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Continuous transformation of a −1/2 wedge disclination line to a +1/2 one

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It is known that, in the order-parameter space S^2/Z_2 (a typical example being a uniaxial nematic liquid crystal in three dimensions), a −1/2 wedge disclination line and a +1/2 one are topologically equivalent and can thus be transformed continuously into each other. Here we report the realization of this transformation in a simulation of a cholesteric blue phase under an electric field.

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Topological defects, found in systems with broken continuous symmetry, can be classified by homotopy groups [1–3]. In the case of a uniaxial nematic liquid crystal whose director rotation is confined in two dimensions (2Ds), the order-parameter space is S^1/Z_2. Its first homotopy group is $\pi_1(S^1/Z_2)=Z$, and due to the equivalence of the head and the tail of the director (or that of $\boldsymbol{n}$ and $-\boldsymbol{n}$), a topological charge of integer or half integer, $m/2$, can be assigned to each defect. The director $\boldsymbol{n}$ rotates by an angle $(m/2)2\pi$ along a contour encircling the defect. In a three-dimensional (3D) system, a topological defect line perpendicular to the plane confining the rotation of $\boldsymbol{n}$ is referred to as a wedge disclination [3].

On the other hand, when the constraint of 2D is released, the order-parameter space is now S^2/Z_2, and its first homotopy group is $\pi_1(S^2/Z_2)=Z_2\equiv\{0,1\}$. It dictates that there is only one class of topologically stable disclinations in a 3D uniaxial nematic liquid crystal. A wedge disclination line with topological charge −1/2 is in fact equivalent to one with +1/2 charge. As first pointed out in a clear manner in [2], and schematically shown in Fig. 1, the former can be transformed into the latter continuously via a twist disclination [3]. Along the contour encircling a twist disclination, $\boldsymbol{n}$ rotates, by an angle π, out of the plane containing the contour.

In spite of the clarity of the above topological argument, to our knowledge a continuous transformation between −1/2 and +1/2 wedge disclinations has been realized neither in experiments nor in computer simulations. This may be one of the reasons why the topological equivalence of wedge disclinations with positive/negative half-integer charge has not been given much attention. In the present Rapid Communication, we report the observation of this transformation in a simulation of a cholesteric blue phase (BP) under an applied electric field. Cholesteric blue phases [4,5] have been known as an intriguing example of liquid crystalline ordered structures involving topological defects. It is now established that cholesteric blue phases contain a network of disclination lines of topological charge −1/2, with cubic symmetry in BP I and II. Their response to an electric field has also been extensively studied [6], with focus on the changes in the symmetry of the ordered phases and the dimension of the unit cell. Recently several numerical studies [7,8] demonstrated various types of possible structural changes under an electric field. One of the main interests of those numerical studies is the dynamics of disclination lines, which is difficult to access experimentally. We carried out an extensive study to show that the structural change of disclination lines sensitively depends on the direction of the electric field and the sign of dielectric anisotropy (ϵ_a) [8]. Here we focus on the change in the director profile of BP I with negative ϵ_a under an electric field parallel to one body diagonal of the cubic unit cell to see the change in the topology of disclination lines.

The details of the numerical calculation are presented in Ref. [8], and here we repeat only the essential part. The orientational order of a liquid crystal is specified by a second-rank tensor. After an appropriate rescaling [8,4] of the order-parameter $\chi_{\alpha\beta}$, length (rescaled pitch of a uniaxial cholesteric helix is set to 4π), and relevant material parameters, the rescaled free-energy density in terms of $\chi_{\alpha\beta}$ is written as $\varphi=\varphi_{\text{local}}\{\chi_{\alpha\beta}\}+\varphi_{\text{grad}}\{\chi_{\alpha\beta},\tilde{\nabla}\}+\varphi_E\{\chi_{\alpha\beta},\boldsymbol{E}\}$, where $\varphi_{\text{local}}\{\chi_{\alpha\beta}\}=\tau\,\text{Tr}\,\chi^2-\sqrt{6}\,\text{Tr}\,\chi^3+(\text{Tr}\,\chi^2)^2$ is the local

