

Flow-induced disclination lines in nematic liquid crystals

Christian Bahr **Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany*

(Received 3 June 2025; accepted 25 September 2025; published 15 October 2025)

We present a numerical study, based on the lattice Boltzmann method, of nematic liquid crystals flowing in microfluidic channels. We show that disclination lines are generated by the interaction between flow and anchoring conditions of the channel walls. In particular, we observe nucleations of pairs of twist disclinations in those regions of the channel where the elastic aligning forces, resulting from the anchoring conditions, are perpendicular to the local shear plane of the flow. The newly formed disclinations either persist or annihilate, depending on the overall configuration of the director field in the channel. We study the behavior at boundaries between different anchoring conditions and describe the formation of flow-induced disclination arcs. We show that the numerical model correctly reproduces the results of an experimental study [Agha and Bahr, *Soft Matter* **12**, 4266 (2016)], thereby validating our numerical results.

DOI: [10.1103/PhysRevE.112.045408](https://doi.org/10.1103/PhysRevE.112.045408)

I. INTRODUCTION

Nematic liquid crystals (NLCs) are liquid phases in which the constituent rod-shaped molecules establish an orientational order by aligning along a common direction, denoted by a unit vector $\vec{n}$ (director). NLCs exhibit a wealth of topological defects [1] and provide thus well-suited model systems for experimental studies of topological defects in general. For example, results obtained on NLCs may be significant for knot theory [2,3], colloid physics [4,5], or even cosmology [6].

The most common defects in NLCs are line defects called disclinations [7–10]. Along any closed loop around a disclination, the orientation of $\vec{n}$ rotates by an angle Ω :

$$\Omega = 2\pi s, \quad (1)$$

where the strength s of the disclination can take values $s = \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \dots$. Usually, only the case $s = \pm\frac{1}{2}$ is observed experimentally and the remainder of this paper is restricted to that case. Another important parameter is the twist angle β between the tangent $\vec{t}$ of the disclination line and the rotation axis $\vec{\Omega}$ around which $\vec{n}$ rotates when the disclination line is circumnavigated on the closed loop. When $\vec{\Omega}$ is parallel to $\vec{t}$ ($\beta = 0, \pi$) we have the well-known configuration of a $+1/2$ or $-1/2$ wedge disclination; for $\beta = \pi/2$ or $\beta = 3\pi/2$ the line defects are denoted as twist disclinations [10]. Note that if the director field is confined to two spatial dimensions only the two wedge disclinations exist (which are point defects in that case), whereas in three dimensions β can take any value

resulting in an infinite number of configurations, all of which are topologically equivalent [11]. More details on the twist and wedge characteristics of disclinations and a procedure to determine β can be found in Ref. [12].

Disclinations are studied not only under fundamental viewpoints [13,14] but also with regard to applications such as guided self-assembly [15–18] or controlled positioning [19–21] and transport [22] of colloidal objects. Also in active NLCs disclinations are studied [12,23] because of their important role in the dynamics of these materials.

Disclinations form spontaneously when a NLC is quenched from the isotropic to the nematic phase by a sudden temperature decrease. However, the thermally induced disclinations tend to annihilate as the NLC relaxes to its equilibrium structure. A common way to induce and stabilize disclinations is to confine the NLC in a cell with conflicting anchoring conditions on its walls. Anchoring denotes the property of a surface to impose a preferred orientation of $\vec{n}$ of a NLC in contact with the surface. Novel techniques of creating arbitrary anchoring patterns [24–26] have enabled the generation of precisely defined disclination networks [27–31] which may be reconfigured by external stimuli [32–34].

In the present study, we focus on a different approach of generating disclination lines, namely, the induction and stabilization of disclinations by means of the interplay between flow and anchoring in microfluidic channels. The effect of flow on disclination lines has been studied in various systems. Most studies are concerned with the disclination loops (so-called Saturn rings [35]) which form around colloidal particles, drops, or bubbles immersed in NLCs [36–43]; other studies consider the flow of NLCs through microchannels [22,44–47] or porous media [48]. All these studies focus mainly on flow-induced transformations of disclination lines which exist also at zero-flow conditions. Giomi *et al.* have shown that junctions of microfluidic channels may be utilized to generate disclinations of different strengths by hydrodynamic forces [49].

*Contact author: christian.bahr@ds.mpg.de

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Already in the 1980s it was observed that shear flows of sufficient strength may lead in low molar mass [50] and polymeric NLCs [51] to textural changes which are accompanied by the appearance of disclination loops. The behavior of these loops in the presence of shear flow was later analyzed theoretically [52]. However, in the present study we concentrate on a more controlled way of creating disclinations. Using lattice Boltzmann simulations, we show that disclination lines can be generated in microfluidic channels by the interaction between flow and anchoring. A key observation is the flow-induced nucleation of one or several pair(s) of twist disclination lines in those regions of the channel where the elastic forces, resulting from the anchoring conditions on the channel walls, tend to align the local director perpendicular to the local shear plane of the flow. Depending on the overall configuration of the director field in the channel, the newly formed disclinations either persist at higher flow rates or they annihilate with other disclinations (which were already present at zero flow or were also newly formed by the flow). We study also the behavior at boundaries between different anchoring conditions and demonstrate the formation of flow-induced disclination arcs originating from the anchoring boundaries. Finally, in order to validate our numerical simulations, we reproduce the results of an experimental study [45] of disclinations in microfluidic channels, thereby also clarifying details of the director field structures which were observed in that study.

II. THEORY AND METHODS

A. Nematic hydrodynamics

The nematic order can be described by the director $\vec{n}$ and the scalar order parameter q , which is a measure of the mean deviation of the individual long molecular axis from $\vec{n}$:

$$q = \left\langle \frac{1}{2} (3 \cos^2 \theta_i - 1) \right\rangle. \quad (2)$$

Here, θ_i is the angle between $\vec{n}$ and the axis of molecule i .

Because the orientations $\vec{n}$ and $-\vec{n}$ are physically equivalent (absence of polar order), it is convenient to use a tensor order parameter $\mathbf{Q}$,

$$Q_{\alpha\beta} = q \left(n_\alpha n_\beta - \frac{1}{3} \delta_{\alpha\beta} \right), \quad (3)$$

with eigenvalue $\frac{2}{3}q$ and eigenvectors $\vec{n}$ and $-\vec{n}$.

A basic principle of nematic hydrodynamics is the coupling between flow, director orientation, and viscosity. A flow in a NLC can change the orientation of $\vec{n}$. The vast majority of NLC compounds show the flow alignment behavior: in a shear flow $\vec{n}$ aligns within the shear plane and approximately (the deviation is of the order of 10°) along the flow direction. Conversely, a change of the orientation of $\vec{n}$ (e.g., by an external field) can induce a flow in the NLC, the so-called backflow. Also, the effective viscosity of a NLC depends on the orientation of $\vec{n}$ with respect to the flow.

The aligning forces of the flow field often compete with elastic aligning forces resulting, e.g., from anchoring conditions at boundaries. This competition is described by the dimensionless Ericksen number, Er , which specifies the ratio between viscous and elastic forces or torques:

$$Er = \frac{\gamma_1 u L}{K}. \quad (4)$$

Here, γ_1 is a viscosity coefficient for director rotation, u the flow velocity, L a relevant length scale (e.g., width or depth of the channel), and K the mean elastic constant of the NLC.

Several theoretical descriptions of nematic hydrodynamics have been proposed [53–65]. The numerical simulations of the present study are based on the Beris-Edwards theory [61,62] of nematic hydrodynamics. In the Beris-Edwards model, the influence of flow on the nematic order is described by a kind of convection-diffusion equation for the order parameter tensor $\mathbf{Q}$, extended by a coupling term $\mathbf{S}$:

$$(\partial_t + \vec{v} \cdot \nabla) \mathbf{Q} = \Gamma \mathbf{H} + \mathbf{S}. \quad (5)$$

Here, Γ is a diffusion coefficient describing the diffusivity of director reorientation and $\mathbf{H}$ is the molecular field driving the system to the free energy minimum. The coupling tensor $\mathbf{S}$ is a function of $\mathbf{Q}$ and the flow gradient tensor $\mathbf{W}$ and may cause both a rotation and an expansion or compression of the order parameter distribution. $\mathbf{S}$ contains also a parameter which determines whether the NLC shows the usual flow-aligning behavior or the rarely observed nonaligning (tumbling) behavior. Here, we consider solely the flow-aligning case. The reverse coupling, i.e., the influence of the nematic order on the flow velocity field $\vec{u}$, is described in the Beris-Edwards model through a modified stress tensor in the Navier-Stokes equation. Further details including equations for these quantities are given in the papers by Denniston *et al.* [66,67], in which also the lattice Boltzmann method is described which is used to solve these equations.

