Novel Defect Structures in a Strongly Confined Liquid-Crystalline Blue Phase

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(Received 10 July 2009; revised manuscript received 23 October 2009; published 4 January 2010)

In our numerical study based on a phenomenological description of strongly confined liquid crystalline blue phase I (BP I), we find several novel structures characterized by specific configurations of topological disclination lines. The thickness of the system is of the order of the dimension of the unit cell of the bulk BP I, and the confining surfaces adopts homeotropic anchoring. The structures include an array of double-helix disclination lines accompanied by an orthorhombic lattice of double-twist cylinders, and two parallel arrays of winding disclination lines almost perpendicular to each other.

DOI: 10.1103/PhysRevLett.104.017801 PACS numbers: 61.30.Dk, 61.30.Hn, 61.30.Mp

Topological defects [1,2], associated with broken continuous symmetry, have long been an important subject of physics, not only in different areas of condensed matter [3], but also in cosmology [4]. Topological defects are universal in the sense that their properties are determined solely by the symmetry of the order parameter space and dimensionality of the system; they do not depend on atomistic details. Liquid crystals have thus served as an ideal model system exhibiting wide variety of topological defects, and allowing direct optical observations of those defects [5]. One intriguing example can be found in cubic blue phases [6] of a nematic liquid crystal (NLC) with strong chirality, in which disclination lines of strength $-1/2$ embedded in between so-called double-twist cylinders [6] form a regular network with cubic symmetry. Blue phases have been regaining greater attention because materials with extended stability range have been discovered [7,8] and, in particular, they have been shown to be applicable to a display with a very fast response [9]. Blue phases have been attracting broader interest also because double-twist cylinders are a typical example of topological excitations called skyrmions. Skyrmions have been known in the context of nuclear physics [10], and exist in a wide variety of physical systems, such as spinor Bose-Einstein condensates [11] and two-dimensional electron systems [12]. Similarities between those systems and blue phases can thus be naturally expected. Indeed, a possibility of structures analogous to blue phases in chiral ferromagnets such as MnSi has been theoretically argued [13–15].

The effect of confining surfaces on the stability of defects is crucial for structures in actual liquid-crystalline systems, which are in some sense confined in most cases. In the case of an achiral NLC, well-known examples include the stability of point defects at the liquid-crystal–air interface [16], and various defect structures, for instance, boojums, hedgehogs, and line disclinations, found in NLC droplets [17]. However, in the case of an NLC with chirality, main attention has been paid to the textures of a cholesteric phase (helical alignment with no disclinations) in droplets [18,19], or in contact with confining glass plates, say, focal conics, Grandjean textures, and fingerprint textures [5]. The interplay between confinement and disclinations associated with strong chirality has never been studied. In this Letter we carry out a numerical study to investigate the effect of strong confinement on the structure of a blue phase and report a discovery of several stable defect structures which, to our knowledge, have never been observed in experiments, nor discussed theoretically.

The numerical procedures to obtain stable (in some cases metastable) structures of a highly chiral NLC is almost the same as those employed in our previous study [20]. Here we present the essential part needed for the present calculation and the difference from our previous study. We employ the rescaling of the order parameter of a second-rank tensor $\chi_{\alpha\beta}$, length, and the material parameters described in Ref. [6]. The rescaled pitch of a uniaxial cholesteric helix becomes 4π. The bulk free energy density is composed of two parts; one is the local part $\varphi_{\mathrm{local}}\{\chi\} = \tau \mathrm{Tr}\chi^2 - \sqrt{6}\mathrm{Tr}\chi^3 + (\mathrm{Tr}\chi^2)^2$, with $\mathrm{Tr}\chi^2$ denoting the trace of a tensor χ^2, and the other takes care of the spatial variation of $\chi_{\alpha\beta}$: $\varphi_{\mathrm{grad}}\{\chi, \nabla\} = \kappa^2\{[(\nabla \times \chi)_{\alpha\beta} + \chi_{\alpha\beta}]^2 + \eta[(\nabla \cdot \chi)_\alpha]^2\}$. The relevant rescaled parameters are the temperature τ, the chirality κ and η that characterizes the anisotropy of liquid-crystal elasticity. Throughout this study, we set $\tau = -1$, $\kappa = 0.7$, and $\eta = 1$ (so-called one-constant approximation). We have checked [20] that, with these parameters, a cubic structure with O_8^- symmetry referred to as blue phase I (BP I) becomes the most stable state.

