A model of crack based on dislocations in smectic A liquid crystals*

Fan Tian-You(范天佑) and Tang Zhi-Yi(唐志毅)†

School of Physics, Beijing Institute of Technology, Beijing 100081, *China*

(Received 5 March 2014; revised manuscript received 17 April 2014; published online 20 August 2014)

A plastic crack model for smectic A liquid crystals under longitudinal shear is suggested. The solution of the screw dislocation in smectic A is the key to the correct result that we obtained by overcoming a longstanding puzzle. We further use the dislocation pile-up principle and the singular integral equation method to construct the solution of the crack in the phase. From the solution, we can determine the size of the plastic zone at the crack tip and the crack tip opening (tearing) displacement, which are the parameters relevant to the local stability/instability of materials. Our results may be useful for developing soft-matter mechanics.

Keywords: smectic A, screw dislocation, dislocation pile-up, plastic crack, local instability

PACS: 61.30.–v, 61.30.Dk, 61.30.Jf **DOI:** 10.1088/1674-1056/23/10/106103

1. Introduction

As is well known, liquid crystals and quasicrystals are important phases in condensed matter, and are fascinating from a fundamental point of view. Liquid crystals are also significant on account of the large number of their current and potential applications. They belong to an intermediate phase between an isotropic liquid and a solid. The mechanical properties of the phase are very interesting and have been extensively studied by de Gennes and Prost,[1] Kleman and Oswald,[2] and Oswald and Pieranski.[3] Owing to the need of basic research and engineering applications, the three-dimensional elasticity, plasticity, defects, and dynamics of the liquid crystals are especially required to be further studied. Among the defects, dislocations and focal conics have been investigated by the above authors,[1–3] as well as Landau and Lishitz,[4] Fujii *et al*.[5] In addition, Brostow *et al*.[6] have carried out numerical simulations on crack formation and propagation in polymer liquid crystals. Liquid crystals, including smectic ones, can be classified as monomer liquid crystals (MLCs), irrespective of whether they can polymerize and form polymer liquid crystals (PLCs). Samuski's[7] classification has been used by a number of researchers.[8,9] The present model is applied to MLCs, particularly smectic A phase MLCs. To develop the pioneering work done by Brostow *et al*.,[6] Fan [10] recently studied a novel defect in liquid crystals. In the respect of dynamics, the hydrodynamics, elastodynamics, and wave propagation have been discussed in the papers and books by de Gennes and Prost,[1] de Gennes and Kleman,[11] Oswald and Pieranski,[3] and Landau and Lishitz.[4] In addition, de Gennes and Prost,[1] and Oswald and Pieranski[3] have done pioneering work on the plasticity of liquid crystals. However, to date, the plastic theory of liquid crystals has not been developed, either microscopically or macroscopically. This leads to some difficulties in studying the plasticities of liquid crystals. There has been preliminary work on the three-dimensional (3D) elasticities of liquid crystals (see, for example, Fan[12]), but more difficult topics have not yet been dealt with. Owing to the difficulty mentioned above, in the present paper we suggest a phenomenological model to cope with a plasticity problem for smectic liquid crystals. An analytic solution of plasticity–crack interaction is presented, which may provide a basis for fundamental research in soft- matter physics and chemistry.

2. Physical model and mathematical solution

There are inherent connections between dislocations and cracks; for example, a piling-up of dislocations can result in a crack, which may strongly influence the mechanical behaviors of liquid crystals. Although cracks affect the plasticities of liquid crystals, the relevant mechanism is not so clear. A coupling between fracture and plasticity makes the problem more complicated. Fan[10] discussed a plastic crack in a smectic liquid based on the dislocation pile-up model. This model has been used for crystals by Bilby *et at*.[13,14] and for quasicrystals by Fan *et al*.[15,16] But the work carried out in Ref. [10] contains some approximations, in which the movement of dislocations does not strictly follow the Peach–Koehler force rule. The reason for this lies in the limitation of the methodology that was adopted. In Ref. [10] the work conducted was based on the edge dislocation pile-up model. The present work takes a screw dislocation pile-up model, in which the movement of the dislocations can strictly follow the Peach–Koehler force rule.

Consider a smectics A liquid crystal whose layers are

*Project supported by the National Natural Science Foundation of China (Grant No. 11272055).

†Corresponding author. E-mail: 7491903@qq.com

© 2014 Chinese Physical Society and IOP Publishing Ltd

in the xy-plane, and a crack dislocation group with length $2l$ along the x axis subjected to a uniform shear stress $\sigma_{yz} = \tau^{(\infty)}$, as shown in Fig. 1, in which the single screw dislocation has Burgers vector $\boldsymbol{b} = (0,0,b)$. Because the deformation is assumed to be independent of variable z, the figure depicts any of transverse sections of the body. At the crack tip there is a screw dislocation pile-up with length d, whose value is unknown and to be determined. We refer to the pile-up as sliding dislocation group. Within the zone defined by $y = 0$, $l \le |x| \le l + d$, a counter direction shear stress τ_c is applied, the value of which represents the yield strength of the material macroscopically. In other words, the dislocation pile-up zone is the plastic zone. The physical meaning of τ_c can be referred to the monograph (p. 499 in Ref. [1]).[1]

The model can be formulated by the following (equivalent) boundary conditions:

$$\begin{cases} (x^2+y^2)^{1/2} \to \infty, & \sigma_{ij} = 0, \\ y = 0, \quad |x| < l, & \sigma_{yz} = -\tau^{(\infty)}, \\ y = 0, \quad l < |x| < l + d, & \sigma_{yz} = -\tau^{(\infty)} + \tau_c. \end{cases} \tag{1}$$

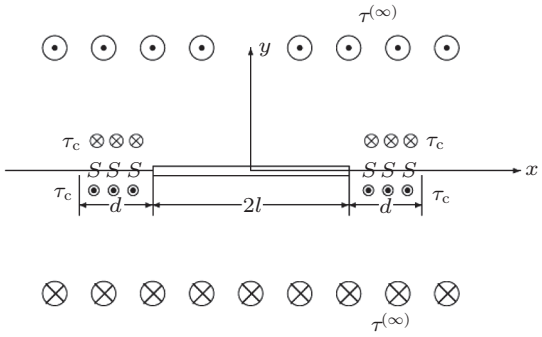


Fig. 1. Plastic crack in a smectics A under longitudinal shear.