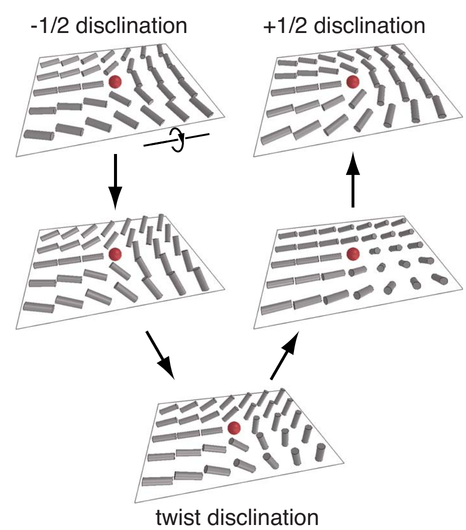

FIG. 1. (Color online) Schematic illustration of the topological equivalence of −1/2 and +1/2 wedge disclinations. Here the director $\boldsymbol{n}$ is indicated by a cylinder and the disclination by a sphere. By a rotation of $\boldsymbol{n}$ about an axis *indicated in the figure*, a −1/2 disclination transforms continuously into a +1/2 disclination via a twist disclination.

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freeenergy in the Landau–de Gennes expansion, and $\varphi_{\rm grad}\{\chi_{\alpha\beta},\tilde{\nabla}\}=\kappa^2\{[(\tilde{\nabla}\times\chi)_{\alpha\beta}+\chi_{\alpha\beta}]^2+\eta[(\tilde{\nabla}\cdot\chi)_\alpha]^2\}$ is the free energy due to the spatial variation of $\chi_{\alpha\beta}$. Here τ and κ are the rescaled temperature and chirality, respectively, and we choose $\tau=-1$ and $\kappa=0.7$. The parameter η characterizes the anisotropy of elasticity, and here we set $\eta=1$ (one-constant approximation). We have checked [8] that with the choice of these parameters BP I is indeed the most stable phase under no electric field. The free energy due to the electric field reads as $\varphi_E\{\chi_{\alpha\beta},\boldsymbol{E}\}=-\tilde{\epsilon}\hat{e}_\alpha\hat{e}_\beta\chi_{\alpha\beta}$, where a unit vector $\hat{\boldsymbol{e}}$ specifies the field direction, the rescaled parameter $\tilde{\epsilon}$ is proportional to the square of the field strength, and its sign is the same as that of $\epsilon_{\rm a}$. In the present study we choose $\hat{\boldsymbol{e}}\parallel[111]$, one body diagonal of the unit cell, and $\tilde{\epsilon}=-1$, corresponding to the field strength $E\sim 20\ \mathrm{V}/\mu\mathrm{m}$ [8,9]. The relaxation of $\chi_{\alpha\beta}$ is governed by a simple relaxation equation via rotational diffusion. We also let the shape and size of the simulation box relax for the system to approach true equilibrium without suffering from the mismatch between the system size and the characteristic size of the equilibrium structure. The details can be found in [8], and we merely notice that the rescaled time t is measured in units of a characteristic time $\tau_\chi\simeq 1\ \mu\mathrm{s}$ proportional to rotational viscosity. Our calculations are carried out on a $32\times32\times32$ parallelepiped lattice with periodic boundary conditions. For clarity, the visualizations in the following are not restricted to the unit cell of our numerical systems. Their inherent periodicity reflects the periodic boundaries of our system.

In Figs. 2–4, we show the time evolution of the director profile under an electric field $\boldsymbol{E}$. We show the director profile at a cross section perpendicular to $\boldsymbol{E}$, and the simulation is started from the equilibrium bulk BP I under no field (Fig. 2). Note that the distance of the viewpoint from the cross section is fixed throughout Figs. 2–4. Therefore the change in the distance between disclinations reflects its actual change.

In the equilibrium structure of BP I, all of the disclination lines, which do not intersect each other, are wedge disclinations with topological charge $-1/2$ as shown in Fig. 2. After the application of $\boldsymbol{E}$, the local director profile around disclination lines parallel to $\boldsymbol{E}$ (for example, one at the center of Fig. 2) stays unchanged because the director in the vicinity of such disclinations experiences no torque from $\boldsymbol{E}$. However, a close inspection of the director profile around a disclination line oblique to $\boldsymbol{E}$ in Fig. 3 reveals that the $-1/2$ wedge disclination before the application of $\boldsymbol{E}$ is transformed to a twist disclination (the director rotates by an angle π out of the plane along the contour encircling it) as shown separately in a magnified manner in Fig. 3; the torque exerted by $\boldsymbol{E}$ in this case can rotate the director. After further elapse of time, in Fig. 4, we see a regular parallel array of $-1/2$ and $+1/2$ wedge disclinations (perpendicular to the plane of the figure) with a hexagonal order significantly different from the original BP I cubic structure [10]. The sequence of Figs. 2–4 clearly demonstrates that some of the wedge disclination lines of topological charge $-1/2$ in the initial bulk structure of BP I have been transformed into $+1/2$ ones continuously via a twist disclination. To show the continuous nature of the transformation in a different manner, we give in Fig. 5 the director variations along the contours in Figs. 2–4 encircling