We assume homeotropic anchoring at the confining surfaces. The surfaces whose normal is along the z direction are located at $z = 0$ and $z = d$, and the surface free energies per unit area are denoted by φ_{s0} and φ_{sd}, respec-

tively. We also assume that the anchoring strengths of two surfaces are equal, and adopt the form [21] $\varphi_{s0}\{\chi\} = \varphi_{sd}\{\chi\} = \frac{1}{2}w\mathrm{Tr}(\chi - \chi_s)^2$, with $\chi_{s\alpha\beta} = S_0(\nu_\alpha\nu_\beta - (1/3)\delta_{\alpha\beta})$, where $\boldsymbol{\nu}$ is the unit vector along the surface normal (or the z direction). We choose $S_0 = 1.44$ so that $\chi_{s\alpha\beta}$ minimizes $\varphi_{\mathrm{local}}\{\chi\}$. We notice that the parameter w characterizes the anchoring strength, and the extrapolation length ξ for $\kappa = 0.7$ is approximately given by $\xi \simeq 1/w$. In our calculations, we choose $w = 0.1$ ($\xi \simeq 10$), 0.5 ($\xi \simeq 2$), and 2.5 ($\xi \simeq 0.4$). Note that as mentioned below, we will consider the cases with system thickness $9 \leq d \leq 18$. Therefore the choices of $w = 0.1$, 0.5, and 2.5 can be classified as weak, intermediate, and strong anchoring, respectively.

The total Landau–de Gennes type free energy of the system F per unit area of the confining surfaces is thus $F = (1/A)\int dxdy[\int_0^d dz(\varphi_{\mathrm{local}}\{\chi\} + \varphi_{\mathrm{grad}}\{\chi, \nabla\}) + \varphi_{s0}\{\chi(z = 0)\} + \varphi_{sd}\{\chi(z = d)\}]$. Here A is the area of the confining surfaces, and the system thickness (distance between confining surfaces) is denoted by d.

We carry out our calculation using a $32 \times 32 \times 33$ parallelepiped lattice in which the unit structure is accommodated. Periodic boundary conditions are imposed along the confining surfaces (or perpendicular to the z direction). We let the shape and size of the system along the confining surfaces vary according to the procedures presented in Ref. [20], while the system thickness d along the z direction is fixed. As the initial condition, we employ the bulk stable structure of BP I for $\tau = -1$, $\kappa = 0.7$, and $\eta = 1$ obtained in Ref. [20], which is dilated or compressed along the z direction to conform to the system thickness d of our numerical system. Depending on w and d, we can obtain various stable (or metastable) structures as shown below. To see if those structures can be (meta)stable for different w and d, we also carry out different calculations employing those structures as initial conditions.

In Fig. 1, we show several (meta)stable structures of disclination lines obtained by our calculations. In addition to those structures similar to the original BP I structure (a and b), we also obtain different profiles, including an array of double-helix disclination lines (c), two parallel arrays of winding disclination lines almost perpendicular to each other (d), and a staggered structure of disclinations attached to the confining surfaces (e). The difference between Figs. 1(a) and 1(b) lies in the distribution of disclination lines. To our knowledge, the latter three structures have never been observed nor discussed in the field of liquid crystals [22]. It may be worthwhile to notice that, in all the structures in Fig. 1, the unit structures projected onto the confining surfaces (the right column) are expanded from that of the bulk BP I (f) (the exception is the structure (a); it is expanded in one direction and shrunk in the other), and are no longer a square in contrast to bulk cubic blue phases [though Figs. 1(b) and 1(d) may look like a square, they are not]; fourfold symmetry about an axis along the z direction is obviously absent. The fourfold symmetry axis

