Topological properties of cholesteric blue phases

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The topological properties of cubic structures which have been proposed as models for the cholesteric blue phases (BP) are considered. When the space of the order parameter is restricted to the standard one for biaxial nematics [$SO(3)/D_2$] then, as a consequence of the cubic symmetry, these structures must have disclinations. The usual classification scheme, wherein defect lines are characterized by the conjugacy classes of the fundamental group appropriate to a biaxial system, is used; some exceptions are also noted. For each of the three groups studied [body-centered-cubic O^5 ($I432$) and O^8 ($I4_132$), and simple-cubic O^2 ($P4_232$)] two aspects are considered: general symmetry constraints on disclinations and the topological properties of equilibrium order-parameter distributions as found from Landau-theory calculations. For O^5 and O^2, there are two nonequivalent symmetry axes upon which there must be disclinations. When they are characterized by a uniaxial order parameter, one must be uniaxial positive and the other uniaxial negative in order for the topology to be consistent with the space-group symmetries. This is not the case for O^8 where only one type of defect line, located on the threefold axes, is topologically required. The order-parameter fields obtained from Landau–free-energy minimization have, except in the case of O^5, additional disclinations. In particular, the three structures described by the O^8 space group are found to have distinctly different networks of defect lines. These, as well as the additional disclination found in the O^2 structure, are examined and their group structures were determined. Finally, some open questions and directions for future work are examined.

I. INTRODUCTION

In the past decade, it has become clear that topological concepts provide a useful approach to the classification and study of defects in ordered media. Several reviews[1–3] dealing with the application of algebraic topology to condensed-matter physics have appeared; standard examples include uniaxial and biaxial liquid crystals and the phases of superfluid helium.

Simultaneously, the unusual blue phases (BP) which appear in cholesteric liquid crystals have been intensively investigated.[4] Theoretically, the analysis of these phases and their properties, particularly via the Landau theory of phase transitions,[5] has been extremely successful; model calculations are in accord with a wide range of experimental observations.

Our objective in this paper is to explore topological features of the cholesteric BP. We shall concentrate on three space groups: body-centered (bcc) O^5 ($I432$) and O^8 ($I4_132$), and simple-cubic (sc) O^2 ($P4_232$). The latter two are believed[4,5] to characterize the structures of the experimentally observed phases BP I and BP II, respectively.

Thermotropic nematics and cholesterics are composed of anisotropic (in most cases, rodlike) molecules which exhibit orientational (not translational) order below a critical temperature.[6] Macroscopically, this order manifests itself as an anisotropy in the material's second-order tensor properties, e.g., the dielectric and diamagnetic tensors. Such a tensor can therefore be used to construct an order parameter which describes quantitatively the orientationally ordered phase or phases. A suitable choice[5] is the anisotropic part of the dielectric tensor

$$\epsilon_{ij}(\mathbf{x})=\epsilon^d_{ij}(\mathbf{x})-\tfrac{1}{3}\,\mathrm{Tr}(\epsilon^d)\delta_{ij}\ . \tag{1}$$

This 3×3 symmetric traceless tensor vanishes in the disordered phase, where all the nonvanishing elements of ϵ^d are equal and located on the tensor's main diagonal. It is nonzero, however, for any orientationally ordered phase, such as a uniaxial or biaxial nematic, the helicoidal cholesteric, or any of the cholesteric BP.

We therefore consider in this paper the topological properties associated with a tensor order parameter $\epsilon_{ij}(\mathbf{x})$ appropriate to the cubic cholesteric BP. To begin, we review some well-known results for the nematic and cholesteric (helicoidal) phases, showing where our approach makes contact with them. We then consider the three cubic space groups which have been put forward[5] as characterizing the symmetry of cholesteric BP structures. For each, we determine the constraints (if any) imposed on the tensor order parameter by the particular space-group symmetry. These constraints will be shown to have topological consequences when the order-parameter space is also constrained.

For each of these space groups, we also consider the order-parameter distributions associated with local minima of the free energy, as obtained from the Landau theory of cholesterics.[5,7,8] Within this framework, the free-energy density of a system is expressed as a functional of the order parameter and its spatial derivatives. In many cases of interest, the physically relevant parameters in such an expression may be limited to those required to

define the phase diagram. Examples are temperature and applied field for the case of nematics and temperature and chirality or, more generally, temperature, chirality, and applied field for the case of cholesterics. By minimizing the free energy with respect to the order parameter, we obtain, in principle, both the equilibrium order parameter distribution and the thermodynamic phase diagram. The latter, in this case, is universal.[5,7,8]

In practice, the global minimization of any realistic free-energy functional for arbitrary values of the parameters is impossible. The approach taken, therefore, has been to consider, individually, possible high-symmetry structures for the cholesteric BP.[5,7,8] As noted, three space groups have been considered as possible structures for the cubic BP. For each of these, an appropriate order parameter was constructed as a linear combination of a limited number of appropriate spatial harmonics. The Fourier amplitudes were then determined by minimizing the associated free energy and a theoretical phase diagram was obtained by comparing the minimized free energies for the cubic, helicoidal, and disordered phases at each point.[7,8] This approach yielded order parameter fields for each of the possible BP structures, whose topological character will be examined by us here.

In the final section, we summarize our results and consider their implications. Some open questions and directions for further studies are also discussed.

II. DEFECTS IN NEMATIC AND CHOLESTERIC PHASES

A. The uniaxial nematic

As noted in Sec. I, the appropriate order parameter to describe a thermotropic nematic or cholesteric liquid-crystal system is a symmetric traceless 3×3 tensor. Such a tensor has five independent elements, each of which can take any real value between $\pm\infty$. The order-parameter space is thus R_5, which is much larger than those usually used to characterize the order of nematic (uniaxial or biaxial) or helicoidal cholesteric phases. For the case of uniaxial nematics, the standard[1-3] topological line and point singularity classification is obtained when the order parameter is taken to be[6] a unit director field $\hat{n}(\mathbf{x})$, satisfying the constraint $\hat{n}^2=1$. Its space is that of the two-dimensional projective plane P_2.

To relate these two viewpoints, we recall that a director representation $\hat{n}(\mathbf{x})$ is equivalent to the symmetric traceless tensor one

$$\epsilon_{ij}^{un}(\mathbf{x})=(\tfrac{3}{2})^{1/2}\epsilon_0[n_i(\mathbf{x})n_j(\mathbf{x})-\tfrac{1}{3}\delta_{ij}]\ , \tag{2}$$

where $\epsilon_0\neq0$ is position independent. Clearly, this tensor is a special case of the more general one defined in Eq. (1). The latter reduces to that in Eq. (2) if we impose two constraints: one, that $\epsilon_{ij}(\mathbf{x})$ be everywhere uniaxial and two, that its magnitude be position-independent. These conditions are satisfied when

$$[\mathrm{Tr}(\epsilon^2)]^3=6[\mathrm{Tr}(\epsilon^3)]^2=\epsilon_0^6\ , \tag{3}$$

independent of $\mathbf{x}$.

Offhand, it might appear that imposing two restrictions on the five independent components of the order parameter should reduce the initial five-dimensional space R_5 to a three rather than a two dimensional one. This is not so in this particular case due to the uniaxially condition, which imposes a constraint on the components of the order-parameter tensor and also ensures that its diagonalization requires two Euler angles only. (A symmetric, uniaxial, 3×3 tensor is diagonalized by two independent rotations rather than the three required for a biaxial one.) Adding the constant magnitude constraint and the physical requirement that $\hat{n}$ and $-\hat{n}$ be the same state reduces the order parameter space from R_5 to P_2.

The standard classification of line and point singularities which occur in nematic liquid crystals is obtained by considering appropriate mappings from real space R_3 to order-parameter space P_2. Note that the latter, and thus the topological properties of a uniaxial nematic, are unaffected if ϵ_0 is position dependent, provided, for example, that it everywhere satisfies the inequalities $0<\epsilon_1\leq\epsilon_0(\mathbf{x})\leq\epsilon_2$. In other words, mathematical singularities occur as a consequence of the restriction that $\epsilon_0\neq0$. This is easy to understand. Suppose that the order parameter had the director form given in Eq. (2) with $\epsilon_0=\epsilon_0(\mathbf{x})$ restricted to a real interval which *included* the origin. Then we could smoothly deform any director configuration $\hat{n}(\mathbf{r})$ in a given local region of real space to any other satisfying the same boundary conditions by (a) bringing $\epsilon_0(\mathbf{x})$ to zero in the region, (b) rotating $\hat{n}(\mathbf{x})$ to the specified director configuration,and (c) returning $\epsilon_0(\mathbf{x})$ to its initial distribution. All mappings on a specified closed surface (e.g., loops or spheres) embedded in this region would then be in the same class and topologically equivalent.

Given the constraint $\epsilon_0\neq0$, there exists[1-3] only one class of topologically stable line defects (see Fig. 1) and a denumerable number of point defects in uniaxial nematics (i.e., the fundamental group $\pi_1=\mathbb{Z}_2$ and the second homotopy group $\pi_2=Z$). However, if this constraint is relaxed (that is, if the space of the order parameter is en-

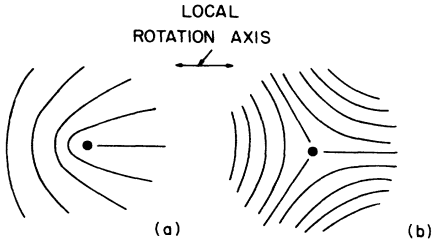

FIG. 1. Cross sections of a representation disclination in a uniaxial nematic system. Shown are the orientations of the director field $\hat{n}(\mathbf{x})$ for (a) $+\pi$ and (b) $-\pi$ configurations. These belong to the same element of the fundamental group and can be deformed into each other by a local rotation of $\hat{n}(\mathbf{x})$ by π around the axis indicated in the figure.

larged from P_2 to, e.g., R_5), then the original topological defects in P_2 may still, in practice, be energetically stable. Also, in real systems, topologically equivalent structures may not necessarily be easily deformable into each other due to energy barriers. Thus, in general, both topological and energetic aspects play important roles. We shall consider them both in Sec. III.