B. Lattice Boltzmann method

The lattice Boltzmann method (LBM) is a numerical method based on a discretization of the Boltzmann equation of the kinetic theory of fluids [68]. The LBM uses a rectangular lattice (two or three dimensional) and to each lattice node a set of distribution functions f_i is assigned which describes the density of fluid particles traveling with velocity $\vec{c}_i$ within one time step to a neighboring grid node i . Macroscopic quantities such as mass density ρ and momentum density $\rho \vec{u}$ at a given node can be obtained from the sum of the discrete distribution functions at the node: $\rho = \sum f_i$, $\rho \vec{u} = \sum \vec{c}_i f_i$ (the index i is running from zero, corresponding to the node currently considered, to the number of neighboring nodes). Macroscopic fluid mechanics can be derived from the Boltzmann equation via the Chapman-Enskog analysis [69] and it is found that the LBM is well suited to simulate the hydrodynamics of liquids, equivalently to solving the Navier-Stokes equation. Compared to simulations based on direct numerical solving of the Navier-Stokes equation using finite element or finite volume methods, the LBM requires considerably less computational effort. Also, the LBM for simple fluids can be extended to other systems, such as thermal flows or multicomponent flows. A drawback might be that the LBM relies on a uniform Cartesian grid, whereas finite element methods can easily handle unstructured meshes or the adaptive refinement of meshes. The LBM is thus usually restricted to mesoscopic resolution.

Extensions of the LBM for flowing NLCs were proposed by Care *et al.* [70,71] and Denniston *et al.* [66,67], the latter being used in the present study. In order to model the nematic

order by the LBM, a second set of distribution functions, $\mathbf{G}_i$, is introduced from which the order parameter tensor is obtained: $\mathbf{Q} = \sum \mathbf{G}_i$. For each time step, the distribution functions f_i and $\mathbf{G}_i$ at a given node and its neighboring nodes are calculated using the results of the previous time step and certain collision and streaming rules. Compared to the LBM for simple fluids, the calculations are extended by coupling terms describing the mutual coupling between the $\bar{\mathbf{u}}$ and $\mathbf{Q}$ fields. Thus, solving the Beris-Edwards model using the LBM gives at each node of a model nematic fluid the flow velocity $\bar{\mathbf{u}}$ and the order parameter tensor $\mathbf{Q}$ while taking into account the mutual coupling between these quantities, including flow alignment, backflow, and viscosity effects, albeit with mesoscopic resolution. Details and all equations required for the implementation of a LBM algorithm for a three-dimensional (3D) model NLC are given in Ref. [67]. The inclusion of external fields into the model, which becomes relevant in Sec. III E, is described in Ref. [72]. A recent example for the application of the LBM to NLCs is found in Ref. [73], in which the internal flow of self-propelling nematic droplets was studied.

For our model NLC we define a cubic grid with either $4 \times 81 \times 81$ or $81 \times 81 \times 81$ nodes. We take the x axis as the central axis of our model channel for which we assume a square cross section with aspect ratio equal to 1. Width (y axis) and height (z axis) of the channel are divided into 81 grid nodes numbered from -40 to $+40$; i.e., the NLC layers with node numbers $N_y = \pm 40$ are in contact with the sidewalls and layers with node numbers $N_z = \pm 40$ are located at the top or bottom wall of the channel. The channel walls are implemented as bounceback boundaries corresponding to solid walls with no-slip conditions. In the direction of flow (x), we implement periodic boundary conditions. The flow of the NLC is induced by applying a body force [74] in the $+x$ direction. Anchoring conditions for the nematic director on the channel walls are implemented by prescribing the desired director orientation to the NLC layers in contact with the walls. In these layers, the orientation of $\bar{\mathbf{n}}$ is held constant during the simulation (so-called strong anchoring). For settings in which the anchoring conditions do not change along the x direction, we have just four lattice nodes in the x direction; otherwise we have the same number of nodes (81) as in the y or z direction. Figure 1(a) gives a sketch of the model channel.

In order to compare the numerical simulation with experimental systems, a mapping of simulation units to physical units is useful. This can be achieved with the help of dimensionless numbers such as the Ericksen number and quantitative results of experiments which can be directly compared to simulation results. A possible procedure, which we apply also for the present study, is described in the supplemental material of Ref. [73]. Thus, the numerical results described in the following should correspond to the behavior of common NLC compounds such as 5CB (4-pentyl-4'-cyanobiphenyl) flowing through a microchannel with a cross section of about $100 \mu\text{m} \times 100 \mu\text{m}$. We specify the strength of the flow in the simulation by means of the Ericksen number Er , which is calculated according to Eq. (4) using the quantities of the numerical model instead of the physical quantities. The behavior observed in our simulations at certain Er values should be comparable to that of experimental systems at similar Er values.

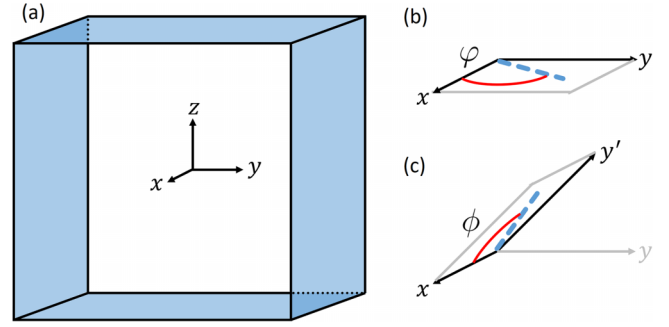


FIG. 1. (a) Sketch of the model channel used in the lattice Boltzmann simulation. The origin of the coordinate system is placed in the channel center. Positions along a given direction i are specified either directly by the node number N_i , or dimensionless by the ratio $2N_i/N_i$ (N_i being the total number of nodes in direction i). Using the latter notation, the top wall is located at $z = 1$, the bottom wall at $z = -1$, and the sidewalls at $y = \pm 1$. In the x direction (direction of flow) the channel is open (periodic boundary conditions). (b) Azimuthal angle φ between the x axis and the projection (dashed blue line) of the director on the xy plane. (c) Angle ϕ between the x axis and the projection (dashed blue line) of the director on the xy' plane. The y' axis is obtained by rotating the y axis by $\pi/4$ around the x axis; φ and ϕ are used for the color-coded visualization of the director field (see Sec. II C).

In addition to the Ericksen number Er , a second dimensionless number, the Deborah number, De , was found to be important for the description of flowing NLCs [63,64], especially for the case of polymeric NLCs [75]. De describes the fluidity of a material (the ratio between relaxation time of an induced strain and a relevant timescale of observation). For $\text{De} > 1$, the flow in NLCs could have a direct effect not only on the orientation of the director but also on the value of the scalar order parameter q . De can be related to Er via the ratio between the two length scales L [see Eq. (4)] and ξ (the nematic correlation length of the Landau-de Gennes theory): $\text{Er}/\text{De} = (L/\xi)^2$ [75]. For standard low-molar-mass nematic compounds, the correlation length ξ is of the order of 10 nm (provided the temperature is well below the nematic-to-isotropic transition). In the present study, typical values of Er are around 100 and the channel width or depth L is of the order of $100 \mu\text{m}$. With these values we obtain $\text{De} = 10^{-6}$; i.e., the direct effect of the flow on the scalar order parameter q is negligible. Nevertheless, the flow can influence the value of q indirectly via the creation of defects.

Because of the restriction of the LBM to mesoscopic length scales, we cannot study the core structure of the disclination or its immediate vicinity. Also, the details of the below-described nucleation processes and physical properties like tension or elasticity of the disclinations are beyond the scope of the present study. The LBM has been applied to the study of the dynamics of defect annihilation [76] and the motion of domain walls and disclination loops [77]. In these studies, the size of the model NLC sample was between 4 and $10 \mu\text{m}$, and the lateral resolution (distance between neighboring nodes) was of the order of 100 nm. In the present study, we consider a model channel the size of which is about one order of magnitude larger (width/depth $\approx 100 \mu\text{m}$), resulting in a resolution not

