - q_o sin\phi) \\
& + 2\nabla_2\theta(k_2 sin\phi + q_o cos\phi) \\
& + 2\nabla_1\phi(\frac{\nabla_2 k_1}{k_1 - k_2} cos^2\theta + cos\theta sin\theta(k_1 sin\phi - q_o cos\phi)) \\
& + 2\nabla_2\phi(\frac{\nabla_1 k_2}{k_1 - k_2} cos^2\theta + cos\theta sin\theta(-k_2 cos\phi + q_o sin\phi)) \\
& + 2\nabla_3\phi(q - q_o)cos^2\theta \\
& - 2q(k_1 - k_2)cos^2\theta cos\phi sin\phi \\
& + 2(-k_2\frac{\nabla_1(k_2)}{k_1 - k_2} - q_o\frac{\nabla_2(k_1)}{k_1 - k_2})cos\theta sin\theta cos\phi \\
& + 2(k_1\frac{\nabla_2(k_1)}{k_1 - k_2} - q_o\frac{\nabla_1(k_2)}{k_1 - k_2})cos\theta sin\theta sin\phi \\
& - k_2^2 cos^2\theta cos^2\phi - k_1^2 cos^2\theta sin^2\phi \\
& + sin^2\theta\left(-\left(\frac{\nabla_2(k_1)}{k_1 - k_2}\right)^2 + \left(\frac{\nabla_1(k_2)}{k_1 - k_2}\right)^2 - (q - q_o)^2 + q_o^2\right) \\
& + \left(\frac{\nabla_2(k_1)}{k_1 - k_2}\right)^2 + \left(\frac{\nabla_1(k_2)}{k_1 - k_2}\right)^2 + (q - q_o)^2 + k_1^2 + k_2^2 + q_o^2.
\end{aligned}
\tag{6}
$$

<u>Double twist condition</u>

Minimization of the energy with respect to the two variables θ and ϕ:

$$\frac{\partial \mathcal{F}}{\partial \phi} = \sum_i \nabla_i \frac{\partial \mathcal{F}}{\partial \nabla_i \phi} + \frac{\partial \mathcal{F}}{\partial \nabla_i \phi} div(\mathbf{e}_i)$$

$$\frac{\partial \mathcal{F}}{\partial \theta} = \sum_i \nabla_i \frac{\partial \mathcal{F}}{\partial \nabla_i \theta} + \frac{\partial \mathcal{F}}{\partial \nabla_i \theta} div(\mathbf{e}_i)$$

leads to the double twist condition expressed in terms of the new coordinates.

As a first approach we look for tangent director field *i.e.* $\theta = 0, \nabla_N \theta = 0$. We obtain the condition for the coordinate in the tangent plane:

$$\begin{aligned}\sum_i \nabla_i^2 \phi = &- \nabla_1 \left(\frac{\nabla_2 k_1}{k_1 - k_2}\right) - \nabla_2 \left(\frac{\nabla_1 k_2}{k_1 - k_2}\right) \\ &- 2q_o(k_1 - k_2)cos2\phi + (k_2^2 - k_1^2)sin2\phi \\ &- \frac{\nabla_1 k_2}{k_1 - k_2}\nabla_1 \phi + \frac{\nabla_2 k_1}{k_1 - k_2}\nabla_2 \phi \\ &- 2(q - q_o)(k_1 - k_2).\end{aligned}$$

This expression is quite general and takes into account the surface properties through the terms in curvature gradient. No simple solution can be extracted in the general case but some simplification occurs if one looks for some specific surfaces.

<u>Surfaces with constant mean curvature.</u>

For surfaces with constant mean curvature C_M, one can write the two principal curvatures as :

$$k_1 = k + \epsilon$$
$$k_2 = -k + \epsilon$$

where $C_M = 2\epsilon$ is constant. The minimization of eq. 6 then reduces to:

$$\begin{aligned}\sum_i \nabla_i^2 \phi = &- 4qkcos2\phi + 4\epsilon ksin2\phi \\ &- \frac{\nabla_1 k_2}{k_1 - k_2}\nabla_1 \phi + \frac{\nabla_2 k_1}{k_1 - k_2}\nabla_2 \phi - 2(q - q_o)(k_1 - k_2).\end{aligned} \tag{7}$$