B. Biaxial nematic

For biaxial nematics, the standard description[1-3] of the order parameter is more complex. At a given point in real space, we require three independent Euler angles in order to diagonalize the biaxial order parameter. The resulting tensor can always be written in the form

$$\epsilon_{ij}(\mathbf{x})=\frac{1}{\sqrt{6}}\,|\,\epsilon_0(\mathbf{x})\,|\begin{bmatrix}[-1+\mu(\mathbf{x})]s(\mathbf{x}) & 0 & 0\\ 0 & [-1-\mu(\mathbf{x})]s(\mathbf{x}) & 0\\ 0 & 0 & 2s(\mathbf{x})\end{bmatrix}, \tag{4a}$$

with

$$\epsilon_0\neq 0,\quad 0<\mu\leq 1,\quad s=\epsilon_0/|\,\epsilon_0\,|\ . \tag{4b}$$

We shall refer to the reduced elements $(-1+\mu)s$, $(-1-\mu)s$, and $2s$ in Eq. (4) as the eigenvalues of the order parameter tensor. It follows that s can be either ± 1; it necessarily changes sign at those points at which $\mu(\mathbf{x})=1$, i.e., where the biaxiality of the tensor is maximum. We shall refer to the locus of these points as the "biaxial surface," noting that it divides the system into regions characterized by positive and negative values of $\epsilon_0(\mathbf{x})$. Where $\mu(\mathbf{x})$ vanishes, the tensor $\epsilon_{ij}(\mathbf{x})$ is uniaxial. We shall label these defects as "uniaxial positive" when $s=+1$ and "uniaxial negative" when $s=-1$. The term uniaxial will be used when the value of s is irrelevant.

By an argument analogous to that given for the uniaxial case, it is easy to show that the topological properties of a system described by the general order parameter in Eq. (4) are identical to those of one in which ϵ_0 and μ are position independent. The effective space of this order parameter is therefore three dimensional. Since the diagonalized tensor is invariant with respect to a rotation by π about any of its principal axes, we see that *the order-parameter space is the quotient group* $SO(3)/D_2$; i.e., the group of proper rotations in three dimensions with the identification of π rotations around three mutually perpendicular axes.[1-3,9]

To classify the topological singularities of the biaxial nematic, one considers, as in the uniaxial case, mappings from real to order-parameter space. Such singularities then exist as a consequence of the restrictions imposed on ϵ_0 and μ. They occur when constraints arising from the symmetry of the structure force us to violate these restrictions locally.

For the order-parameter space $SO(3)/D_2$, there are no topologically stable point defects, but there are four different classes of stable line defects.[1-3] In group-theoretical terms, $\pi_1=Q$ (the quaternion group) and $\pi_2=0$. We show,[1-3] in Fig. 2, cross sections of representative line defects for each of these classes. (Rigorously, these cross sections are planar only asymptotically in the neighborhood of the dislocation.) Let us consider their realization in a biaxial nematic system.

The first three defects, shown in parts 2(a) to 2(c) of the

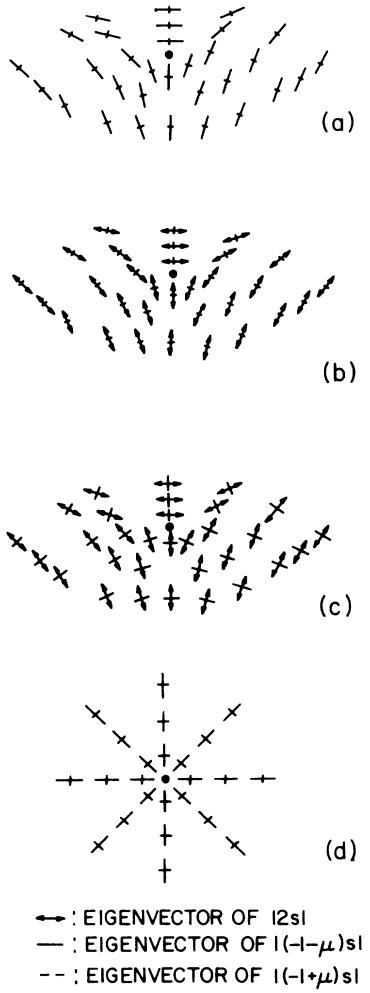

FIG. 2. Cross sections of representative disclinations in biaxial nematic systems. Shown in (a), (b), and (c) are the three nonequivalent classes of π disclinations, each in a $-\pi$ configuration. The nonrotating eigenvector (perpendicular to the plane of the figure) is that of the eigenvalue with the greatest $|\,2s\,|$, intermediate $|\,(-1-\mu)s\,|$, and smallest $|\,(-1+\mu)s\,|$ absolute value, respectively. Shown in (d) is a 2π disclination.

figure, are similar. In each, there is a π rotation of two of the principal axes characterizing the biaxial order parameter on any closed path which encircles the dislocation axis. The third principal axis is perpendicular to the cross section. When the order parameter has the explicit form of Eq. (4), this is equivalent to stating that the eigenvector associated with one of the three eigenvalues of the tensor is perpendicular to the plane of the figure. Note that it is not necessary that the tangent to the disclination and the nonrotating eigenvector to be parallel to each other.

Insofar as the group-theoretical classification of biaxial line defects is concerned, the question of which of the topological constraints (nonuniaxiality or nonvanishing of the order parameter) is violated at the disclination is irrelevant. However, when energetics are considered together with the specific order-parameter realization given in Eq. (1) or Eq. (4) (i.e., the order-parameter space is enlarged to R_5), it becomes meaningful. Note that when the nonrotating eigenvector is not associated with the $2s=\pm 2$ eigenvalue, the amplitude ϵ_0 of the order parameter must vanish at the disclination. In the remaining case, where the rotating eigenvectors are associated with $(-1-\mu)s$ and $(-1+\mu)s$, either $\epsilon_0=0$ or $\mu=0$ is, in principle, possible at the disclination, depending upon the energetics. For example if the physical system is one which first undergoes a transition from a disordered to a uniaxial state and then to a biaxial one, it is likely that the structure having the lower free energy would have a uniaxial core. This is what occurs in the lyotropic *rubidium laurate, 1-decanol,* H_2O system.[10] Kutka and Trebin[11] call singularities of this type "semidefects" and have discussed their topological properties.

Figure 2(d) shows a representative 2π line defect. Unlike the π case, there is only one topological class of defects of this type. That is, we can always rotate the order parameter within a local region surrounding the disclination so that any of the three eigenvectors is the nonrotating one. Topologically, there is no distinction among these configurations. Energetically, however, there can be significant differences. For example, when the eigenvector of the $2s=\pm 2$ eigenvalue is nonrotating, the system can "melt" to a uniaxial state (semidefect[11]) at the disclination whereas, in the alternate configurations, it must melt to an isotropic core. In real systems, the free energy differences between these topologically equivalent defect structures is likely to be considerable.

C. Blue phases

From the topological point of view, there is a fundamental difference between cholesteric BP structures and those discussed above. For a uniaxial or biaxial nematic (and also for the helicoidal cholesteric phase), there is always a singularity-free order-parameter configuration (energetically, the ground state). The three cubic space groups, however, *must have topological singularities when the order-parameter space is taken to be* $SO(3)/D_2$. That is, even when the order-parameter distribution conforms exactly to one of these space groups (e.g., there are no edge or screw dislocations), there will always be line defects and, in some cases, isolated point singularities located on them. We shall consider this aspect in detail in Sec. III.

Our approach to studying dislocations in the cholesteric BP will be a physical one: Close to a defect line or, in other words, on a length scale small with respect to a unit cell dimension,[4,5,7,8] the order-parameter field in the BP is the same as in a biaxial nematic. We therefore expect the structures of disclinations in perfect BP structures to be similar to those in biaxial nematics. They can, therefore, be associated with conjugacy classes of the same fundamental group.[1-3] However, since our structures have additional symmetry, there is no guarantee that defects in the same class are topologically equivalent.[1] We shall indeed see that, in some cases, they are not.

In Sec. III, we consider the three cubic space groups in detail. For each, we determine the general symmetry constraints, if any, on disclinations and consider the topological properties of the equilibrium order-parameter distributions found from Landau-theory calculations.[8]

III. CUBIC BLUE PHASES AS PERIODIC DEFECT STRUCTURES

Since the tensor order parameter $\epsilon_{ij}(\mathbf{x})$ is periodic in the cubic BP, it is sufficient to specify it within a unit cell. For our purposes, a convenient choice is the so-called asymmetric unit. By definition, this is a simply connected part of space from which, by repreated application of the group's symmetry operations, space can be completely filled.[12] For the cubic space groups, these units have been described in detail by Koch and Fischer[13] and may be found in standard tables.[12] For the three space groups of interest to us, the relevant asymmetric units are shown in Figs. 3–5 and their specifications are summarized in Table I. Note that threefold and fourfold rotation axes can only be edges of these units; twofold axes can be ei-

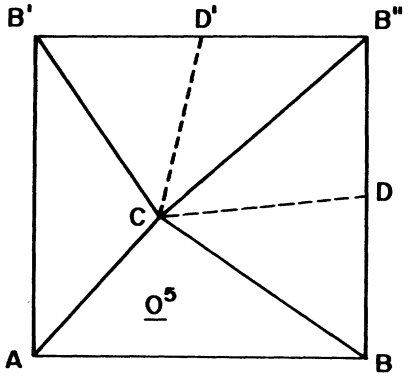

FIG. 3. The O^5 asymmetric unit. Its vertices are at A: (0,0,0); B: $(\frac{1}{2},0,0)$; B': $(0,\frac{1}{2},0)$; B'': $(0,0,\frac{1}{2})$; and C: $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$. The points D,D' bisect the edges BB'', $B'B''$, respectively. AC is a threefold axis, AB and AB' are fourfold axes, BB'', $B'B''$, CD, and CD' are twofold axes. B,B', etc., designate points which are equivalent under operations of the space group. The exact bounds of the unit are given in Table I.