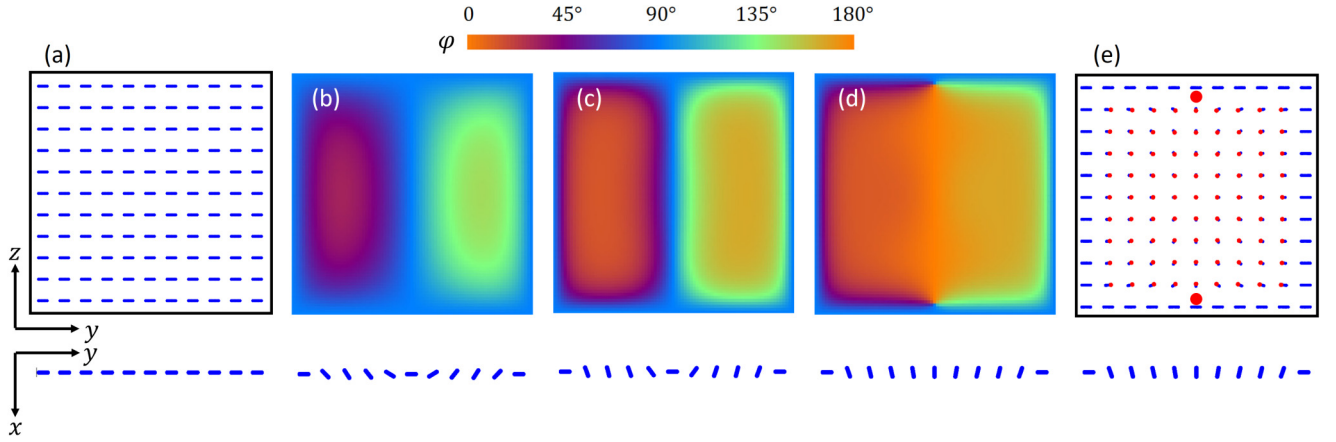


FIG. 2. Model channel with planar anchoring on top and bottom walls and homeotropic anchoring on the sidewalls. (a) Director field in the channel cross section at zero flow. [(b)–(d)] Azimuthal angle φ [see Fig. 1(b)] in the channel cross section for three different Ericksen numbers: (b) $Er = 24$, (c) $Er = 117$, and (d) $Er = 128$; two disclination lines run along x near the middle of the top and bottom walls. (e) Director field at $Er = 128$ [same data as in (d)]. The big red dots indicate the two disclination lines. The schematics below the images show the orientation of the local director in the horizontal midplane.

better than $1\ \mu\text{m}$. We thus aim primarily at the detection of the presence, location, and configuration (wedge or twist) of the disclinations in the channel under various flow and anchoring conditions.

C. Director field visualization and detection of disclination lines

The presence of a disclination influences the surrounding director field well over mesoscopic length scales and the location of a disclination can be deduced from the shape of the director field and the sudden change of the director orientation by $\pi/2$. Also, we observed that the value of the scalar order parameter q is significantly decreased in those voxels of our model channel in which we expect, because of the geometry of the director field, the presence of a disclination. We thus use the decrease of q as an additional marker for a disclination.

In the following, we visualize the director fields in the various settings mainly in two ways. The first consists of a direct display of the local directors, symbolized by small blue rods, at the grid nodes of a given channel section. Local directors which are not parallel to the plane of the image (within an interval of $\pm 5^\circ$) are drawn with reduced length (corresponding to their projection onto the image plane) and are assigned with a red dot indicating the “end” of the director pointing toward the observer. If solely the red dot is visible, the local director is perpendicular to the image plane. For the sake of clarity, only every eighth node along one spatial direction is shown (unless stated otherwise in the captions).

The second way of visualization is a color-coded representation of the angular orientation of the local directors. Shown is either the azimuthal angle φ , which is the angle between the x axis and the projection of the director onto the xy plane [Fig. 1(b)], or the angle ϕ , which is the angle between the x axis and the projection of the director onto the xy' plane [this plane is obtained by rotating the xy plane by $\pi/4$ around the x axis; see Fig. 1(c)]. In the different configurations considered below, the majority of local directors is oriented nearly parallel either to the xy or to the xy' plane and φ or ϕ correspond essentially to the angle between flow direction and local di-

rector. This kind of representation, which can be given in the full resolution of the simulation, is useful for a more precise localization of disclination lines, which are accompanied by a sudden change of director orientation by $\pi/2$ which appears as a sharp color contrast in the image.

In a few cases, we use the decrease of the scalar order parameter q for the visualization of a disclination: all voxels in which q is below a certain threshold are marked with black while all other voxels are set transparent. This is a convenient way to show just the shape of the disclination line without the director field of the sample.

III. RESULTS

A. Homogeneous director field

We first consider a completely homogeneous director field as start configuration: the anchoring conditions on all four walls align the local director along the y direction [homeotropic anchoring on the sidewalls, planar anchoring on top and bottom walls; see Fig. 2(a)] and, at zero flow, this orientation is adopted by all local directors in the sample volume.

When the flow sets in, the first deviation from the uniform y alignment, $\vec{n} = (0, 1, 0)$, is observed in the horizontal midplane ($z = 0$) in the two regions at $y \approx \pm 0.6$, where the local director adopts a nonzero value of its component n_x . With increasing flow, the two regions with $n_x \neq 0$ (and $n_z \neq 0$ for positions above and below the horizontal midplane) spread rapidly over almost the entire sample volume with the exception of the immediate vicinity of the walls (where strong anchoring along y is enforced) and a narrow band around the vertical midplane ($y = 0$) where the orientation of $\vec{n}$ remains unchanged for a wide range of the Ericksen number ($0 < Er < 125$). For $Er > 125$, a structural transition occurs and $\vec{n}$ becomes aligned along x in the major part of vertical midplane. The transition is accompanied by the formation of two disclination lines near the top and the bottom end of the vertical midplane. Figure 2 shows the distribution of the azimuthal angle φ in the director field of the cross section of

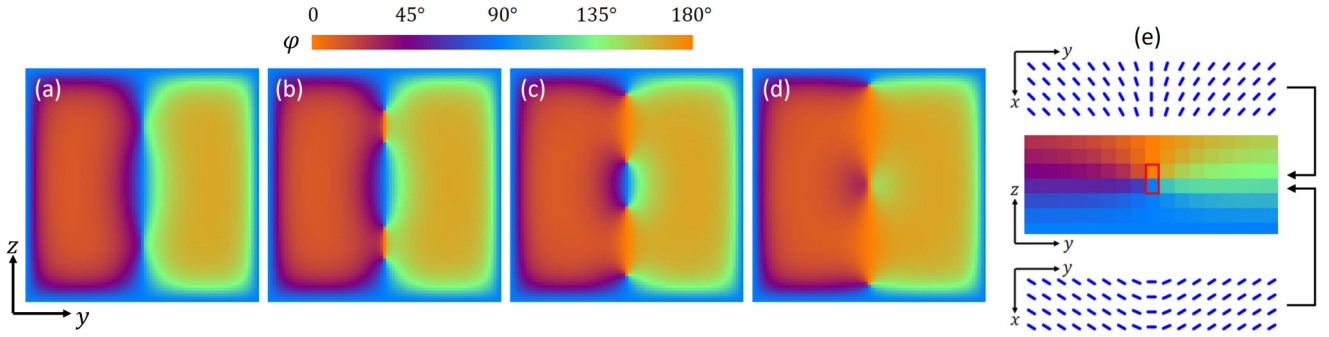


FIG. 3. Model channel with planar anchoring on top and bottom walls and homeotropic anchoring on the sidewalls. [(a)–(d)] Transient states, visualized by the azimuthal angle φ in the channel cross section, at four different times after starting a flow with $Er = 128$. In the vertical midplane two pairs of disclination lines appear in a nucleation process (b). The two inner lines annihilate each other, whereas the lines near the top and bottom walls persist (d). Image (d) shows the structure just after the annihilation of the two inner disclinations and displays transient elastic deformations in the center which are not present in the final steady state [shown in Fig. 2(e)]. (e) Middle: Azimuthal angle φ in the proximity of the disclination line near the bottom wall [enlarged section of Fig. 2(e)]. The disclination line (running along x) is located at the boundary between the two red-framed voxels in the center. Upper and lower panels show the local director orientation in the grid planes just above and below the disclination line, respectively.

the model channel for three different values of Er . Our model square channel may be seen as a combination of two special configurations which are realized in the two (horizontal and vertical) midplanes. In the horizontal midplane, all local directors are, when the flow sets in, perpendicular to the flow direction and parallel to the shear plane of the flow, corresponding to the configuration for measuring the Miesowicz viscosity η_2 [78] (or η_c in the book by de Gennes and Prost [79]). The effect of flow on this configuration has been studied experimentally [80–82], theoretically [80,83,84], and in simulations [81,83,85–87]. Our results confirm the results of the previous studies. In particular, our data concerning the azimuthal orientation φ of the local director in the horizontal midplane correspond to the relation $\varphi - \varphi_0 \propto y - y^3$ (φ_0 being the value at the boundary), which is expected for lower Er and strong anchoring [86].