For $q = q_o$, one trivial solution is:

$$\phi = 1/2 Arctg(-q/\epsilon) + n\pi/2. \tag{8}$$

or

$$cos2\phi = \pm \frac{\epsilon}{\sqrt{\epsilon^2 + q^2}}.$$

Let us notice that a stable solution is:

$$cos2\phi = -\frac{\epsilon}{\sqrt{\epsilon^2 + q^2}}.$$

which leads to the following energy:

$$\mathcal{E} = -\int [2k\sqrt{\epsilon^2 + q^2}]vol + \int [g(k, \epsilon,)]vol$$

where $g(k, \epsilon,)$ does not depend on ϕ but only on the surface properties. Equation (8) shows that the director field remains at a constant angle from the principal directions. We recover the solution $\phi = \pi/4$ and $\phi = 3\pi/4$ for a minimal surface $\epsilon = 0$ *i.e.* the director field is along the asymptotic directions.(12) Let us remark that asymptotic directions always exist for a minimal surface (but not always in the case of a general surface). It is also interesting to notice that solution (8) also leads to a director field reminiscent of the double twist cylinder one. Principal directions are along the usual cylindrical frame $\mathbf{e}_\theta, \mathbf{e}_\mathbf{Z}$ tangent to the circle and along the Z axis. The director field for a cylinder of radius $\frac{1}{R} = 2\epsilon$ is:

$$tg(2\phi) = -2q_oR$$

which is of the predicted type for double twist cylinders (fig. 2). A nice engraving has been performed by P. Jeener (fig. 3) illustrating and extrapolating our results. We can see the director field as predicted on the minimal surface, on the cylinders and also inbetween as a dream.

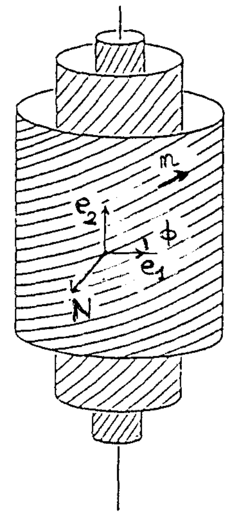

FIGURE 2 Director field **n** in a double twist cylinder.

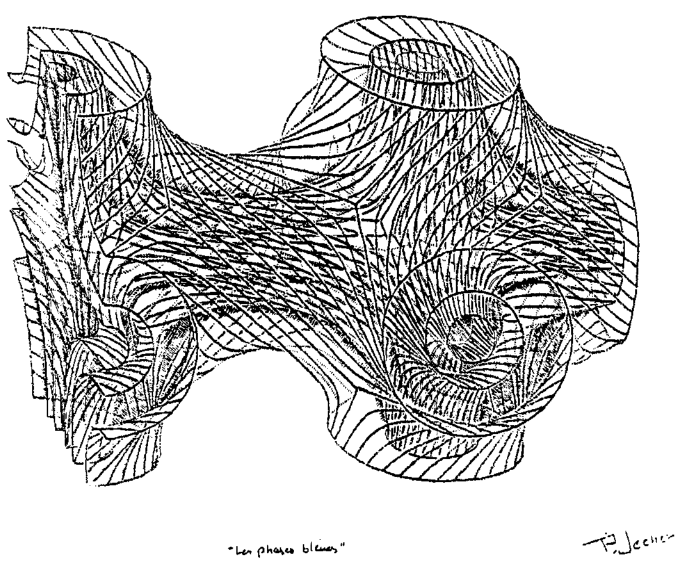

FIGURE 3 Blue phase as engraved by the artist P. Jeener, Paris 1990.

CONCLUSION.

In this paper we have derived the elastic free energy and the double twist condition in terms of general properties of surfaces, namely in terms of curvatures and principal directions. We looked for tangent director field and exhibit solutions in the case of surfaces with constant mean curvature. We recovered solutions already known in the case of double twist cylinders and minimal surfaces. This paper is a first attempt for a description of blue phases in terms of stratification of the space by a series of surfaces. Simplification occurs for surfaces with constant mean curvature. But the main point which remains is to know if such a stratification may exist filling the space between the double twist axes.

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