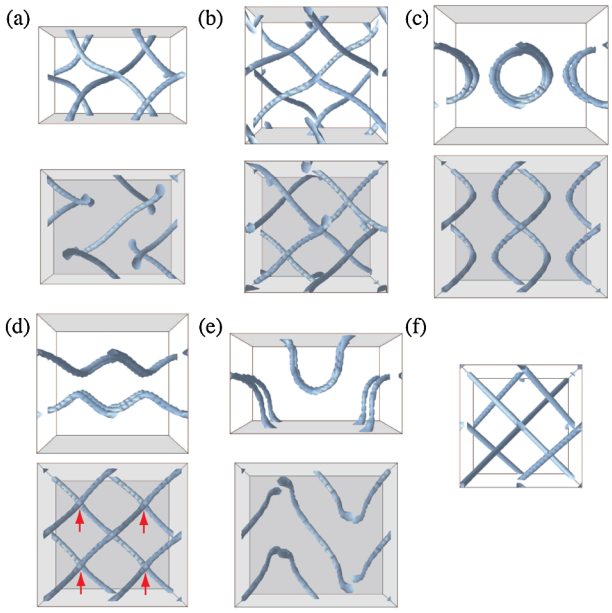

FIG. 1 (color online). Various (meta)stable structures of disclination lines. Shaded planes represent confining surfaces. The view directions are along (top) and perpendicular to (bottom) the confining surfaces. The parameters used are $w = 0.5$ (for all the figures), $d = 10$ (a and e), and $d = 14$ (b, c, and d). Here we show a "unit structure", in which four faces other than the confining surfaces are periodic boundaries. For reference, we also present the structure of the bulk BP I in (f). Note that the distance of the viewpoint from the center of those structures are the same for all the figures, and therefore the dimensions of the figures reflect the actual size of the unit structures.

in bulk cubic blue phases is in fact a screw axis, which implies that fourfold symmetry is associated with translational symmetry along the axis. The absence of translational symmetry due to confinement thus results in the absence of a fourfold symmetry axis in a confined system.

To investigate the energetic stability of those defect structures, we plot in Fig. 2 the free energy per unit surface area $\mathcal{F} = F - f_0 d$ as a function of the system thickness d for $9 \leq d \leq 18$, with f_0 being the free energy density of cubic blue phase I in the bulk. In Fig. 2, we also give the free energy of a cholesteric phase for comparison [23]. Note that we are dealing with the cases where d is of the order of the dimension of the unit cell of BP I structure (12.60 for the parameters used here). In the case of weak anchoring [$w = 0.1$, Fig. 2(a)], energetically stable structures with the variation of d are a staggered structure [Fig. 1(e)] at $d \simeq 9$, one similar to that of the original BP I [Figs. 1(a)] at $9 \lesssim d \lesssim 12$, an array of double-helix disclination lines [Fig. 1(c)] in a very narrow region around $d = 12$, orthogonal sets of winding disclinations [1(d)] at $12 \lesssim d \lesssim 14$, and another structure similar to that of the original BP I [Figs. 1(b)] at $d \gtrsim 14$. The stability of BP I–like structures in a wide range of d is a reasonable result because surfaces with weak anchoring do not disturb so much the stable BP I structure that is stable in the bulk.