We now consider the structural transition which proceeds at higher Er through a nucleation process in the vertical midplane as shown in Fig. 3. In the vertical midplane, all local directors are at lower Er oriented perpendicular to the shear plane of the flow, corresponding to the configuration for measuring the Miesowicz viscosity η_3 [78] (or η_a in the book by de Gennes and Prost [79]). The effect of flow on this configuration has been studied in Refs. [88–92]. It was found that the director orientation remains unchanged at low Er , whereas different instabilities can develop if Er exceeds a certain threshold Er_c . However, in the experiments described in Refs. [88–91] a flow cell with a large aspect ratio was used (width up to 100 times larger than depth), resulting in a quasi-two-dimensional flow field which is quite different from our model flow field. Thus, the origin of the transition in our study is probably the reduction of the elastic energy as described in the theoretical models in Refs. [80,84]. The transition via nucleation of topological defects was also observed in earlier simulation studies [85,87] on essentially two-dimensional systems.

In the present study, we observe two simultaneous nucleation processes in the vertical midplane at positions $z \approx \pm 0.6$ [Figs. 3(a) and 3(b)] where the orientation of the local director

changes abruptly by $\pi/2$, resulting in the formation of two pairs of twist disclination lines. Of each pair, one disclination line moves toward the center and the second line migrates to the top or bottom wall, respectively [Figs. 3(b) and 3(c)]. The two disclination lines in the center annihilate each other whereas the two lines at the top and bottom walls persist [Figs. 3(d), 2(d), and 2(e)].

Figure 3(e) shows the structure of the disclination line near the bottom wall. The presence of the disclination is indicated by the abrupt change of the director orientation by $\pi/2$ at two neighboring grid nodes [red frame in the middle panel of Fig. 3(e)]. Along any closed loop around the disclination line the director rotates, within the xy plane, by π ; i.e., the rotation vector is parallel to the z axis. The angle β between the rotation vector and the disclination line (which is parallel to x) amounts thus to $\pi/2$, indicating a pure twist configuration of the disclination.

The nucleation process, which leads to the formation of the two disclination lines at the top and bottom walls, takes place when the Ericksen number Er reaches a value of about 125. On a further increase of Er , the two lines just persist near the walls. Decreasing Er from 125 leaves the two disclinations at first unchanged; then, for $Er < 60$, the position of the two lines depends on the value of Er : The position of the line near the bottom wall is at $z = -0.9$ (the position of the wall is $z = -1$) for $Er > 60$ and changes to $z = -0.33$ when the Ericksen number is lowered to $Er = 8$ (Fig. 4). The line at the top wall shows the same (laterally reversed) behavior; i.e., with decreasing Er the lines move away from the walls toward the center. If $Er < 8$ the disclination lines are no longer stabilized by the flow field; rather they approach each other and annihilate in the channel center although the flow is maintained, resulting in a weakly deformed director field as shown in Fig. 2(b). This behavior is readily understood because the two lines attract each other with a force $F \propto d^{-1}$ (d being the distance between the lines) [93]. Thus, with decreasing Er the attractive force increases and overcomes the effect of the flow field if Er is below a certain critical value (≈ 8 in our case). However, if Er is kept above 8 it is possible to control

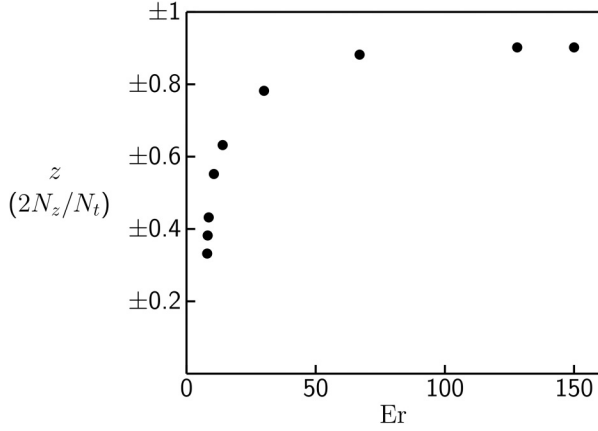


FIG. 4. Model channel with planar anchoring on top and bottom walls and homeotropic anchoring on the sidewalls. Position z (see caption of Fig. 1) of the persisting disclination lines (after their nucleation) as a function of Ericksen number Er .

the position of the two disclination lines (once they were created by the nucleation process at larger Er) in the range between $z = \pm 0.33$ and ± 0.9 by adjusting the flow velocity.

B. Frustrated director field

In the previous section we have shown how disclination lines are created by the interplay between flow and anchoring in an initially homogeneous director field. Here, we study the opposite case: We start with a director field containing disclination lines in the absence of flow and we expect a transformation to a defect-free structure by the flow. A corresponding director field is obtained by enforcing homeotropic anchoring on all four channel walls. Minimizing the elastic energy gives the structure shown in Fig. 5(a) with two disclination lines located in diagonally opposite corners of the channel. The structure is similar to that observed in a recent experimental study [94] in which the behavior of NLCs in cylindrical and square capillaries with homeotropic anchor-

ing was studied. In square capillaries, different configurations with disclinations in two corners were observed, not only in diagonally opposite but also in neighboring corners, and it was found that the lines may switch corners when going along the channel axis. In the present simulation, such a behavior cannot be observed because we have only four lattice nodes in the x direction.

Apart from the presence of the disclination lines, the main difference from the structure considered in the previous section is the orientation of the plane in which the local directors are perpendicular to the local shear plane of the flow: In the case of the homogeneous director field this plane corresponds to the vertical midplane (the xz plane), whereas in the present case the corresponding plane is the diagonal plane from the upper left to the lower right corner, containing the two disclination lines.

In the presence of flow, we see a similar behavior as in the previous case: At low Ericksen number, continuous deformations, consisting of a partial alignment along the flow direction, appear in the regions possessing a larger distance to both the diagonal symmetry plane and the channel walls. With increasing Er , the flow-aligned regions spread over the whole channel volume apart from the regions near the walls and around the diagonal plane in which all local directors are perpendicular to the shear plane of the flow [Fig. 5(b)]. Also, the two disclination lines in the corners of the channel remain unchanged by the flow. For $Er \geq 80$ we observe the nucleation of two pairs of twist disclination lines in the diagonal symmetry plane [Figs. 5(c) and 5(d)]. Of each pair, the line which is closer to the center migrates toward it and annihilates there with the line of the other pair. The second line of each pair (the line which is closer to the corner) migrates to the corner where it annihilates with the disclination that was formed at zero flow. The final steady state for $Er \geq 80$ is then a defect-free escaped configuration [95,96] in which the local directors are aligned approximately along the channel axis, except near the channel walls where the director field is continuously deformed in order to cope with the homeotropic anchoring conditions [Fig. 5(e)].

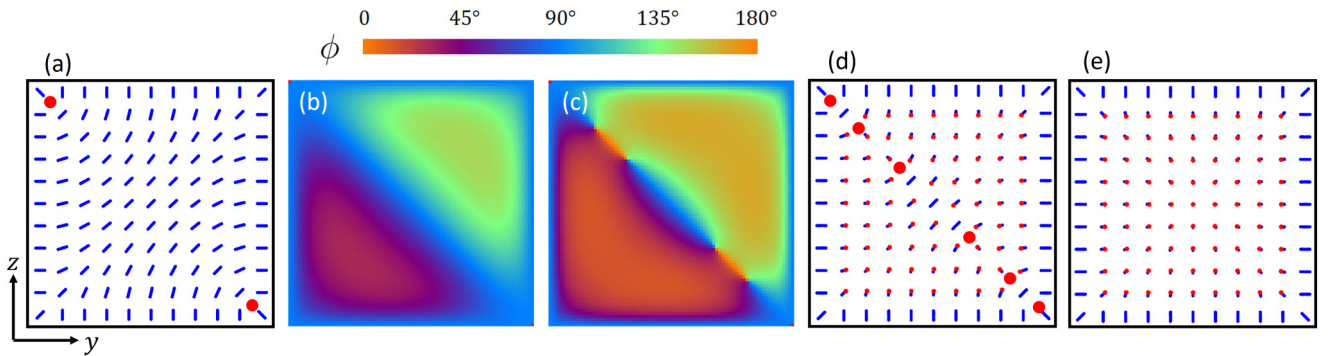


FIG. 5. Model channel with homeotropic anchoring on all walls. (a) Director field in the channel cross section at zero flow, obtained by minimizing the elastic energy starting from an “isotropic” director field with random orientation of all local directors. Two disclination lines are present in the upper left and lower right corner. [(b), (c)] Alignment angle ϕ [see Fig. 1(c)] in the channel cross section (yz plane). Image (b) shows the final steady state for $Er = 20$. Partial flow alignment is observed except near the walls and near the diagonal plane spanning from the upper left to the lower right corner. Image (c) shows a transient state after the nucleation of two pairs of twist disclinations in the diagonal plane at $Er = 80$. [(d), (e)] Director field in the channel cross section (yz plane) at $Er = 80$. Panel (d) shows the same data as in (c). Panel (e) shows the final steady state (escaped configuration with local directors in the channel center aligned along the flow direction).