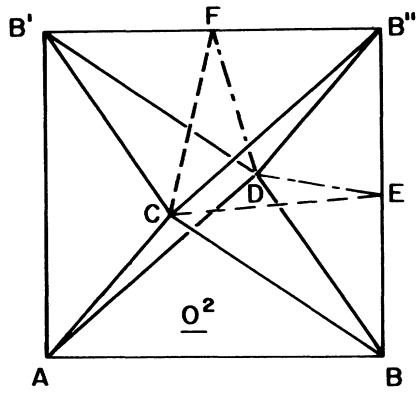

FIG. 4. The O^2 asymmetric unit. Its vertices are at A: (0,0,0); B: $(\frac{1}{2},0,0)$; B': $(0,\frac{1}{2},0)$; B'': $(0,0,\frac{1}{2})$; C: $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$; and D: $(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$. The points E,F bisect the edges BB'', $B'B''$, respectively. AC and AD are threefold axes, BB'', $B'B''$, CD, CF, DE, and DF are twofold axes. B, B', etc., designate points which are equivalent under operations of the space group. The exact bounds of the unit are given in Table I.

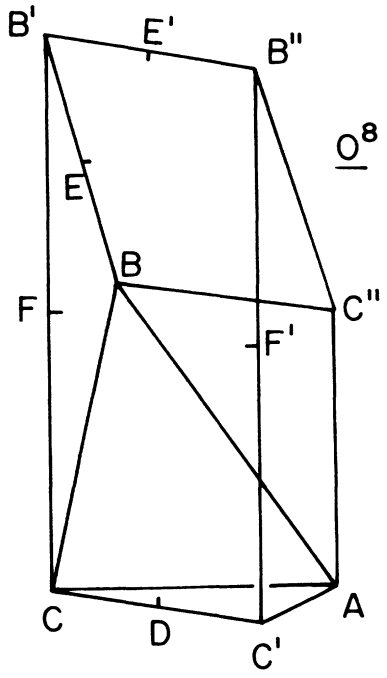

FIG. 5. The O^8 asymmetric unit. Its vertices are at A: $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$; B: $(-\frac{1}{4},-\frac{1}{4},-\frac{1}{4})$; B': $(-\frac{3}{4},-\frac{1}{4},\frac{1}{4})$; B'': $(-\frac{3}{4},\frac{1}{4},\frac{3}{4})$; C: $(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$; C': $(\frac{1}{4},\frac{1}{4},\frac{3}{4})$; and C'': $(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$. The points D, E, E', F, F'' bisect the edges CC', BB', $B'B''$, $B'C$, $B''C'$, respectively. AB is a threefold axis, BB', $B'B''$, $B'C'$, CC', AD, AF', DE', and EF are twofold axes (the last four are not drawn in the figure). B, B', etc., designate points which are equivalent under operations of the space group. The exact bounds of the unit are given in Table I.

ther edges or bisectors of boundary planes. (In exceptional cases, a boundary plane may be composed of two distinct regions which are coplanar. In such a case, a twofold axis lying in the plane need bisect only one of the regions. The asymmetric unit for O^8 shown in Fig. 5 is one of these exceptions.)

A. bcc O^5 ($I432$)

The first cubic space group proposed as a possible structure for a cholesteric BP, based upon structural[14] and energetic considerations,[15] was bcc O^5 ($I432$). This group has no center of symmetry (as is the case for all BP structures) and is symmorphic. A general point has 48 equivalent positions in the bcc cell; thus the volume of the asymmetric unit (see Fig. 3 and Table I) is $\frac{1}{48}$ that of the standard bcc cell. The unit has the form of a regular pyramid with a square base. Although the O^5 space group is not believed to describe either of the experimentally observed cubic BP, it has been argued that it should appear at sufficiently short cholesteric pitch.[7,16] Its topological properties are of interest in any case.

The O^5 space group has both threefold and fourfold rotation axes. Upon them, the tensor order parameter given in Eq. (4) must either vanish or be uniaxial, with its unique axis aligned with the rotation axis. Thus both of these symmetry axes are necessarily disclinations. In addition, there are points in the structure with cubic (432) symmetry, represented by the origin of the asymmetric unit in Fig. 3. Here threefold and fourfold axes intersect and the biaxial tensor order parameter must vanish.

Symmetry requires that all physical properties be invariant to $\pi/2$ rotations about a fourfold axis. It follows that the order-parameter distribution, in the neighborhood of such an axis, is characterized by the singularity class of Fig. 2(d). On the axis, the tensor vanishes unless the eigenvector of its $2s=\pm 2$ eigenvalue is parallel to the axis, in which case it can be uniaxial. Turning to the threefold axis, the disclination, insofar as the local topology is concerned, can belong to any of the four nontrivial biaxial classes. For those shown in Figs. 2(b) and 2(c), the eigenvector of the $2s=\pm 2$ eigenvalue rotates about the symmetry axis in its immediate neighborhood and the tensor must therefore vanish on the entire axis. For the remaining two classes [Figs. 2(a) and 2(d)], the tensor can be uniaxial on the threefold axis. Since the $2s=\pm 2$ eigenvector is along the axis, only one of the three topologically equivalent 2π configurations is compatible with the symmetry.

While the above classification is identical to that used for the biaxial nematic and helicoidal cholesteric phases, there is a significant difference. For the latter, one can always convert singular configurations belonging to the same class into each other by a continuous transformation. Consider, for example, the two topologically equivalent π disclinations shown in Fig. 6. In group-theoretical terms, these two configurations are characterized by different elements of the fundamental group π_1 of the biaxial nematic, with both elements belonging to the same conjugacy class.[1] When, however, the disclination is also a threefold rotation axis, the configuration in Fig.

TABLE I. The asymmetric units for O^5, O^2, and O^8. Given are the bounding planes and the portions of these planes, their edges, and the vertices included in each unit. The vertices are defined in Figs. 3–5. See Ref. 13.

Group	Bounding planes	Planes	Edges	Vertices
O^5 ($I432$)	(a) $z=0$	$a(x-y\geq 0)$	AB, AC	$A;B;C$
	(b) $x-z=0$	$c(y\leq \frac{1}{4})$	$BC;BD$	
	(c) $x+z=\frac{1}{2}$	$d;e(x\geq \frac{1}{4})$		
	(d) $y-z=0$			
	(e) $y+z=\frac{1}{2}$			
O^2 ($P4_232$)	(a) $x-z=0$	$c(y\leq \frac{1}{4})$	$AB;AC;AD$	$A;B;C;D$
	(b) $x+z=0$	$d(y\leq \frac{1}{4})$	$BC;BD;BE$	
	(c) $x-z=\frac{1}{2}$	$e;f$	$B''F$	
	(d) $x+z=\frac{1}{2}$	$g(x\geq \frac{1}{4})$		
	(e) $y-z=0$	$h(x\geq \frac{1}{4})$		
	(f) $y+z=0$			
	(g) $y-z=\frac{1}{2}$			
	(h) $y+z=\frac{1}{2}$			
O^8 ($I4_132$)	(a) $x=\frac{1}{8}$	$a(y+z\leq \frac{1}{4})$	$AC;AB;BC$	$A;B;C$
	(b) $y=\frac{1}{8}$	$b(x+z\leq 4)$	$BC'';CD;B'E'$	
	(c) $y=-\frac{1}{8}$	$c(z-x\geq \frac{1}{4})$		
	(d) $x-z=0$	$e;f(y\leq 0)$		
	(e) $y-z=0$	$g(y-x\leq \frac{1}{4})$		
	(f) $-y+z=\frac{1}{4}$			
	(g) $-x+y-z=\frac{1}{8}$			

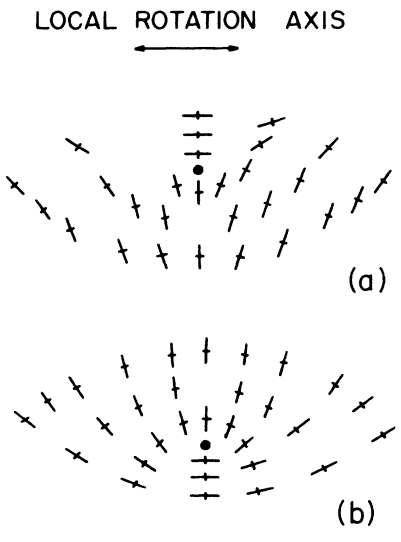

FIG. 6. Cross sections of two possible configurations (a) $-\pi$, (b) $+\pi$ for a π dislocation line, characterized by different elements of the fundamental group belonging to the same conjugacy class. They can be continuously transformed into each other by a π rotation of each of the elements about the axis indicated in the figure. Only $-\pi$ defects are consistent with threefold symmetry on the defect line. The disclinations shown here are in the same conjugacy class as that in Fig. 2(a); similar examples can be given for those in Figs. 2(b) and 2(c).

6(b) is not compatible with the point-group symmetry. Thus, in certain cases, the classification of line singularities in the BP can be with an *element* of the fundamental group rather than with a conjugacy class. The need to augment the topological theory of line defects by considering the point symmetry of the order parameter at the disclination has been discussed by Balinskii, Volovik, and Kats.[17]

Based upon energetic considerations, we now restrict ourselves to configurations in which $\epsilon_0\neq 0$ everywhere except at points of cubic symmetry and consider the following question: It is topologically possible to have an order-parameter distribution consistent with O^5 symmetry which exhibits uniaxial positive disclinations only? Equivalently, can we define an $\epsilon_{ij}(\mathbf{x})$ in the O^5 asymmetric unit of Fig. 3 which has no biaxial surface? If so, we can obtain a uniaxial director order-parameter field which is invariant under O^5 by simply aligning $\hat{n}(\mathbf{x})$ with the eigenvector of the $+2$ eigenvalue of $\epsilon_{ij}(\mathbf{x})$. This distribution would have point singularities only. We now show, however, that this is impossible.