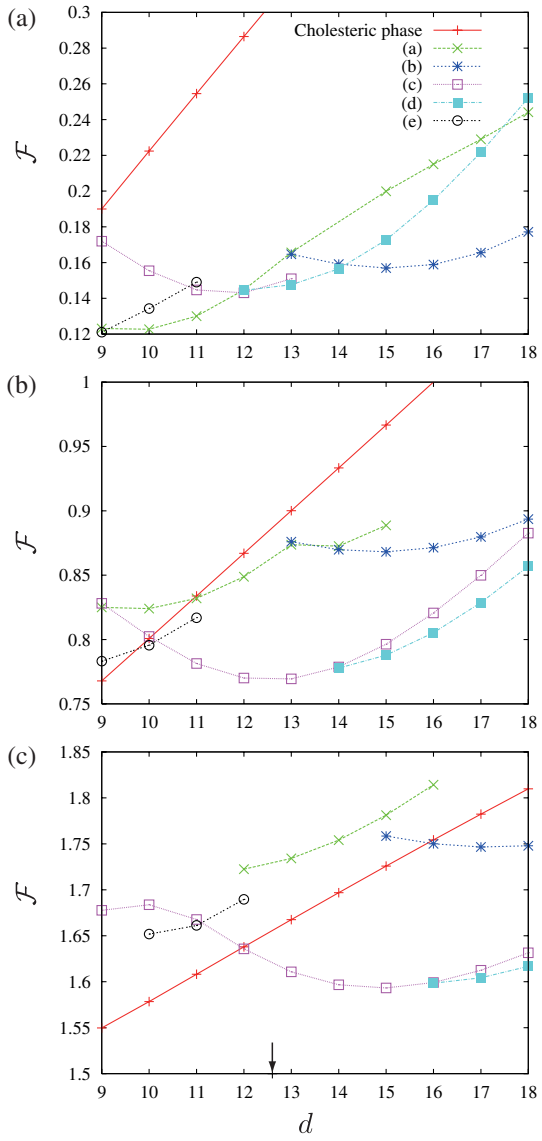

FIG. 2 (color online). Plots of the free energy $\mathcal{F}$ as a function of the system thickness d for $w =$ (a)0.1, (b) 0.5, and (c) 2.5. The legends in (a) are common for all graphs, and the labels (a)–(e) in the legends correspond to those in Fig. 1. In (c), we also indicate by an arrow the dimension of the unit structure of a bulk BP I (12.60).

The stability of those structures in Fig. 1 is significantly altered when the anchoring strength w is increased. For $w = 0.5$, the range of stable double-helix disclinations [Fig. 1(c)] becomes larger to $10 \lesssim d \lesssim 14$ and for $d \gtrsim 14$, orthogonal sets of disclinations [Fig. 1(d)] are stable. In the range of d we study, BP I–like structures no longer give the smallest free energy. Notice also that in a very narrow region around $d \simeq 10$, the most stable structure is a staggered one [Fig. 1(e)]. In the case of strong anchoring, $w = 2.5$, we find that for $12 \lesssim d \lesssim 16$, double-helix disclinations [Fig. 1(c)] is energetically the most favorable, while for smaller d, a cholesteric phase is the most stable. At $d \gtrsim 16$, orthogonal sets of winding disclinations [Fig. 1(d)] is the most stable. These results clearly indicate that confinement and surface anchoring significantly influences the stability of disclination structures in confined blue phases.

That the BP I–like structures lose their stability for larger w can be attributed to the energy loss of disclination lines in contact with confining surfaces; disclination lines in Figs. 1(c) and 1(d) do not touch the surfaces. The stability of double-helix disclinations [Fig. 1(c)] over orthogonal ones [Fig. 1(d)] for relatively small d can again be understood in an intuitive manner. When the system is compressed to smaller d, orthogonal disclinations becomes closer to each other, and feel repulsion. Eventually, it is more energetically favorable if the reconnection of disclination lines occurs at the points indicated by arrows in Fig. 1(d) and the disclination lines transform to double helix, Fig. 1(c). It can be also seen that double-helix disclinations do not suffer from repulsion between disclination even in the case of small d (of course, for small d, interaction between disclinations and confining surfaces becomes important. However, such interaction plays a significant role in the orthogonal-disclination configuration as well).