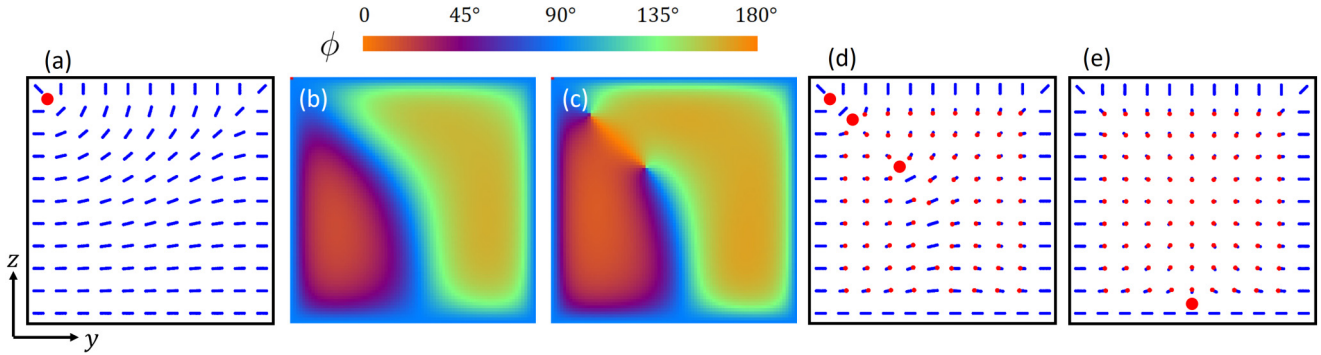


FIG. 6. Model channel with planar anchoring on the bottom wall and homeotropic anchoring on the other three walls. (a) Director field in the channel cross section at zero flow, obtained by minimizing the elastic energy starting from an “isotropic” director field with random orientation of all local directors. One disclination line is present in the upper left corner. [(b), (c)] Alignment angle ϕ (see caption of Fig. 5) in the channel cross section (yz plane). Image (b) shows the final steady state for $Er = 20$. Partial flow alignment is observed except near the walls and in a narrow region spanning from the upper left corner to the center of the bottom wall. Image (c) shows a transient state after the nucleation of one pair of twist disclinations in the diagonal plane near the upper left corner at $Er = 80$. [(d), (e)] Director field in the channel cross section (yz plane) at $Er = 80$. Panel (d) shows the same data as in (c). Panel (e) shows the final steady state (partially escaped configuration with one disclination line running near the center of the bottom wall).

Note that the value of Er , at which the nucleation of the two disclination pairs occurs ($Er \approx 80$), is significantly lower compared to the previous setting of the homogeneous (at zero flow) director field where the nucleation occurs at $Er \approx 125$. A reason might be that in the present case the director field already contains elastic deformations at zero flow so that the elastic threshold, which must be overcome by the flow field for the nucleation of a disclination, is somewhat lower compared to the case where the director field is completely undistorted in the absence of flow.

Once the escaped configuration has been formed, it remains regardless whether the flow is reduced or even decreased to zero. The only structural change occurring with decreasing flow is a relaxation of the bend deformation which is at higher flow rates concentrated in the regions near the channel walls. At lower or zero flow, the deformation stretches out over the whole channel volume, thereby minimizing the total elastic energy.

C. Partially frustrated director field

Here, we briefly consider a configuration which is between those of the two previous sections; i.e., we have homeotropic anchoring on three channel walls and planar anchoring on the fourth (bottom) wall. Minimizing the elastic energy in the absence of flow gives the structure shown in Fig. 6(a) with one disclination line. The disclination is localized either in the upper left corner (as shown in the figure) or, equivalently, in the upper right corner. In the presence of flow, we first observe continuous deformations (partial flow alignment) of the director field except near the walls (where anchoring dominates) and a narrow band spanning from the upper left corner, where the disclination is located, to the middle region of the bottom wall [Fig. 6(b)]. This band indicates those regions in the director field in which local directors are perpendicular to both the flow direction and the local shear plane of the flow.

Increasing the flow to $Er = 80$ or larger leads to the nucleation of one pair of twist disclinations in the above-described band near the corner where the disclination, which

was formed at zero flow, is located [Figs. 6(c) and 6(d)]. Of the newly formed pair of disclinations, the disclination which is closer to the corner migrates toward it and annihilates there with the already existing disclination. The second newly formed disclination moves across the channel toward the middle of the bottom wall where it stays, apparently even for arbitrarily large flow rates. The final steady state for $Er \geq 80$ is thus a combination of the escaped configuration [Fig. 5(e)], which is present in the upper half of the channel, and the configuration with flow-induced disclinations near the walls [Fig. 2(e)], which here exists in the lower half of the channel [Fig. 6(e)].

Lowering Er below 80 results in a similar behavior as described in Sec. III A: With decreasing Er , the disclination stays within the vertical midplane but moves away from the bottom wall. In contrast to the setting of Sec. III A, there is no second disclination in the upper half of the channel. Thus, the single disclination will not be attracted by and annihilate with another disclination; rather it remains stably located in the vertical midplane even if Er is decreased to unity. The vertical position of the disclination line changes from $z = -0.9$ for $Er \geq 80$ to $z = +0.5$ for $Er \approx 1$ (note that the top and bottom walls are located at $z = +1$ and $z = -1$, respectively). For $Er < 1$, the position of the disclination line in the vertical midplane becomes unstable and the line migrates toward either of the two upper corners, thereby reestablishing the initial zero-flow configuration.

D. Alternating anchoring conditions

In the previous sections, the anchoring conditions on the channel walls were constant in the flow (x) direction. Here, we want to explore the behavior at boundaries that separate channel segments which, by means of their anchoring conditions, either favor or disfavor the induction of disclination lines by flow. Thus, we combine the two settings considered in Secs. III A and III B. Our model channel is extended along the flow direction and we have now the same number of nodes (81) along all three spatial directions. We divide the channel

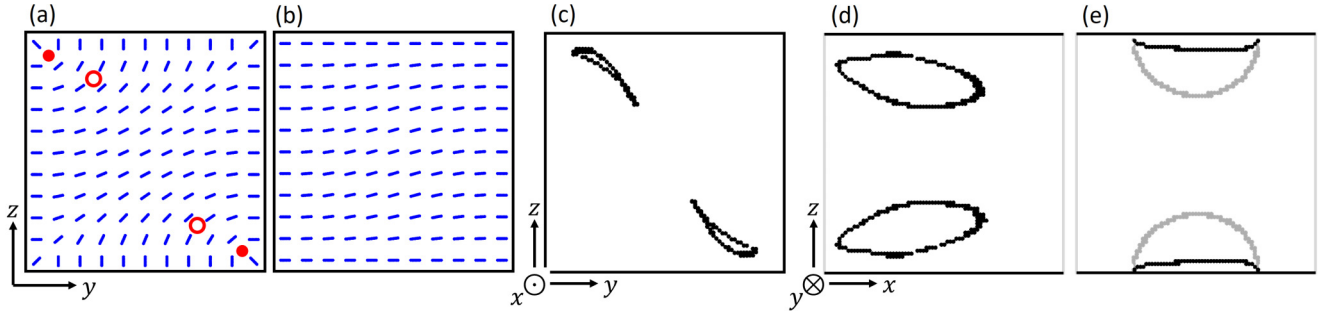


FIG. 7. Model channel with alternating anchoring conditions. (a) Director field in the channel cross section (yz plane) in the region with homeotropic anchoring on all four walls [compare with Fig. 5(a)]. Shown is the director field in the absence of flow, obtained by minimizing the elastic energy starting from an “isotropic” director field with random orientation of all local directors. Two disclination lines (red dots) are present in the upper left and lower right corners. Red circles mark the positions where the nucleation of disclination loops start for $Er \geq 80$. (b) Director field (zero flow) in the neighboring region with planar anchoring on top and bottom walls and homeotropic anchoring on the sidewalls [compare with Fig. 2(a)]. [(c), (d)] Snapshot (transient state) of the two growing disclination loops after nucleation. Shown is the complete volume of the model channel with viewing direction either against the flow direction (cross-sectional view, c) or along the y axis (side view, d). Voxels in which the scalar order parameter q is below 0.25 (indicating the presence of a disclination) are marked with a black dot; all other voxels are set transparent. (e) Final steady states: Black dots indicate the two disclination arcs which remain near the top and bottom walls between the two anchoring boundaries at $Er \geq 80$. Grey dots show the shape of the disclination arcs in the steady state obtained after decreasing Er to unity. Shown is the complete channel volume with viewing direction as in (d); however, in contrast to (d) the disclinations are located exactly in the center plane (xz plane with $y = 0$) of the channel.

in the x direction into three zones: For the first 20 nodes, the anchoring is homeotropic on all four walls (corresponding to Sec. III B). For the next 41 nodes, the anchoring is homeotropic on the two sidewalls and planar on the top and bottom walls (corresponding to Sec. III A). The last 20 nodes have the same anchoring conditions as the first 20 nodes. Because of the periodic boundary conditions in the x direction, the model channel corresponds to an arbitrarily long channel with alternating anchoring conditions that change after each 40th or 41st node.