We refer to Fig. 3. By hypothesis, $\epsilon_0>0$, i.e., $s=1$ everywhere, except at the point of origin. Then, on the fourfold axis, the eigenvector associated with the $+2$ eigenvalue must be *parallel* to the axis itself and, at the vertices B and B' (B, B', etc., designate points which are

equivalent under symmetry operations of the space group), it must be perpendicular to the edges BB'' and $B'B''$. Since these are both twofold axes, the eigenvectors associated with the $+2$ eigenvalue must remain *perpendicular* to these axes as we move from B to B'' and from B' to B'' (we return to this point below). Of course, the order-parameter tensor need not be uniaxial on a twofold axis. Consider now the midpoints of BB'' and $B'B''$, labeled D and D', respectively, in the figure. Since CD and CD' are both twofold axes,[12] the eigenvectors of $+2$ at D and D' must be either along these axes or parallel to the normals to the planes $BB''C$ and $B'B''C$, respectively. The crucial point, however, is that the points D and D' are symmetry related via a $\pi/2$ rotation about the fourfold axis passing through B'' and perpendicular to the plane ABB'. Thus if the eigenvector at D is along CD, that at D' is perpendicular to CD', and vice versa. In either case, at vertex C the eigenvector associated with the $+2$ eigenvalue must be *perpendicular* to the threefold axis AC. This, however, *contradicts* our original hypothesis, according to which this eigenvector is *parallel* to this axis.

We now return to the claim in the previous paragraph that the eigenvector associated with a $+2$ eigenvalue on a twofold axis cannot change its direction from parallel to perpendicular to the axis at any point upon it. This could occur only if there existed a uniaxial negative disclination which intersected this axis (see Fig. 7). One hypothesis, however, *forbids* such defect lines. This completes the proof that it is impossible to define a tensor order parameter with $s=+1$ everywhere (i.e., no biaxial surface) in the O^5 asymmetric unit. Note that the proof did not depend upon the singularity type (π or 2π) on the threefold axis.

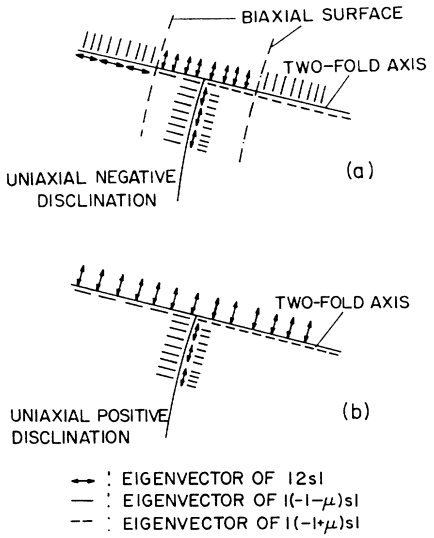

FIG. 7. Examples of eigenvector configurations in the neighborhood of the intersection of a (a) uniaxial negative, (b) uniaxial positive disclination with a twofold symmetry axis. At any point, the eigenvector not shown in perpendicular to the plane of the figure. In (a), $s=-1$ in the region between the intersection of the biaxial surface with the plane of the figure and including the defect line. External to this region, $s=+1$. On the biaxial surface, $\mu=1$. In (b), $s=+1$ everywhere.

The above analysis indicates that the O^5 structure *has at least two distinct line singularities,* located on its threefold and fourfold rotation axes. The disclination on the fourfold axis must be of the 2π type. That on the threefold axis, if of the π type, can be associated with only one of the two elements belonging to this conjugacy class. When the defect cores are uniaxial (i.e., not isotropic) and there are no other uniaxial negative defect lines, we must have $s=+1$ on one of the symmetry axes and $s=-1$ on the other; these axes are separated by a biaxial surface.

Are these two disclinations, which are required by symmetry, sufficient as well as necessary? The answer to this question is obviously positive if we can find an order-parameter distribution $\epsilon_{ij}(\mathbf{x})$ with O^5 symmetry having only these defect lines. Let us therefore consider the topological properties of a particularly interesting distribution, that corresponding to the minimum free energy for this structure. It was obtained[8] via Landau theory using a trial order parameter consisting of selected symmetry-allowed[7,8,18] Fourier components characterized by $\langle 111\rangle$, $\langle 211\rangle$, and $\langle 220\rangle$ wave vectors. The resulting order parameter is given in the Appendix.

Upon examining the order parameter field for O^5 given in the Appendix, we find the following. (a) It vanishes only at points having cubic symmetry. (b) The only disclinations are on the threefold and fourfold axes. (c) The former is uniaxial negative and the latter uniaxial positive. (d) On the threefold axis, the eigenvector of the -2 eigenvalue is aligned with the axis. In its neighborhood, those associated with the eigenvalues $(1+\mu)$ and $(1-\mu)$ rotate through an angle of $-\pi$ along a closed loop enclosing the defect [see Fig. 2(a)] as expected. Energetically, it is not surprising that this disclination is of the π rather than the 2π type as the energy cost of the latter is approximately four times greater than that of the former.[6] (e) On the fourfold axis, the eigenvector of the $+2$ eigenvector is along the axis. In its neighborhood, the two other eigenvectors rotate through 2π as the axis is encircled. This is, of course, expected as a π disclination cannot occur on a fourfold axis. (f) The biaxial surface consists of a collection of sleeves which enclose the threefold axes and coalesce with them at points of cubic symmetry. They thus form a three dimensional net of connected sausagelike objects; eight of which meet at each point having (432) symmetry.

Given a distribution $\epsilon_{ij}(\mathbf{x})$ for the O^5 structure, we can also characterize it by a uniaxial director by the following procedure: One, set $\mu=0$ in $s=1$ regions. In the same regions, replace $\epsilon_0(\mathbf{x})$ by its average value. Two, set $\epsilon_0=0$ in the region between the threefold axis and the biaxial surface. (In principle, we could, instead, "shrink" the sleeve defining the biaxial surface onto the axis. This would make the energy of the defect infinite.[6]) The resulting director configuration has defects on the threefold axes only. If the sleeve is shrunk to zero, they are of the type shown in Fig. 1.

The free energy of the constrained O^5 director configuration obtained via the process described above (with a nonzero sleeve diameter) can be lowered by allowing the director field $\hat{n}(\mathbf{x})$ to rotate locally. Such an approach to the energetics of BP was used by Meiboom *et al.*[19]

B. sc O^2 ($P4_232$)

The possibility that one of the cubic BP might have a sc O^2 structure was noted by us[20] and by Alexander.[21] A wide range of experimental[4] and theoretical[5–7] evidence has confirmed this suggestion, and this space group is believed to characterize BP II. It is nonsymmorphic and noncentrosymmetric and a general point has 24 equivalent positions in the standard sc cell. The volume of the O^2 asymmetric unit is thus $\frac{1}{24}$ that of the standard cell. As shown in Fig. 4, it has the form of a regular double pyramid with a square base. Its bounds are listed in Table I.

The nonsymmorphic O^2 space group has among its elements fourfold screw axes and two nonequilvalent threefold axes. At the origin of the asymmetric unit four threefold axes intersect and the biaxial tensor must therefore vanish at this point. Elsewhere on the threefold axes, the limitations on the order parameter are the same as for the case of O^5. That is, these axes are necessarily disclinations and, unless ϵ_{ij} vanishes, it must be uniaxial upon them. If the disclination is uniaxial and has a rotation angle of π, it must be described by the element of the fundamental group represented by Fig. 6(a) and not by that (in the same conjugacy class) shown in Fig. 6(b).

Restricting ourselves to a nonvanishing order-parameter tensor on the threefold axes, is it topologically possible for the two different threefold axes to be characterized by disclinations of the same type (i.e., both uniaxial positive or negative)? Using an argument similar to that given for the case of O^5, we demonstrate that this is impossible.

Referring to Fig. 4, let us assume $s=1$ everyone in the asymmetric unit and that the order-parameter tensor is uniaxial on the disclinations. This, then, includes both of the threefold axes, *AC* and *AD*. At vertex *C*, therefore, the eigenvector of the $+2$ eigenvalue is *perpendicular* to the twofold axis *CE* and, at vertex *D*, the same eigenvector is *perpendicular* to twofold *DE*. Thus, at point *E*, this eigenvector must be *parallel* to the twofold axis *BB''*. By exactly similar reasoning, we see that the eigenvector of the $+2$ eigenvector at *F* must be along *B'B''*. (The bisectors *CF*, *DF*, and the edge *B'B''* are all twofold axes.) Since, by hypothesis, there cannot be a change from parallel to perpendicular in the direction of this eigenvector along a twofold axis, we have a *contradiction* at vertex *B''* and our original assumption is invalid. Thus either the axes *AC*, *AD* are separated by a biaxial surface or, if both have $+2$ eigenvalues, there must be a disclination with a -2 eigenvalue elsewhere in the asymmetric cell.

Given the above result, is there a topologically-allowed biaxial order-parameter distribution in which, in the asymmetric unit, only the two threefold axes are disclinations (one with a $+2$, the other with a -2 eigenvalue)? That is, are these two line defects sufficient as well as necessary? Here, unlike the O^5 case, the disclination pattern corresponding to the order-parameter distribution minimizing the free energy [see Fig. 8(a)] does not give a definite answer. It was obtained using Landau theory and an order parameter with $\langle 100 \rangle$ and $\langle 110 \rangle$ Fourier components.[7,8,18] The resulting expression is given in the Appendix. As expected, the disclinations on the threefold axes are of opposite sign ($s=-1$ on *AC* and $+1$ on *AD*), with the uniaxial eigenvectors along the symmetry direction. Both are $-\pi$ defects of the type shown in Fig. 2(a). The biaxial surface is a collection of narrow sleeves, which surround the uniaxial negative disclinations and coalesce with them at the isotropic points.

However, in addition to these two disclinations, there is a third one upon which the order parameter is uniaxial positive. Its end points P_1, P_2 are on the twofold axes, *AB* and *CF*, respectively, and two of the principal axes of the biaxial tensor rotate through an angle of $+\pi$ when traversing a loop encircling this defect line. Generating the standard sc cell from the asymmetric one, we find that equivalent points on this helicoidal disclination differ by two lattice constants. Another way of seeing this is to consider the "group of the line,"[22] that is, the set of operations which leaves this defect line invariant. These are the elements of a group which is necessarily a subgroup of O^2. For the disclination we are considering the appropriate group is[22] $P4_2(22)$, with a primitive translation twice that of the cubic cell. Here 4_2 denotes the screw displacement symmetry operation about the axis of the helical line (which is the same screw axis in the O^2 space group), and (22) that the helix, in addition, is invariant with respect to two twofold rotations perpendicular to this axis. If we define the sc cell as a closed torus (translation group T^3) embedded in a four-dimensional space, then the segment of the disclination between P_1 and P_2 in the O^2 asymmetric unit generates a line defect in T^3 with a winding number of two. In other words, there are two such helical disclinations sharing the same axis of the O^2 space group (i.e., they form a "double helix"). In the cubic O^2 cell, there are a total of six helical disclinations (two about each of the structure's 4_2 axes).