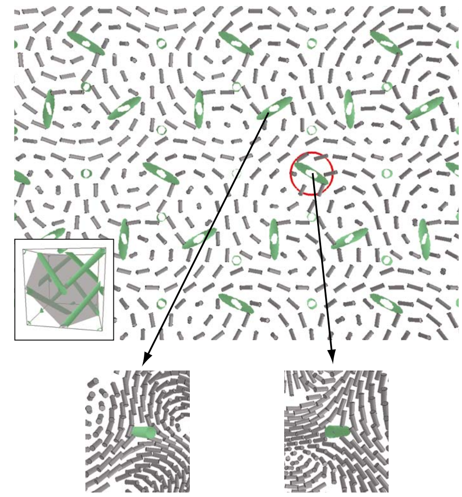

FIG. 2. (Color online) The director profile at a cross section at $t=0$, just after the application of the electric field $\boldsymbol{E}$ perpendicular to the plane of the figure. The director is shown by a cylinder, and the curved surfaces (green) are the isosurfaces with Tr $Q^2=0.7$, indicating the position of disclination lines. The isosurfaces are shown only in a region sandwiched by two planes whose distance from the cross section is $\sqrt{3}/6$. The location of the cross section with respect to the unit cell of BP I is shown by a gray plane in the inset. To clarify that all the disclination lines are of topological charge $-1/2$, we also show the director profiles around two disclination lines at a different cross section perpendicular to the disclination line. The circle (red) indicates the contour along which the director variation is shown in Fig. 5.

the identical disclination. The director variations are presented as a contour on a unit sphere representing the order-parameter space of the director. The time evolution of the contours indicates that the transformation is indeed a continuous one. From Fig. 5, one can also see clearly that the final profile (Fig. 4) is that of a $+1/2$ disclination [11].

The inevitability of the change in the charge from $-1/2$ to $+1/2$ can be understood by a simple topological argument.

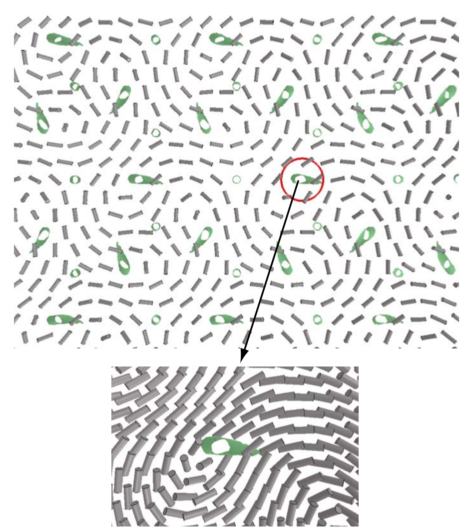

FIG. 3. (Color online) The director profile at $t=18.9$. The local director profile around one disclination line is shown separately to emphasize that it is a twist disclination.

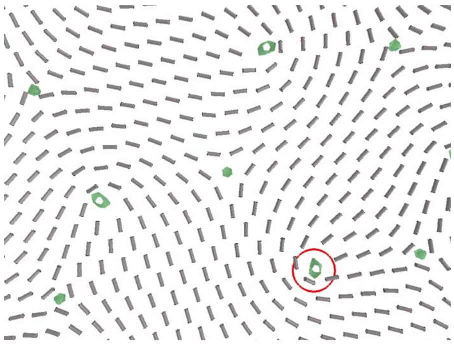

FIG. 4. (Color online) The director profile at $t=38.5$. In this region three disclination lines of charge $+1/2$ and five ones of charge $-1/2$, which are almost perpendicular to the cross section, can be seen. The number of $+1/2$ disclination is the same as that of $-1/2$ disclination in the infinite system not shown here.