Figures 7(a) and 7(b) show the director field in the two different anchoring regions obtained for zero flow. The structures are similar to those shown in Figs. 2(a) and 5(a) with small deviations in the bulk regions resulting from the mutual influence between the two structures.

When the flow is started, we observe at lower Ericksen numbers ($Er < 80$) the same continuous deformations of the director field as described in the previous sections [see Figs. 2(a), 2(b), and 5(a)]. When Er reaches a value of 80, two simultaneous nucleation processes are observed. In the previous settings the channel structure did not change along the x direction. Accordingly, all changes in the director field, such as the nucleation of the disclinations, appeared simultaneously along x ; i.e., the nucleation occurred on a line parallel to x . Here, the nucleation occurs at two points with (x, y, z) coordinates $(-0.7, -0.6, +0.65)$ and $(-0.7, +0.6, -0.65)$; i.e., the nucleations occur near the upstream boundary in x (which is located at $x = -1$) and in the plane in which the local director is perpendicular to the local shear plane [see marks in Fig. 7(a)]. Starting from these two points of nucleation, we observe the development of two disclination loops which rapidly extend their diameter, mainly in the downstream direction [Figs. 7(c) and 7(d)]. When the extension of the disclination loops reaches the downstream boundary in x , each loop transforms into two lines. The first line floats near the channel center, where it annihilates with

the corresponding line stemming from the other loop. The second line exists near the top (or bottom) wall. A part of the line annihilates with the disclination line formed at zero flow in the channel corner while the remaining part is preserved as a flat disclination arc spanning the middle part of the model channel near its top (or bottom) wall. The final steady state for $Er \geq 80$ is then a combination of the fully escaped configuration in the channel region with all-homeotropic anchoring and the partly escaped configuration with two disclination lines near the top and bottom walls (walls with planar anchoring) in the second channel region. These flow-induced disclination lines possess a bent shape with their ends being located near the anchoring boundaries on the walls while their middle parts are slightly more distant from the walls [Fig. 7(e)].

When Er is decreased below 80 after the formation of the above-described steady state, the structures remain qualitatively unchanged except that the regions with continuous deformations of the director field grow toward the channel center at the expense of the flow-aligned regions. As a result, the flow-induced disclination lines adopt the shape of an approximate half circle; i.e., the distance between the walls and the middle parts of the disclination lines increases with decreasing Er [Fig. 7(e)]. The flow-induced disclination arcs remain stable even if Er is decreased to unity.

The flow-induced disclination arcs at $Er = 1$ are shown in more detail in Fig. 8. An interesting feature is that the configuration of the disclination arcs changes along x . For several points on the disclination, we have determined the twist angle β between the rotation vector $\vec{\Omega}$ and the tangent $\vec{t}$ to the disclination. The procedure is described in Ref. [12]. In brief, for a given point on the disclination the tangent $\vec{t}$ is defined. For a closed loop around the disclination in the plane perpendicular to $\vec{t}$ the local directors are determined and plotted on a unit sphere, where they form a semicircle (because $\vec{n}$ rotates by π along any closed loop around the disclination). The normal to the plane defined by this semicircle then corresponds to

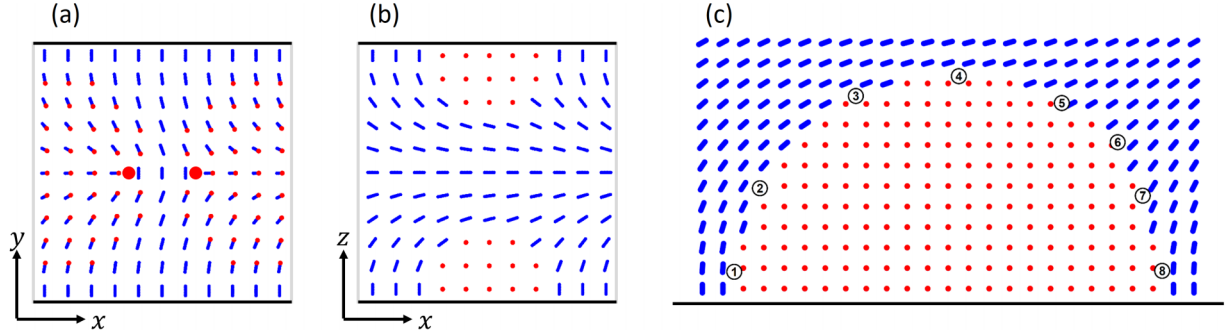


FIG. 8. Model channel with alternating anchoring conditions, director field around the flow-induced disclination arcs [$Er = 1$, same state as shown in Fig. 7(e)]. (a) Cross section parallel to the xy plane in the lower half of the model channel at $z = -0.5$. The two larger red dots indicate the cross sections through the lower disclination arc. (b) Director field in the central xz plane ($y = 0$) of the model channel. (c) Director field near the disclination arc at the bottom wall in higher resolution (shown is every second node along x and z). The encircled numbers ① give the points on the disclination line for which the angle β was determined. The values of β are at point 1, 87° ; point 2, 88° ; point 3, 89° ; point 4, 105° ; point 5, 134° ; point 6, 180° ; point 7, 210° ; and point 8, 265° .

$\bar{\Omega}$. The values of β are given in Fig. 8(c). For the upstream side of the disclination arc we find $\beta \approx \pi/2$, corresponding to the configuration of a twist disclination. In the middle part of the disclination arc, β increases continuously and reaches a value of π at a certain point. Here, the disclination has the configuration of $-1/2$ wedge disclination [point 6 in Fig. 8(c)]. Toward the downstream end of the disclination arc, β increases further and reaches finally a value around $3\pi/2$, corresponding again to the configuration of a twist disclination. The structural evolution along the disclination arc, from twist over $-1/2$ wedge to twist configuration, does not depend on the Ericksen number Er . The exact position of the point, where the configuration corresponds to a $-1/2$ wedge disclination [point 6 in Fig. 8(c)], shifts slightly in the downstream direction with increasing Er .

The flow-induced disclination arcs resemble in some aspects disclination arcs connecting $+1/2$ and $-1/2$ surface defects in static (i.e., without flow) settings [11,33,97]. In these anchoring-induced disclination arcs, the twist angle β also changes by π (from $+1/2$ wedge over twist to $-1/2$ wedge configuration).

Once created at $Er \geq 80$, the flow-induced disclination arcs are stable provided Er is kept in the range $Er \geq 1$. The shape of the arcs varies from approximately half circular at low Er to flat at high Er . However, when Er is decreased below unity, the disclination arcs are no longer stable but decompose via an interesting transformation process. Figure 9 illustrates two transient states of this process observed on decreasing Er from 1 to 0.5: The disclination arcs first change their shape from circular to approximately elliptical by extending toward the channel center. When the two arcs get in contact, they transform into two almost straight lines which connect the bottom and the top walls [Fig. 9(a)]. Similar to the disclination arcs, these disclination lines show a continuous variation of their configuration: near the walls, their structure corresponds to twist disclinations, whereas in the channel center we find either a $+1/2$ (line at upstream position) or a $-1/2$ (line at downstream position) wedge disclination [Figs. 9(b) and 9(c)]. Preliminary studies, in which we vary the aspect ratio of the channel, indicate that the two disclination lines can be stabilized in a steady state if the channel has a more shal-

low shape (height less than width). However, in the present setting (height equal to width), the two lines are not stable but undergo, at constant Er , a further transformation and the final steady state is defect-free with only continuous deformations of the director field [Fig. 9(d)]. These continuous deformations correspond mainly to a twist deformation along the x direction, with the director rotating by π between the upstream and the downstream boundary of the model channel. The twisted structure remains when the flow is decreased to zero, resulting in a different zero-flow configuration compared to the structure that is obtained by minimizing the elastic energy starting from an isotropic state [shown in Figs. 7(a), 7(b), and 9(e)]. However, starting the flow again leads to the same sequence of structures as described above.

The homeotropic or planar anchoring pattern described here might be difficult to realize experimentally because of the following reason. Experimental microchannels are usually based on soft lithography: First, an open channel (or a network of several open channels) is created in the surface of a block of an elastomeric polymer (poly(dimethylsiloxane), PDMS) and then the PDMS block is bonded to a flat glass substrate. The final channel possesses, thus, three PDMS walls and one glass wall (either the top or bottom wall). The intrinsic anchoring condition of a PDMS surface is homeotropic and can be changed only with methods [98] which prevent the creation of sharp homeotropic or planar anchoring boundaries. However, on the glass substrate, which becomes the top or bottom wall of the channel, a well-defined homeotropic or planar anchoring pattern could be created using the method described in Ref. [26] and the flow-induced disclination arcs could be studied at least near one wall of the microchannel. In the following section, we consider results obtained for a similar experimental setting (which possesses anchoring boundaries between two different planar alignments on one channel wall) and we compare these results with predictions of the LBM simulation.