In Fig. 8(b) we give some details of the minimum free-energy order-parameter configuration on the symmetry axes within the asymmetric unit. In particular, we show which of the three principal axes of the biaxial tensor is along each of these axes. Note the interchange in the directions of two of the principal axes at the points P_1 and P_2.

Interestingly, although the minimum energy configuration summarized in Fig. 8 has a third disclination, such a defect is not a topological requirement. To establish this, we shall use the following (note, however, the points raised in the following paragraph): One, since the O^2 system has no fourfold axes, we can always have a topologically stable configuration without 2π disclinations. The basis for this statement is that, topologically, we can take the defects on the threefold axes to be of the

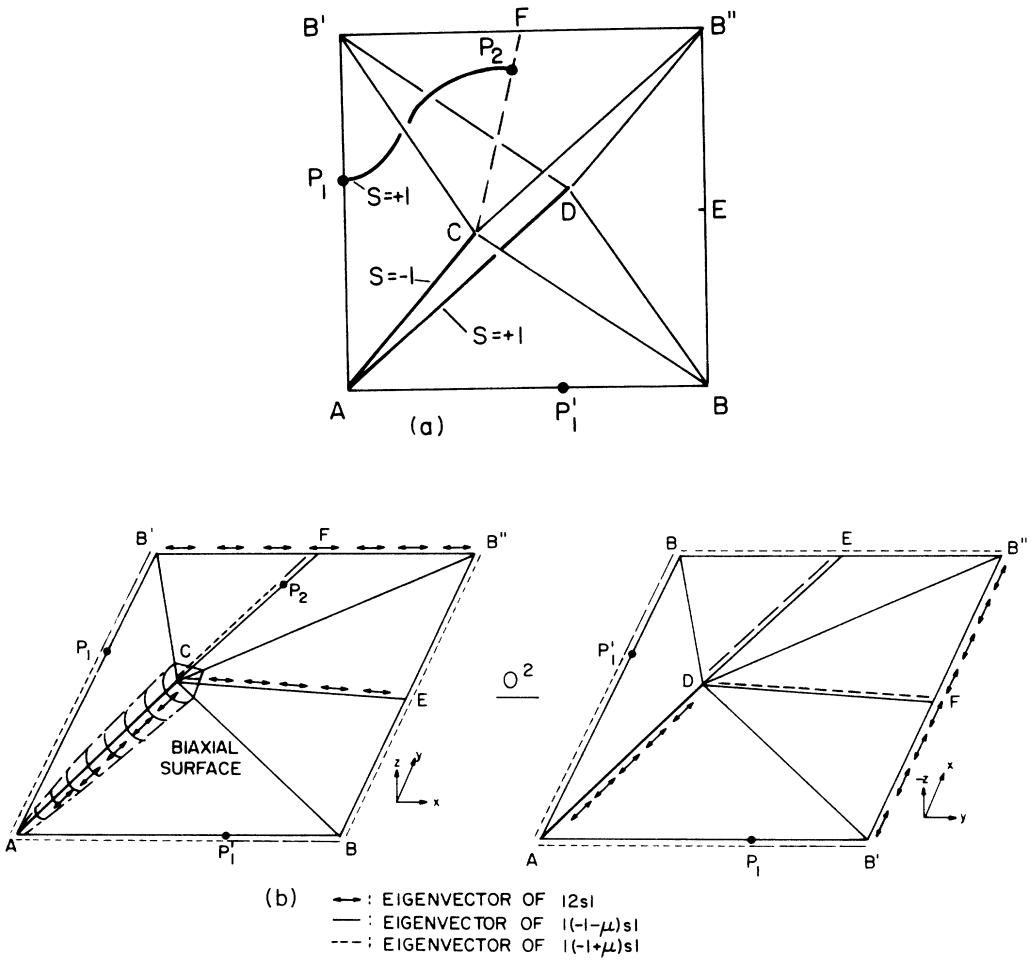

FIG. 8. Minimum free-energy configuration with O^2 symmetry. Shown are (a) the type ($s=+1$: uniaxial positive; $s=-1$: uniaxial negative) and location of the disclinations in the asymmetric unit, and (b) the principal axes of the biaxial order parameter tensor parallel to the threefold and twofold axes and the location of the biaxial surface. At vertex A the order parameter vanishes.

π type and use the fact that the presence of a π disclination serves to catalyze the decay of any 2π one which is not symmetry imposed.[1] Second, it is sufficient, in order to determine whether there exists an order-parameter configuration compatible with O^2 symmetry and without additional disclinations, to examine the principal axes of the biaxial tensor on the twofold axes of the asymmetric unit and, in particular, to determine whether any disclinations necessarily intersect these axes. This follows by observing the following. (1) If there is a π disclination which does not intersect a twofold axis at all points at which it exists the asymmetric unit, there must be a second disclination belonging to the same element of the fundamental group and symmetrically located with respect to the twofold axes; an example for a simple system characterized by a director order-parameter field is shown in Fig. 9. (2) Topologically, these two disclinations can be combined so as to put the new end points on twofold axes; the resulting disclination, if any, is then the 2π type.[1] We have already pointed out, however, that in a system with O^2 symmetry such a disclination is topologically unstable. Thus it is sufficient to examine the dis-

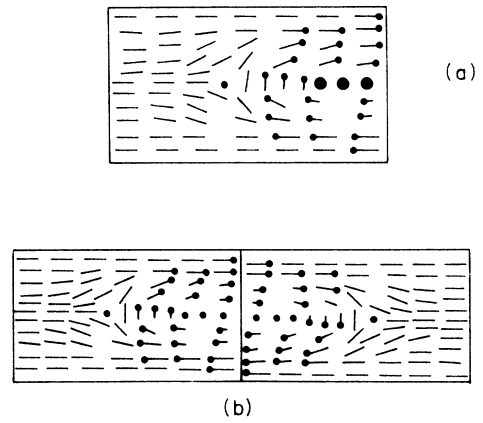

FIG. 9. Possible director order-parameter field with a $-\pi$ singularity in (a) a region bounded by four nonequivalent twofold axes, and (b) the same field in two adjacent regions. Directors which are canted with respect to the plane of the figure are drawn with a dot at that end of $\hat{n}$ which inclines upward. The structure in (b) contains two $-\pi$ and a 2π disclination, which combine to give a defect-free structure.

tribution of the biaxial tensor on the twofold symmetry axes, as claimed.

We stress, however, that the argument in the previous paragraph must be viewed with caution. As noted in Sec. II, for nontranslationally invariant structures, the space-group symmetry can break the topological equivalence of defects belonging to the same conjugacy class. There is thus the possibility that, in the space groups characterizing BP, the combination rules for defects will not always be identical with those applicable to translationally invariant biaxial systems,[1-3] as used by us in the argument given above. In other words, it is not obvious to us that, in all cases, we have homotopies (i.e., continuously deformations of the order-parameter field) which combine defects and also satisfy the space-group symmetry at all intermediate configurations. If this is not so, then combining defects as discussed in the previous paragraph may require, at intermediate stages, distortions of the physical medium. Having stated all this, however, we shall continue to assume that the usual rules are valid (or, alternatively, that any distortions required do not entail prohibitive energy barriers) and that it is therefore sufficient, in order to determine whether there are additional topologically required disclinations, to study the order-parameter configuration on the symmetry axes.

To demonstrate that no topologically required disclinations are required for O^2 symmetry in addition to those on the threefold axes, we give, in Fig. 10, an example of a configuration satisfying this condition. Shown is the orientation of the principal axes of $\epsilon_{ij}(\mathbf{x})$ on the symmetry axes. A self-consistent pattern is obtained without any interchange of principal axes except at the intersection points with the threefold symmetry axes. Thus additional defect lines are *not* required.

Finally, consider the characterization of an O^2 system by a uniaxial order parameter (i.e., one whose space is $P_2 = S_2/\mathbb{Z}_2$). The same procedure used for the O^5 case results in a structure which is singularity-free except on those threefold axes upon which the biaxial tensor had a -2 eigenvector. Here the defects are of the type shown in Fig. 1. This is the uniaxial O^2 configuration used as a starting point by Meiboom *et al.*[19] in their analysis of BP structures with director order parameters.

C. bcc O^8 ($I4_132$)

When experimental studies[4] made it clear that there exist two cubic cholesteric BP, it was suggested[20] that the O^8 space group could characterize the structure of one of them. This assignment has since been confirmed for BP I.[4,5,8]

The bcc space group O^8 is nonsymmorphic and noncentrosymmetric and a general point has 48 equivalent positions in the standard cell. Its asymmetric unit, given in Fig. 5 and Table I, is quite different from those for the space groups O^5 and O^2. In particular, the threefold axes of O^8 do not intersect and there are both positive and negative fourfold screw axes. There are no points in the O^8 structure at which the biaxial order-parameter tensor necessarily vanishes.

As in the two other space groups considered, there must be a disclination on the threefold axis of the asymmetric unit. In principle, it can be either the π or 2π type; if the former, it is, as discussed earlier, described by the fundamental group element of Fig. 6(a) rather than that in Fig. 6(b). When the order parameter is uniaxial on this symmetry axis, it can have either a $+2$ or -2 eigenvalue. Again, the first question is whether there must be other topologically required dislocations in O^8 structures characterized by a biaxial tensor order parameter?