Since the dielectric anisotropy ϵ_a is negative and the field is strong, the electric field forces the director $\boldsymbol{n}$ to lie in a 2D plane perpendicular to it. In the 2D plane, as mentioned at the beginning of this Rapid Communication, a topological defect is characterized by its charge of half integer, and defects with different charges cannot be transformed interchangeably by a continuous process. Moreover, the net topological charge must be zero because we deal with an infinite system with periodic boundaries. Therefore, as noted in Fig. 4, if $-1/2$ defects exist in the 2D plane, there must be as many $+1/2$ defects, which is why some of the $-1/2$ defects are forced to transform to $+1/2$ ones. Recall that the above argument does not hold in 3D; the presence of $-1/2$ disclination lines without the compensation by $+1/2$ ones in the initial cholesteric blue phase does not break any topological rules.

Finally we comment that chirality does not play an important role in the dynamical process of the transformation of disclination lines; we have just utilized a blue phase of a chiral liquid crystal as an initial system containing disclination lines. Indeed, chirality is irrelevant to topological arguments so long as cholesteric planes play no role as in the present case. Therefore the transformation shown here can occur in an achiral nematic liquid crystal. Our observation demonstrates that a field oblique to a disclination line can induce the transformation when ϵ_a is negative; that is, the field can exert a torque to the director $\boldsymbol{n}$ and restricts $\boldsymbol{n}$ to a 2D plane perpendicular to it. Therefore this transformation is expected to be observed experimentally in a simple setup of a nematic cell. We believe that we have presented an interesting numerical realization of a transformation of topological defects and thus hope that the present study will promote further experimental or numerical studies concerning the topological nature of liquid crystals in a different way from previous work.

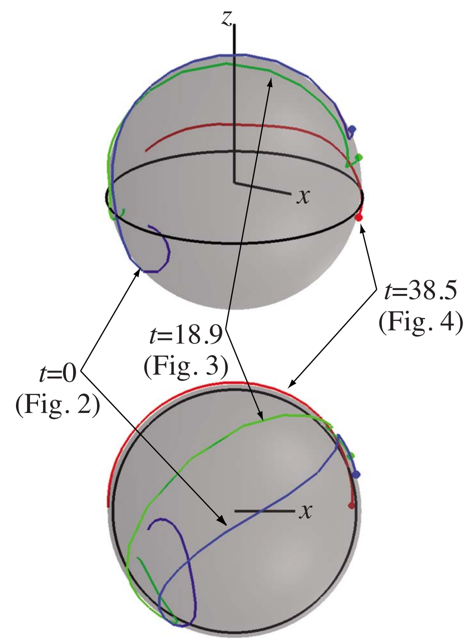

FIG. 5. (Color online) The director variations along the counterclockwise contours in Figs. 2–4, shown as a contour on a unit sphere. Two figures from different viewpoints are presented for clarity. The starting point of the contour of the director is shown by a small sphere. The plane of Figs. 2–4, or the xy plane, is presented by a black circle, and the axis perpendicular to the xy plane, or the z axis, is indicated by a straight line. The direction of the horizontal axis of Figs. 2–4, or the x axis, is shown by a short line. The figure below is drawn from the $+z$ point as in Figs. 2–4, and the z axis cannot be seen. This illustration follows the idea of Fig. 12.15 in [3].

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[9] In Ref. [8], we showed that with other choices of the field direction ([100] and [110]), disclination lines eventually annihilate to result in a helical (cholesteric) state without disclinations. We also note that for positive ϵ_a, the final director profile is a uniform one parallel to $\boldsymbol{E}$ without disclination, irrespective of the field direction. This is the reason why in the present study we concentrate on the case with negative ϵ_a and the field along [111], where annihilation of disclination is not observed (see [10] below).

[10] We should mention that this regular array of $-1/2$ and $+1/2$ disclination lines must be regarded as a transient, not a stable, state. The ground state under $\boldsymbol{E}$ is a helical state with its pitch axis parallel to $\boldsymbol{E}$. In simulations in the present Rapid Communication and [8], we could not observe a helical state as a final structure, possibly due to the perfectness of the prepared initial condition; threefold symmetry of the defect array (Fig. 4) remains unchanged, though a gradual increase of the defect distance is observed. A small perturbation would be necessary for the system to reach a helical state.

[11] It is not clear enough from Fig. 5 that the initial profile (Fig. 2) is that of *a* $-1/2$ disclination. It is because the plane of the contour (the plane of Fig. 2) is not perpendicular to the disclination line.