E. Comparison with experiment

To what extent do the results presented in the previous sections describe real experiments? In order to address this question, we consider the experimental study described

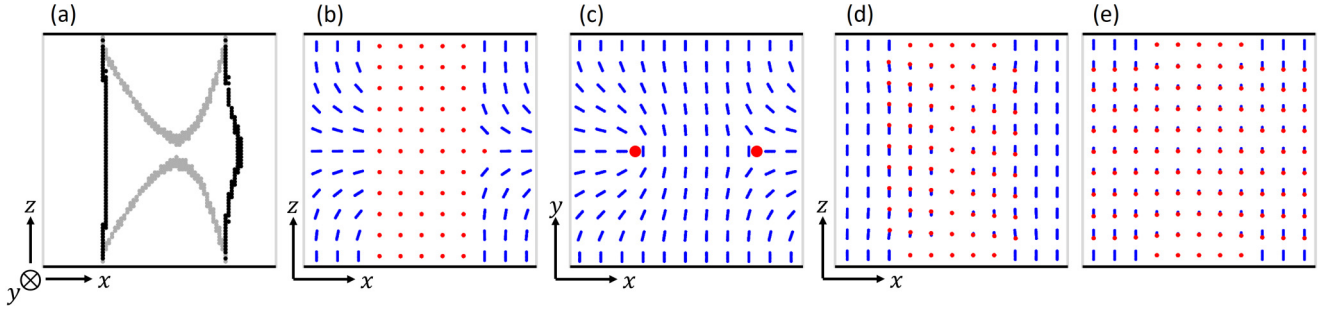


FIG. 9. Model channel with alternating anchoring conditions. (a) Transient shapes of the disclination lines after Er has been decreased from 1 to 0.5. The two disclination arcs, possessing initially the shape of an approximate half circle (see Fig. 8), first extend toward the channel center (gray dots). After touching each other in the channel center, they transform into two almost straight lines (black dots) which connect the bottom and the top walls. Shown is the complete channel volume with viewing direction along the y axis [see caption of Figs. 7(c)–7(e) for more details of this kind of depiction]. (b) Director field in the central xz plane ($y = 0$). Shown is the same transient state as represented by the black dots in (a). (c) Director field in the horizontal midplane (xy plane with $z = 0$). Shown is the same transient state as in (b). Red dots mark the position of the two disclination lines [black dots in (a)] showing a $+1/2$ (upstream line) or $-1/2$ wedge configuration (downstream line). (d) Director field in the central xz plane ($y = 0$) in the final steady state at $Er = 0.5$ (after decreasing from $Er = 1$). Note the difference from the configuration at zero flow, shown in (e), obtained by minimizing the elastic energy starting from an isotropic state.

in Ref. [45], which is concerned with the configuration of disclination lines in microfluidic channels under different anchoring, flow, and external field conditions. In particular, it was shown that two disclination lines, which exist at constant flow in two separate regions of the channel, can be connected by the application of an electric field.

The experimental system consisted of a straight microchannel with anchoring conditions corresponding to those described in Sec. III C: homeotropic anchoring on the two sidewalls and the top wall, and planar anchoring, perpendicular to the flow direction, on the bottom wall. In a short section in the channel center, the bottom wall was provided with a different type of anchoring: planar but parallel to the flow direction. In the following, we designate the two different types of anchoring at the bottom wall as “planar-perpendicular” and “planar-parallel.”

At constant flow, in each of the two major parts of the channel (with planar-perpendicular anchoring), a disclination line, located near the vertical midplane, was observed in accordance with our simulation results described in Sec. III C. These lines terminated at the boundaries to the short section with planar-parallel anchoring, where a defect-free escaped configuration existed [similar to the structure shown in Fig. 5(e)]. It was studied how this flow-stabilized configuration could be changed by the application of an electric field. The used compound possessed positive dielectric anisotropy. Thus, the aligning force of an electric field applied perpendicular to the flow direction was expected to compete with the aligning force of the flow (which acts in a direction nearly parallel to the flow). When the field was switched on, the disclination line in the upstream part of the channel extended as a half loop in the downstream direction, i.e., into the central channel region where the escaped structure existed. Eventually, the half loop got in contact with the second disclination line in the downstream part of the channel and in the final steady state in the presence of flow and field a continuous straight disclination line near the top wall of the whole channel was formed together with a disclination arc at the bottom wall which spanned the short sec-

tion with planar-parallel anchoring. More details are given in Ref. [45].

In order to study this setting in our simulation framework, we provide our model channel with the corresponding anchoring conditions: the top wall and both sidewalls possess homeotropic anchoring, whereas the bottom wall is designed with the two planar anchoring types: planar-perpendicular anchoring at the first 27 and the last 27 nodes and planar-parallel anchoring for the 27 nodes in the center. We start from an isotropic state with random director orientation, minimize the elastic energy at zero flow, and then start a flow along x which is strong enough ($Er \geq 80$) to induce potential disclination lines as described in the previous sections. After establishing a steady state at constant flow, an electric field is applied in the y direction, the strength of which is comparable to the experimental field. (In the experiment, a sinusoidal AC field was used in order to avoid ionic currents. In the present simulation, a simple DC field is applied.)

Figure 10 gives the structure of the steady state at constant flow with $Er \geq 80$ and zero applied field. As expected, we observe a defect-free escaped configuration in the center of the model channel with planar-parallel anchoring on the bottom wall, whereas we find a twist disclination near the bottom wall in the two regions with planar-perpendicular anchoring on the bottom wall (these two regions show the same configuration as described in Sec. III C). The disclination lines terminate at the anchoring boundary between the regions with planar-perpendicular and planar-parallel anchoring on the bottom wall, thereby forming one partial disclination arc in the upstream-located third of the model channel and another partial arc in the downstream-located third. Because of the periodic boundary conditions in the x direction, the two partial arcs may be seen as one complete arc existing in the two-thirds of the channel with planar-perpendicular anchoring on the bottom wall.

When the field is switched on, the upstream-located disclination arc forms a half loop which extends in the downstream direction [Figs. 11(a)–11(c)] until it gets in contact with the downstream-located disclination arc. Then, the disclination

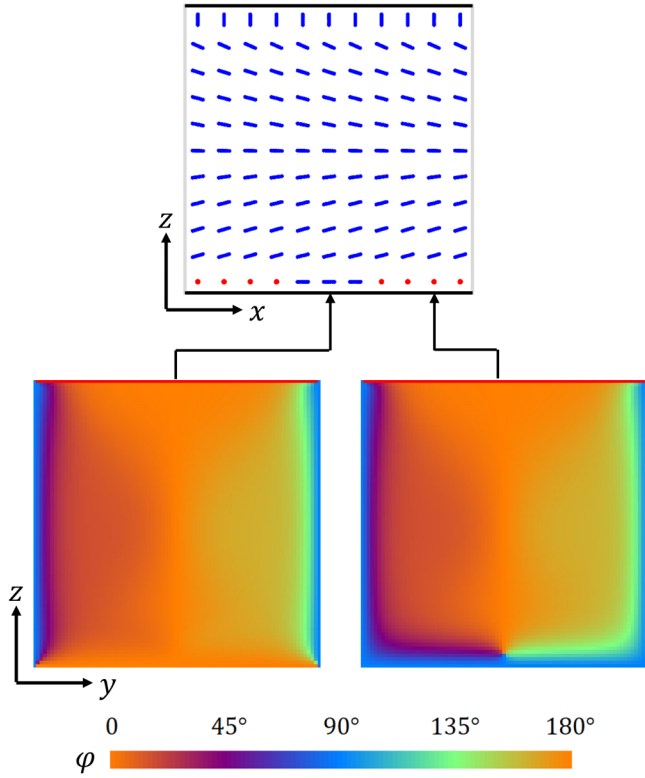


FIG. 10. Model channel with two different planar anchoring conditions on the bottom wall, steady state at $Er = 80$, and zero external field. Top: Director field in the central xz plane ($y = 0$). Bottom: Azimuthal angle φ for two different cross sections (yz planes). Left: Cross section in the central region with planar-parallel anchoring on the bottom wall, showing a defect-free state (mainly flow aligned, $\varphi \approx 0$) with continuous deformations near the top wall and sidewalls only. Right: Cross section in the downstream part of the channel with planar-perpendicular anchoring on the bottom wall, showing a twist disclination near the bottom wall [see also Figs. 2(d) and 3(e)].

lines undergo a reconfiguration, after which a new disclination arc near the bottom wall spans the central third of the model channel and a second disclination line runs through the whole channel, connecting the upstream and downstream boundaries [Figs. 11(d) and 11(e)]. The second disclination line migrates toward the top wall of the channel, where it remains in the final steady state with constant flow and field, as shown in Fig. 12. When the field is switched off, the above-described transformation of the disclination lines takes place in reverse order, establishing again the steady state shown in Fig. 10.