As discussed in Sec. III B, taking the disclination on the threefold axis to be of the π type reduces this question to determining whether additional π disclinations must intersect the twofold axes of the asymmetric unit. We therefore assume that the threefold axis is a $-\pi$ disclination and, without loss of generality, take it to be uniaxial positive. We next divide the problem into two parts: First, must there be a biaxial surface and a uniaxi-

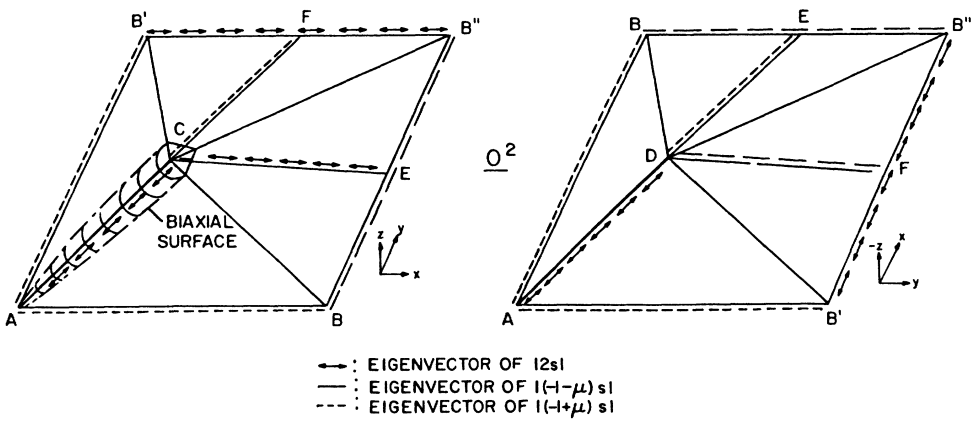

FIG. 10. A topologically acceptable order-parameter configuration in the O^2 asymmetric unit with disclinations on the threefold axes of the structure only. Shown are the principal axes of the order parameter parallel to the threefold and twofold axes and the location of the biaxial surface. The order parameter vanishes at vertex A.

al negative disclination in the unit, given the above configuration on the threefold axis? Second, if the answer to the above is negative, must there be uniaxial positive disclinations in addition to the one on the threefold axis?

We show, by demonstration, that the answer to the first part is negative. There are three nonsymmetry related types of twofold axes in the O^8 structure, two of which intersect the threefold axes. In Fig. 11, one of these is represented by the segments AD, AF', and EF, the second by BB', $B'B''$, $B'C''$, and CC'. The third type of twofold axis appears as DE' in the figure. Since the first two types are both perpendicular to the threefold axis (AB in the figure), the eigenvector of the $+2$ eigenvalue on any of these axes will be everywhere *perpendicular* to it in the absence of a biaxial surface. Of course, this eigenvector can (and will) rotate about the symmetry axis in order to satisfy the conditions we now specify at their intersections. These points, where axes of different types cross, are D, E, and E' (at E and E', one of the twofold axes is external to the unit shown). At each of them, the three different axis types are at right angles to each other. Then, again in the absence of a biaxial surface, the eigenvector of the $+2$ eigenvalue must be *parallel* to DE' at all points upon it. We thus have a realizable configuration for the eigenvector of the $+2$ eigenvalue everywhere on the twofold axes which is *consistent with the initial assumption that no uniaxial negative defect lines exist.* This demonstrates that the answer to the first part of our problem is indeed negative.

We now turn to the second part. Take the configuration of the $+2$ eigenvector on the twofold axes to be as in Fig. 11 and consider the orientation of the other two eigenvectors. Clearly, it is sufficient, upon the twofold axes, to specify the eigenvector parallel to them. What we must show is that there is a configuration wherein the eigenvectors of $(-1-\mu)$ and $(-1+\mu)$ do not interchange directions at any points on the twofold axes except where they cross the threefold one. At the latter, of course, an interchange must take place.

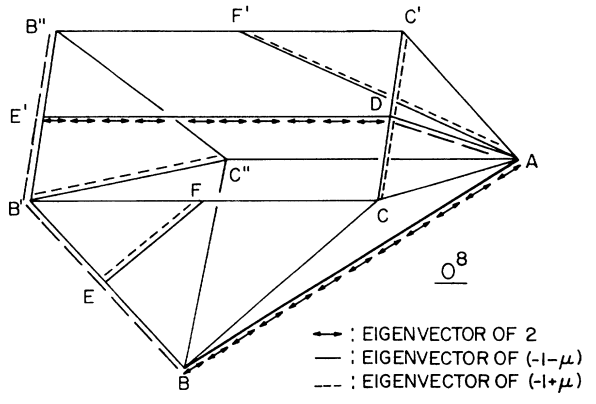

FIG. 11. A topologically acceptable order-parameter configuration in the O^8 asymmetric unit with a uniaxial positive ($s=+1$) disclination on the threefold axis of the structure only. Shown are the principal axes of the order parameter parallel to the threefold and twofold axes of the structure. The order parameter is nonzero everywhere.

In Fig. 11, we show a configuration satisfying the above conditions. In it, the eigenvector of $(-1-\mu)$ is *parallel* to the segments of the twofold axes AD, BB', and $B'B''$ while that of $(-1+\mu)$ is *parallel* to AF', EF, CC', and $B'C''$. Both these eigenvectors are *perpendicular* to DE' and rotate about this axis. Thus, by demonstration, we have shown (somewhat to our surprise) that *there are no topologically required uniaxial positive disclinations in addition to that on the threefold symmetry axis.* We conclude that the only topologically required disclination in any O^8 structure with a biaxial tensor order parameter is the one on the threefold axis. It, of course, can be either uniaxial positive or negative.

What are the topological properties of the minimum-energy structure? The Landau theory analysis for the O^8 structure, based upon an order parameter with $\langle 110\rangle$, $\langle 200\rangle$, $\langle 211\rangle$, and $\langle 220\rangle$ Fourier components[8,18] yields three local minima for the free energy. These are summarized in the Appendix and their defect structures are given in Figs. 12 and 13.

Consider first Fig. 12. We see that all three structures have disclinations in addition to the required one on the threefold axis. In particular, for O_a^8 and O_b^8, the disclination on this symmetry axis is uniaxial positive and there is also a uniaxial negative disclination and a second uniaxial positive one in the asymmetric unit. In O_c^8 which is believed[5,8,19] to be the structure of BP I), the topology is different; the threefold axis is a uniaxial negative disclination and there are, in addition, two uniaxial positive ones in the asymmetric unit.

1. O_a^8

The simplest disclination structure is that of O_a^8 [see Fig. 12(a)]. Here the segment of the uniaxial negative disclination in the asymmetric unit has its end points P_1, P_2 on the twofold axes DE' and $B'C''$, respectively. The end points of the additional uniaxial positive one (P_3,P_4) are on the twofold axes DE' and AF'. These are both π disclinations (uniaxial negative: $+\pi$, positive: $-\pi$) and the resulting eigenvector orientation on the symmetry axes for this structure is shown in Fig. 13(a). Both have a helical structure; their symmetry groups ("group of the line") are $P4_3(22)$ (negative) and $P4_1(22)$ (positive).[22] The screw orientation of the uniaxial negative defect line is opposite to that of the positive one and their axes are the 4_3 and 4_1 screw axes, respectively, of the O^8 space group. For both, the primitive translation is identical to that of the cubic cell, thus the winding number of these helicies on the torus T^3 is unity. Each has a unique (unshared) helical axis and there are six of both the uniaxial positive and negative helicoidal disclinations within a cubic unit cell. The biaxial surface is a collection of disjoint helical tubes, one of which surrounds each of the uniaxial negative helical defect lines.

2. O_b^8

Consider next O_b^8. The uniaxial negative disclination is essentially the same as in the O_a^8 structure, with its end points (P_1,P_2) on DE' and $B'C''$. The additional uniaxi-

al positive one, however, is quite different. We see, in Fig. 12(b), that it has four segments within the asymmetric unit and, like the uniaxial negative defect line, intersects the twofold axes DE' and $B'C''$ (at P_3 and P_4). All four segments are "connected" when the symmetry operations of the space group are applied; thus they must have the same defect structure. It is in this sense that we consider them as a single disclination—this does not imply that these segments are connected in the standard cubic cell. Both disclinations (the uniaxial positive and negative helicies) are of the $+\pi$ type and the resulting eigenvector orientation on the symmetry axes is shown in Fig. 13(b). The group of the uniaxial negative helix is again $P4_3(22)$ and its axis is the screw axis of the O^8 space group. Its winding number is unity and there are six such defect lines in the cubic unit cell. The biaxial surface is the same as for O_a^8; i.e., a set of disjoint helical tubes, one surrounding each of the uniaxial negative disclinations.

The uniaxial positive helical disclination is more interesting. Its structure is characterized by the line group $P4_1(22)$. However, the axis of the helix is not the 4_1 screw axis of the O^8 space group but, rather, the structure's 4_3 axis! This is connected with the fact that