It is instructive to illustrate how liquid crystals are aligned in the presence of those disclinations with nontrivial geometry. Because of space limitations, we give a detailed presentation only for the case of double-helix disclinations in Fig. 1(c). The orientation profiles at three cross sections are presented in Fig. 3(a). We find local double-twist orientation profiles [5,6], which are indicated by circles (○). As in cubic blue phases in the bulk, disclination lines run in between those double-twist cylinders. Schematic illustration of the arrangement of double-twist cylinders is given in Fig. 3(b). Double-twist cylinders in this configuration constitute a simple orthorhombic lattice, in contrast to a body-centered-cubic lattice in BP I. We note that the structure with orthogonal sets of winding disclinations, Fig. 1(d), has almost the same arrangement of double-twist cylinders, which demonstrates in a different manner the similarity between the structures in Figs. 1(c) and 1(d) mentioned above.

Here we comment on the possibility of experimental observations of those disclination structures. Cano-wedge geometry might be useful in the investigation of the effect of sample thickness variations [24]. Lack of a fourfold symmetry axis normal to the confining surfaces as mentioned above may be detected in a careful scattering experiment. Notice also that three-dimensional lasing of blue phases [25] might be affected by strong confinement. We also point out the possibility of obtaining direct evidence of the symmetry of the structures by freeze-fracture microscopy [26,27].

In conclusion, by numerical calculations based on a tensor description of orientational order, we have shown that various defect structures that have not been previously discussed are possible in a strongly confined liquid-crystalline blue phase. Those structures include an array of double-helix disclinations, two orthogonal sets of par-

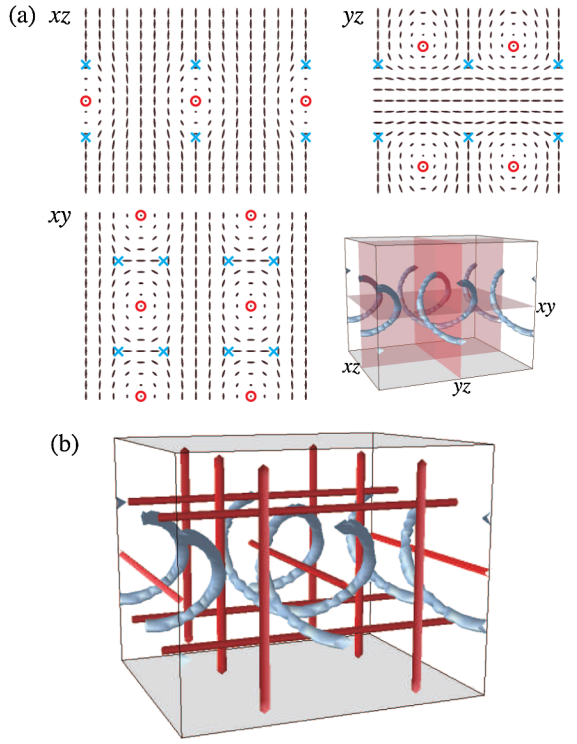

FIG. 3 (color online). (a) Orientation profiles at three given cross sections for the structure in Fig. 1(c). The locations of the three cross sections are also shown. The positions of disclinations and axes of double-twist cylinders are indicated by crosses (×) and open circles (○), respectively. (b) Schematic illustration of the arrangement of double-twist cylinders with respect to the disclination lines.

allel winding disclinations, and a staggered structure of disclinations contacting the confining surfaces. In the present study, we have focused on the case in which blue phase I is stable in the bulk. The effect of temperature change and the stability of other phases such as blue phase II will be the subject of future studies. Nevertheless, we believe that we have presented a novel aspect of the interplay between topological defects and confinement in a liquid crystal, and that topological defects under an appropriate control can show far richer structures than we have already known. Therefore we hope that our present study will stimulate further theoretical and experimental studies to find novel defect structures and perhaps also their use in electro-optical applications. Furthermore, we expect that our study will stimulate a search of confined structures in chiral magnets.