The simulation results described in this section, especially the transformation of the disclination lines, agree well with the experimental observations, thereby confirming that the results of the previous sections could be observed in real experiments. We should also note that the structures presented here in Figs. 10–12 provide a more realistic description of the nematic director field compared to the schematic structures proposed in Ref. [45].

IV. CONCLUSIONS

We have reported a simulation study, based on lattice Boltzmann calculations, concerning the flow of nematic liquid

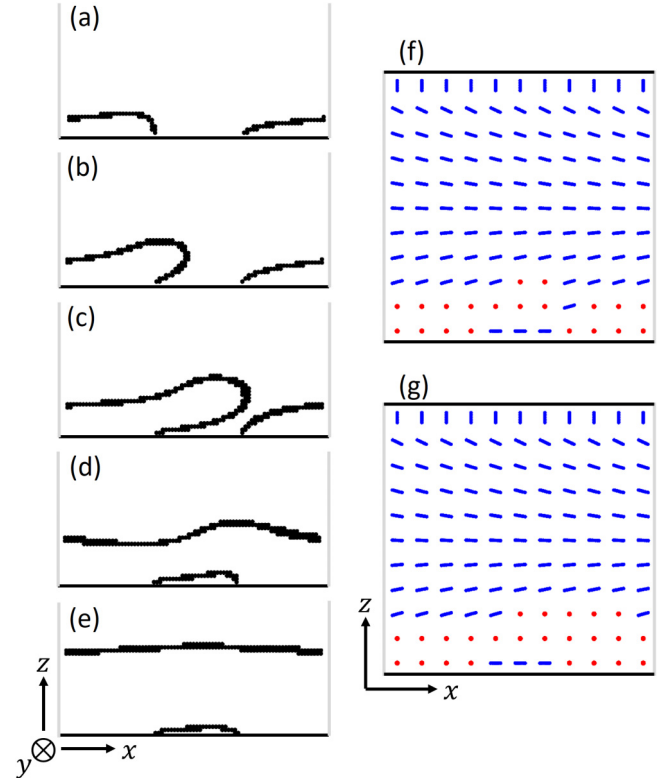


FIG. 11. Model channel with two different planar anchoring conditions on the bottom wall; transient states at $Er = 80$ after a constant electric field along y has been switched on. [(a)–(e)] Transient shapes of the disclination lines: lower half of the channel volume with viewing direction along the y axis (side view, see caption of Figs. 7(c) and 7(d) for more details of this kind of depiction). After the field is switched on, the upstream-located partial disclination arc extends in the downstream direction [(a), (b)], forming a half loop that eventually touches the downstream-located partial disclination arc (c). Then, the disclination lines transform to an arc spanning the central region of the bottom wall with planar-parallel anchoring and a second line which connects the upstream and downstream boundary (d) and migrates toward the top wall of the model channel (e). [(f), (g)] The director field in the central xz plane ($y = 0$) just before and after the transformation [same states as shown in (c) and (d)].

crystals through linear microchannels. In particular, we have studied the interplay between anchoring conditions, flow, and disclination lines. An important observation is a nucleation process, resulting in the creation of at least one pair of twist disclinations, which takes place under two conditions: the orientation of the local director is perpendicular to the local shear plane of the flow, and the magnitude of the Ericksen number Er is above a certain level. When the flow is maintained at this level, the newly created disclination lines either persist or they annihilate with other disclination lines, which were also newly created or which existed already under zero flow conditions. A requirement for the persistence of a disclination line is a certain anchoring condition on at least one of the channel walls. This anchoring condition should support the same director alignment which is required for the nucleation process, namely, an orientation of the director perpendicular to the shear plane of the flow (corresponding to planar

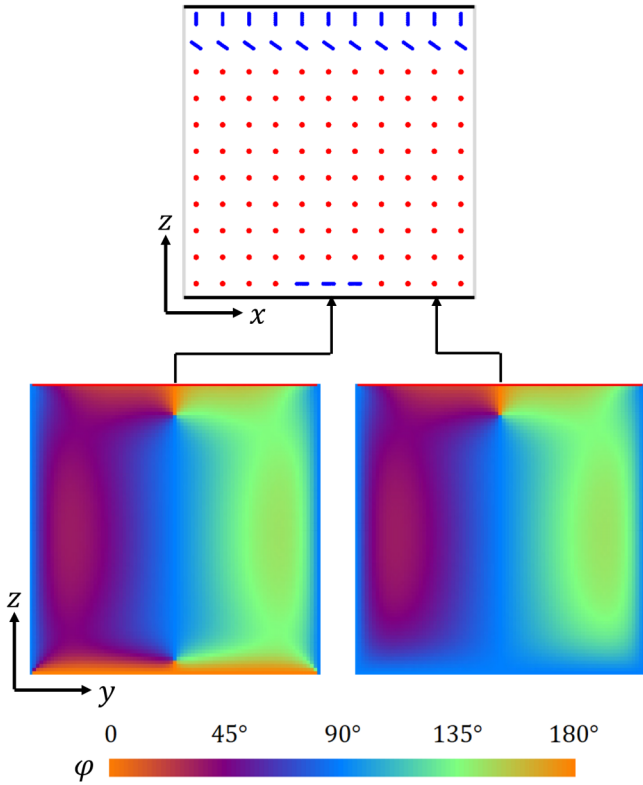


FIG. 12. Model channel with two different planar anchoring conditions on the bottom wall; steady state at $Er = 80$ with constant electric field applied along y . Top: Director field in the central xz plane ($y = 0$). In the major part of the channel volume, the aligning force of the field overcomes the aligning force of the flow, resulting in an orientation of the director along y except near the top and the central bottom wall (compare with Fig. 10). Bottom: Azimuthal angle φ for two different cross sections (yz planes). Left: Cross section in the central region with planar-parallel anchoring on the bottom wall, showing a twist disclination near the bottom wall and a second disclination near the top wall. Right: Cross section in the downstream part of the channel with planar-perpendicular anchoring on the bottom wall, showing just one twist disclination near the top wall.

anchoring perpendicular to the flow direction). The persistent disclination line migrates toward this wall and remains there near the central region (i.e., at equal distance from the two neighboring channel walls) of the wall surface.

The nucleation of the disclination lines requires large values of the Ericksen number ($Er \geq 80$). A persistent line, once created, is stable even if Er is decreased to 10 or smaller values. The distance between the line and the wall increases with decreasing Er ; thus, the line position marks a kind of boundary between the region where the anchoring forces of the wall dominate and the region in which the aligning forces of the flow prevail.

The number of channel walls possessing the planar-perpendicular anchoring condition determines the number of disclination lines which persist at high Er values. The configuration described in Sec. III A possesses two such walls (top and bottom walls) and in the configuration of Sec. III C only one wall possesses the plane-parallel anchoring condition. We thus find in the final steady state at large Er two or one persisting disclination lines. We have checked also that configurations in which three or all four walls possess the planar-perpendicular anchoring show three or four persisting disclinations in their steady states at large Er . In Sec. III B we consider a configuration in which none of the walls possesses a planar-perpendicular anchoring. Accordingly, all disclination lines created by nucleation processes annihilate either with other newly created disclinations or with disclinations which already existed at zero flow and no lines persist in the final steady state. We have also studied the behavior in channels with varying or alternating anchoring conditions and demonstrated the existence of disclination arcs which start and terminate at boundaries between regions with different anchoring conditions.

In the present study, we used so-called strong anchoring conditions; i.e., the orientation of the director in the nematic layer adjacent to the wall is a fixed boundary condition and cannot be changed by the flow or external fields. In a real experiment, however, the anchoring strength is always finite. Thus, it might be that at very large Er numbers the final steady state corresponds to a defect-free completely flow-aligned configuration as shown in Fig. 5(e), regardless of the anchoring conditions on the channel walls. On the other hand, we have demonstrated that the lattice Boltzmann model gives an appropriate description of an experimental study of disclination lines and their transformation by the interplay between anchoring, flow, and electric field in microfluidic channels. In particular, the two steady states in the presence of flow (with and without electric field), and the rearrangement of the disclination lines by the combined action of flow and field, are correctly reproduced. Thus, we are confident that the behavior found in our simulations will be observed also in experimental studies.

ACKNOWLEDGMENT

We thank Stephan Herminghaus for continuous support and stimulating discussions.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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