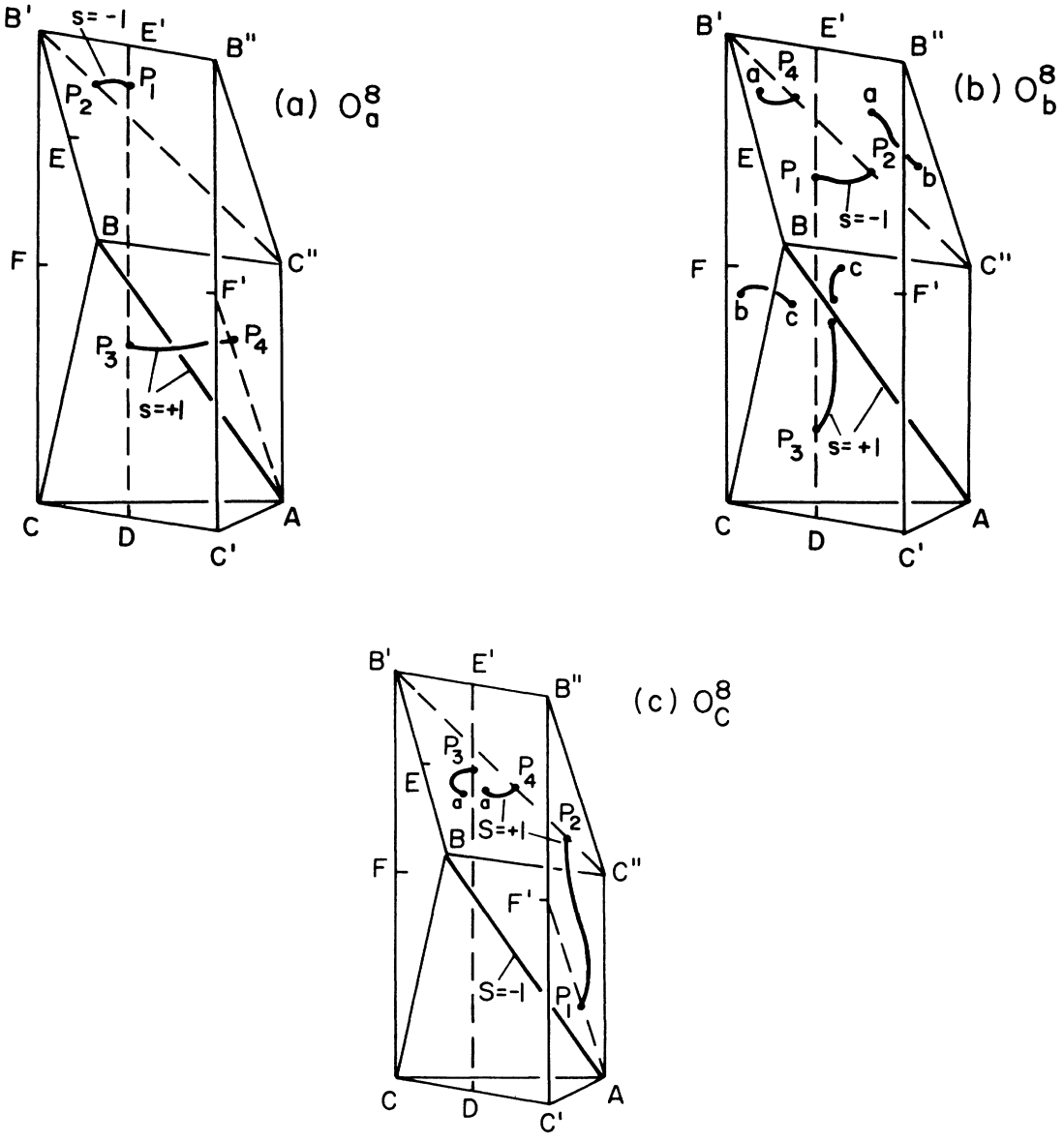

FIG. 12. Disclinations in the O^8 structure for the three local minimum free-energy distributions of the biaxial order parameter found in Ref. 8 and summarized in the Appendix. Shown are the type ($s=+1$: uniaxial positive, $s=-1$: uniaxial negative) and location of the disclinations for (a) O_a^8, (b) O_b^8, and (c) O_c^8. The letters a,b,c denote points at which disclinations "leave" and "reenter" the asymmetric unit.

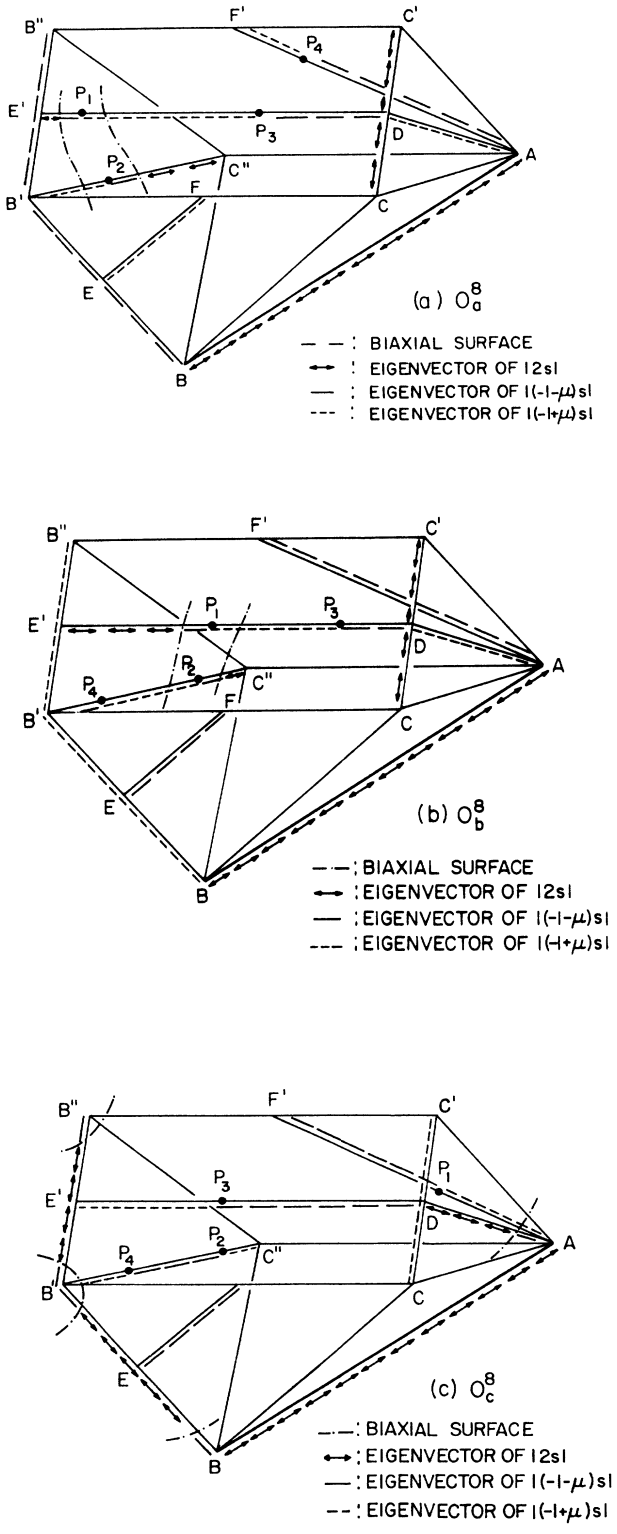

FIG. 13. Principal axes of the order parameter parallel to the threefold and twofold symmetry axes in the asymmetric unit for (a) O_a^8, (b) O_b^8, and (c) O_c^8.

the winding number of this defect line in the space T^3 is three. That is, the primitive translation of the line group is thrice that of the cubic cell, or, in other words, there are three such defect lines (a "triple helix") associated with each of the 4_3 axes in the cubic unit cell. The 4_3 operation of the space group takes us sequentially from one of these three lines to the other, so that this symmetry operation must be invoked three times in order to return to the original disclination. These three 4_3 operations are equivalent to a single 4_1 screw operation in the group of the line. In a cubic unit cell, there are 18 uniaxial positive helicoidal defect lines. This number is not a factor of 48, the number of equivalent points in the unit cell, reflecting the fact that some of the rotation operations take a point on one of the disclinations to an equivalent point lying on the same disclination. It is, of course, a factor of $144=3\times48$, the addition factor of three taking into account the enlarged unit cell of the line group. Finally, as in the case of O_a^8, both the helical disclinations (positive and negative) are of the $-\pi$ type and their senses of rotation are opposite.

3. O_c^8

Finally, consider O_c^8, the third structure with this space group which is also a local minimum of the Landau free-energy functional [see Fig. 12(c)]. It differs from the two discussed previously in that its threefold axis has a uniaxial negative rather than positive character. This is the only such defect in the structure; there are no uniaxial negative helicoidal disclinations. There are, however, two uniaxial positive ones. The first is represented by a single segment in the asymmetric unit and has its end points P_1, P_2 on the twofold axes AF' and $B'C''$. The other has two segments in the asymmetric unit, connected by a twofold rotation about DE'. It intersects the twofold axes DE' and $B'C''$, at the points P_3 and P_4. Both these disclinations are of the $-\pi$ type. The eigenvector configuration on the symmetry axes of the O_c^8 structure is shown in Fig. 13(c). Here again the biaxial surface is a collection of disjoint tubes, one of which surrounds each of the threefold (uniaxial negative) axes.

The line group of the defect going through the points P_1, P_2 is[22] $P3_2(21)$. Thus this helical disclination, unlike all those (both positive and negative) discussed previously, does *not* have as its axis one of the fourfold screw axes of the O^8 space group. Its primitive translation is $\sqrt{3}/2$ that of the cubic cell, i.e., the distance between the bcc lattice points at a vertex and the body center of a cell, and the winding number in the space T^3 is unity. This is a $+\pi$ disclination and there are three equivalent defect lines of this type in the cubic cell.

The other two uniaxial positive segments in Fig. 12(c) belong to the same helical disclination in the cubic cell. It is of the $+\pi$ type and its line group is $P4_3(22)$. The helical axis is the 4_3 axis of the space group. The primitive translation is equal to that of the cubic cell (winding number of unity in T^3) and there are six equivalent disclinations in the cell.

Finally, we consider the characterization of an O^8 structure by a uniaxial order parameter. Unlike the two

previous cases (O^5 and O^2), it is, in principle, possible here to define a direction field which is both invariant under the O^8 space group and also defect-free. This can be done, for example, by beginning with a biaxial tensor field consistent with the configuration of the principal axes shown in Fig. 11 and then taking $\hat{n}(\mathbf{x})$ to be parallel to the eigenvector of the $+2$ eigenvalue at every point in the asymmetric unit. Of course, there is no reason to expect that the resulting director configuration will be attractive energetically.

In fact, both of the director distributions with O^8 symmetry which have been suggested as structures for the cholesteric BP (Ref. 19) have disclinations. One of these was obtained by beginning with O_c^8 and introducing the director field in the same manner discussed earlier for the cases of O^5 and O^2. The resulting structure than has disclinations on its threefold axes. In the second O^8 uniaxial structure, the disclination was placed on the 4_3 axis of the space group. This is not the position of the uniaxial negative defect line in either O_a^8 or O_b^8, but is rather their (common) axis. Here, unlike the other uniaxial structures considered as models for the cubic BP, the position of the disclination is not dictated by symmetry and should therefore be determined by minimizing the free energy. This was not done in the approximation used by Meiboom *et al.*[19] Also there is no distinction between the O_a^8 and the O_b^8 structures when the order parameter is constrained to be uniaxial.

IV. DISCUSSION

In this paper we first considered the possible order-parameter spaces which can be used to describe the cholesteric BP. When this space is restricted to that commonly used for biaxial nematics [$SO(3)/D_2$], there are topological consequences. Then, as a consequence of the cubic symmetry, *there must be disclinations in these structures.* This is not the case, of course, for the nematic and usual helicoidal cholesteric phases. The classification scheme used for the defect lines was the standard one for biaxial nematics, wherein disclinations are identified with the conjugacy classes of the fundamental group of the system (i.e., the eight element quaternion group). In addition, however, we pointed out that, in certain cases, where the disclination is a threefold rotation axis of the space group, one can identify it with a element of the fundamental group rather than a conjugacy class only.