This work was carried out while J. F. was staying at the Department of Physics, University of Ljubljana. He thanks Slovenian Research Agency (ARRS research program P1-0099 and project J1-2335) for generous financial support for his stay. J. F. is in part supported also by KAKENHI (Grant-in-Aid for Scientific Research) on Priority Area "Soft Matter Physics" from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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[1] N. D. Mermin, Rev. Mod. Phys. **51**, 591 (1979).
[2] H.-R. Trebin, Adv. Phys. **31**, 195 (1982).
[3] P. Chaikin and T. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge, England, 1995).
[4] T. W. B. Kibble, J. Phys. A **9**, 1387 (1976).
[5] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals* (Oxford University Press, Oxford, 1993), 2nd ed.
[6] D. C. Wright and N. D. Mermin, Rev. Mod. Phys. **61**, 385 (1989).
[7] H. Kikuchi *et al.*, Nature Mater. **1**, 64 (2002).
[8] H. J. Coles and M. N. Pivnenko, Nature (London) **436**, 997 (2005).
[9] Samsung Electronics Co., Ltd., "15 inch Blue Phase Mode LC Display", presented at SID2008 (Los Angeles, 2008).
[10] G. E. Brown and M. Rho, Phys. Rep. **363**, 85 (2002).
[11] T. L. Ho, Phys. Rev. Lett. **81**, 742 (1998).
[12] S. E. Barrett *et al.*, Phys. Rev. Lett. **74**, 5112 (1995).
[13] B. Binz, A. Vishwanath, and V. Aji, Phys. Rev. Lett. **96**, 207202 (2006).
[14] U. K. Rößler, A. N. Bogdanov, and C. Pfleiderer, Nature (London) **442**, 797 (2006).
[15] I. Fischer, N. Shah, and A. Rosch, Phys. Rev. B **77**, 024415 (2008).
[16] R. B. Meyer, Mol. Cryst. Liq. Cryst. **16**, 355 (1972).
[17] G. E. Volovik and O. D. Lavrentovich, Zh. Eksp. Teor. Fiz. **85**, 1997 (1983) [Sov. Phys. JETP **58**, 1159 (1983)]; O. D. Lavrentovich, Liq. Cryst. **24**, 117 (1998).
[18] M. V. Kurik and O. D. Lavrentovich, Pis'ma Zh. Eksp. Teor. Fiz. **35**, 362 (1982) [JETP Lett. **35**, 444 (1982)].
[19] Y. Bouligand and F. Livolant, J. Phys. (Paris) **45**, 1899 (1984).
[20] J. Fukuda, M. Yoneya, and H. Yokoyama, Phys. Rev. E **80**, 031706 (2009).
[21] M. Nobili and G. Durand, Phys. Rev. A **46**, R6174 (1992).
[22] Though structures similar to those in Figs. 1(c) and 1(d) have been reported in G. P. Alexander and D. Marenduzzo, Europhys. Lett. **81**, 66 004 (2008), they are transient ones when a strong field is applied to bulk blue phase II.
[23] For the alignment of the cholesteric phase, the uniform lying helix (ULH) configuration (helical axis parallel to the confining surfaces) rather than the Grandjean configuration has been employed. We have checked that the former is energetically more favorable. In the ULH configuration, the director is uniform along the z-direction, except close to the surfaces. The total free energy F thus depends linearly on d as found in Fig. 2.
[24] A. I. Feldman, P. P. Crooker, and L. M. Goh, Phys. Rev. A **35**, 842 (1987).
[25] W. Cao *et al.*, Nature Mater. **1**, 111 (2002).
[26] B. Donnio *et al.*, Liq. Cryst. **23**, 147 (1997).
[27] J. Yamamoto *et al.*, Nature (London) **437**, 525 (2005).