We considered in detail three cubic space groups which have been suggested as possible structures for cholesteric BP. For two of these, bcc O^5 and sc O^2, there are two nonequivalent symmetry axes upon which there must be disclinations. Assuming that these defects are characterized by a uniaxial (rather than vanishing) order parameter, we showed that, in both structures, one of the disclinations must be uniaxial positive and the second uniaxial negative in order for the topology to be consistent with the space group symmetries. Thus any model for a cubic BP based upon a unit director field with the symmetry of either one of these two space groups *must necessarily have disclinations.* This was not the case, however, for the third space group we considered, bcc O^8. Here we found that uniaxial order parameter distributions (i.e., director fields) consistent with the absence of defects *are* topologically possible. They do not, however, occur in any of the configurations found by minimizing the free energy.

In addition, we considered the topological properties of order-parameter configurations obtained[5,7,8] by minimizing the Landau free-energy functional. For O^5, we found that the defect structure of the minimum energy configuration had the minimal number of disclinations and isotropic points required by the space-group symmetry. This was not the case, however, for the nonsymmorphic groups O^2 and O^8. The structures with these group symmetries contained additional uniaxial disclinations having a helical character. That is, they formed helicies about a screw axis of the space group. For these, we specified the group of the line, i.e., the group which leaves the defect line invariant, and also their winding number. In some cases, the axis of a helical disclination was shared by two or three defects, giving a double or triple helix structure.

We also considered the limit wherein the order parameter is constrained to be uniaxial everywhere except on defects lines. Except for the case of the bcc structures O_a^8 and O_b^8, the director configurations used in the literature[19] had defect lines in the same symmetry-prescribed locations obtained from Landau free energy minimization. For these two structures, however, the disclination was taken to be a straight line, contiguous with the axis of the line group, rather than a helical structure.

The results obtained for O^8, where three different structures corresponding to local minima in the free energy was examined, were particularly interesting. While invariant under the same space group, these three order-parameter configurations differ significantly when considered as nets of disclination lines. They have in common, however, a single (within the asymmetric unit) uniaxial negative disclination, even though this is not topologically required and, considered in isolation, raises the free energy. In two of the structures (O_a^8 and O_b^8), these defects are helical and thus have the same line group and helical axis. The helical uniaxial positive defect lines in these structures do, however, differ considerably. In the third structure (O_c^8), the uniaxial defect is on the threefold axis and, of course, is nonhelicoidal. As in the other two O^8 structures, there are two uniaxial positive disclinations, here both are helicoidal.

For all the structures obtained from Landau–free-energy minimization, the biaxial surfaces are essentially narrow tubes, one surrounding each of the uniaxial negative defect lines. This is *not* a topological requirement but rather, as expected, the result of taking order-parameter configurations corresponding to free-energy minima. Other order-parameter configurations exhibit different biaxial surfaces; for example, structures having the same uniaxial negative disclination networks as O_a^8 and O_b^8 can have a single, multiply connected biaxial surface, one with the topology of a Schwarz surface.[23]

We again stress that all our results are based upon an order parameter restricted to the space $SO(3)/D_2$. When "escape" to a large space is permitted, many or all of the

topological defects disappear. This is well known, for example, for the case of uniaxial nematics, when an escape to a biaxial parameter space [i.e., from P_2 to $SO(3)/D_2$] is allowed.[19,24,25]

The analysis presented here was restricted to the three cubic space groups which have been introduced in theoretical studies[5] of the BP structures which appear in the absence of an external field. We remark in passing that similar disclinations lines (both uniaxial positive and negative) appear also in icosahedral models[26] considered in connection with BP III. When a field is present, other structures become thermodynamically stable, including two different hexagonal phases and a tetragonal one.[4,27] A study of their topological properties, similar to that reported here, would also be of interest. However, only partial Landau–free-energy calculations for these structures are presently available.[28]

We again note that this study was concerned with the topological properties of "perfect" BP structures; in other words, ground-state disclination networks compatible with a given space-group symmetry. The more general problem of the classification of defects in nonideal structures, e.g., those with edge or screw dislocations, should also be considered. It is particularly relevant as such dislocations have been observed in cholesteric BP.[29]

Finally, there is the question of direct experimental observation of defects in the BP. Uniaxial negative disclinations, in particular, are analogous to those usually seen[6] in nematic and cholesteric phases and should, under appropriate conditions, be observable. Note, in this connection, that while dislocations have not yet been observed, isolated screw dislocations have been seen in the hexagonal BP which exists in an external field.[29] Direct confirmation that the uniaxial negative disclinations in BP I are contiguous with the threefold symmetry axes would support the Landau-theory prediction that the structure of this phase is O_c^8 rather than O_a^8 or O_b^8. More generally, studies of defect structures in the BP could help to resolve unanswered questions[1] on the application of homotopy theory to systems which are not translationally invariant.

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APPENDIX

The states with minimum free energy for the three cubic space groups were obtained by using an order parameter of the form[5,7,8]

$$\epsilon_{ij}(\mathbf{x})=\sum_{h,k,l} N^{-1/2}\epsilon_2(\sigma)[M_2(h,k,l)]e^{i\psi_2(h,k,l)} \times\exp[i\kappa(h\xi+k\eta+l\zeta)r/\sqrt{2}] . \quad \text{(A1)}$$

Here (ξ,η,ζ) are the components (in appropriate units) of $\mathbf{x}$ (h,k,l) are Miller indices, $\sigma=h^2+k^2+l^2$, the multiplicity $N=(3!)2^{3-n_0}/(n_1!)$, where $n_0(n_1)$ is the number of vanishing (equal) $|h|, |k|, |l|$, κ is the chirality, the amplitude $\epsilon_2(\sigma)\geq 0$, and the phases satisfy $\psi_2(h,k,l)=-\psi_2(-h,-k,-l)$. The basis matrix $[M_2(h,k,l)]$ is defined such that $[h,k,l]$ is along the polar axis of a local coordinate system (defined separately for each value of $[h,k,l]$ in which it has the form

$$[M_2]=\frac{1}{2}\begin{bmatrix}1 & i & 0\\ i & -1 & 0\\ 0 & 0 & 0\end{bmatrix} . \quad \text{(A2)}$$

The parameter r (which determines the unit-cell dimension) is fixed by minimizing the free energy.

(1) O^5: For all bcc groups, the four lowest-lying states are those with $\sigma=2$, 4, 6, and 8. For O^5, the $\sigma=4$ state is forbidden,[7,8,18] thus $\epsilon_2(4)=0$. With the coordinate system used in Table I, the phases $\psi_2(h,k,l)=\psi_2(\sigma)$ and the independent phases $\psi_2(110)$, $\psi_2(112)$, and $\psi_2(220)$ must be equal to either 0 or π; we set them at 0. From the free-energy minimum, we obtain[8] at a typical point (chirality $\kappa=1.5$, temperature $t=2.9$) in the phase diagram,

$$\epsilon_2(2)=0.48;\ \epsilon_2(6)=0.06 ;\quad \epsilon_2(8)=0.01;\ r=0.98 . \quad \text{(A3)}$$

(2) O^2: For sc groups, the four lowest-lying states are those with $\sigma=1$, 2, 3, and 4. For O^2, the latter two values are symmetry forbidden[7,8,18] and $\epsilon_2(3)=\epsilon_2(4)=0$. For the O^2 coordinate system in Table I, we again have $\psi_2(h,k,l)=\psi_2(\sigma)$ and the independent phases $\psi_2(100)$, $\psi_2(110)$ are again equal to either 0 or π. Setting them equal to π, we obtain[8] at the free-energy minimum for $(\kappa=1.3, t=2.5)$

$$\epsilon_2(1)=0.41;\ \epsilon_2(2)=0.23;\ r/\sqrt{2}=0.89 . \quad \text{(A4)}$$

(3) O^8: For this bcc structure, the values $\sigma=2$, 4, 6, and 8 are all allowed.[7,8,18] Using the coordinate to system given in Table I, the phases are[8]

$$\begin{aligned}&\psi_2(110)=-\psi_2(\bar{1}\,1\,0)-\pi/2=0 \text{ or } \pi ,\\ &\psi_2(200)=-\pi/2 \text{ or } +\pi/2 ,\\ &\psi_2(112)=\psi_2(\bar{1}\,\bar{1}\,2)=-\psi_2(1\,1\,2)-\pi/2\\ &\qquad=-\psi_2(\bar{1}\,1\,2)-\pi/2=0 \text{ or } \pi ,\\ &\psi_2(220)=\psi_2(\bar{2}\,2\,0)+\pi=0 \text{ or } \pi .\end{aligned} \quad \text{(A5)}$$

All other phases can be obtained from the above by cyclic permutation of the (h,k,l) indices. Taking the first-mentioned value for each phase [except $\psi_2(110)=\pi$ for the case of O_c^8], we obtain[8] the following free-energy minima at $\kappa=0.9$, $t=1.6$: for O_a^8,

$$\epsilon_2(2)=0.33;\ \epsilon_2(4)=0.16;\ \epsilon_2(6)=0.01 ;\quad \epsilon_2(8)=0.02;\ r=0.90 , \quad \text{(A6)}$$

for O_b^8,

$$\epsilon_2(2)=0.43;\quad \epsilon_2(4)=0.03;\quad \epsilon_2(6)=0.18\ ;$$
$$\epsilon_2(8)=0.08;\quad r=0.82\ , \tag{A7}$$

for O_c^8,

$$\epsilon_2(2)=0.36;\quad \epsilon_2(4)=0.28;\quad \epsilon_2(6)=0.18\ ;$$
$$\epsilon_2(8)=0.01;\quad r=0.77\ . \tag{A8}$$

The values given here for $\epsilon_2(\sigma)$ are those used to obtain the BP topologies given in Sec. III. We stress, however, that the topological properties of the three cubic BP are *independent* of the particular point in the (κ,t) plane at which the local minimum of the Landau free energy is calculated.

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