A quantitative description of the problem needs to introduce relevant basic governing equations. The mathematical model (1) requires the nonlinear (plastic) problem to be linearized, although it contains an unknown constant d. This greatly simplifies the mathematical solution and allows us to choose linear governing equations.

According to Refs. [1] and [4], the stress tensor for smectic liquid crystal (exactly speaking for smectics A) is

$$\begin{cases} \sigma_{xx} = \sigma_{yy} = K_1 \nabla^2 \dfrac{\partial u}{\partial z}, \\ \sigma_{zz} = \rho_0 B' \dfrac{\partial u}{\partial z}, \\ \sigma_{zx} = \sigma_{xz} = -K_1 \nabla^2 \dfrac{\partial u}{\partial x}, \\ \sigma_{zy} = \sigma_{yz} = -K_1 \nabla^2 \dfrac{\partial u}{\partial y}, \\ \sigma_{xy} = \sigma_{yx} = 0, \end{cases} \tag{2}$$

where $u \equiv u_z$ is the displacement of the z component, $B' = B - C^2/A$, ρ_0 and K_1 are material constants (see Ref. [4]). Physically, the constant B' describes material modulus relating to deformation arising from displacements, while K_1 describes material modulus relating to deformation arising from curvature. It is evident that for the stress tensor (2) only the symmetric part (the elastic part), according to the Landau's terminology (i.e., the de Gennes' terminology), is considered; the fluid part is omitted here according to the method adopted in the liquid crystal study community.

Substituting Eq. (2) into the equilibrium equations

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{3}$$

yields the final governing equation

$$\rho_0 B' \frac{\partial^2 u}{\partial z^2} - K_1 \nabla^2 \nabla^2 u = 0,$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

Because the field variables are independent of variable z, the equation is reduced to

$$\nabla^2 \nabla^2 u = 0. \tag{4}$$

Equation (4), which can also be derived from the energy minimization, is identical to those given by de Gennes and Prost,[1] Oswald and Pieranski,[3] and Landau and Lishitz.[4]

The solution of the plastic crack is reduced to solving Eq. (4) under boundary conditions (Eq. (1)), which can be called the "boundary value problem (4), (1)".

To solve the "boundary value problem (4), (1)", we can refer to the experiences in crystals[13,14] and quasicrystals,[15,16] we can also refer to the experience in liquid crystals for edge dislocation more recently, that is, to transform the problem into the following singular integral equations:

$$\int_L \frac{f(\xi)\,\mathrm{d}\xi}{\xi - x} = \frac{\tau(x)}{G}, \tag{5}$$

in which $f(\xi)$ is a dislocation density function, ξ the dislocation source point coordinate, and x the field point coordinate on the real axis, L represents interval $(-(l+d), l+d)$, and $\tau(x)$ the shear stress distribution in the region $z = 0, |x| \le l + d$, that is,

$$\tau(x) = \begin{cases} -\tau^{(\infty)}, & |x| < l, \\ -\tau^{(\infty)} + \tau_c, & l < |x| < l + d, \end{cases} \tag{6}$$

and the key point is how to choose constant G. This depends upon the solution of the screw dislocation of smectic A liquid crystal. Kleman[17] and Pershan[18] obtained the solution long ago, but it is wrong. This results in a longstanding puzzle in the study, which can be named the de-Gennes–Kleman–Pershan paradox.

Fan and Li[19] have clarified the puzzle, and gave a correct solution:

$$G=\left(\frac{b}{\pi}\right)K_1D_1,$$

$$D_1=\frac{-\frac{8}{3}\pi\alpha}{(R_0+r_0)\left(\frac{\pi}{4}\alpha\beta+\frac{b^2K_1}{8\pi}\right)\ln\frac{R_0}{r_0}+\frac{\pi}{320}\alpha\gamma(R_0-r_0)}, \tag{7}$$

in which

$$\begin{cases}\alpha=\left(\dfrac{b}{2\pi}\right)^4\rho_0B',\\ \beta=2+\dfrac{32\pi^2}{3},\\ \gamma=75-160\pi^2+256\pi^4.\end{cases} \tag{8}$$

In terms of the singular integral equation theory of Muskhelishvili (p. 251 in Ref. [20]), the integral equations (5) under condition (6) have the solution

$$\begin{aligned}f(x) &= -\frac{1}{\pi^2G}\sqrt{\frac{x+(l+d)}{x-(l+d)}}\int_L\sqrt{\frac{\xi-(l+d)}{\xi+(L+d)}}\tau(\xi)\frac{d\xi}{\xi-x}\\ &= -\frac{1}{\pi^2G}\sqrt{\frac{x+(l+d)}{x-(l+d)}}\\ &\quad\times\left\{\mathrm{i}\left[2\tau_c\arccos\left(\frac{l}{l+d}\right)-\tau^{(\infty)}\pi\right]\right\}\\ &\quad+\frac{\tau_c}{\pi^2G}\left[\operatorname{arccosh}\left|\frac{(l+d)^2-lx}{(l+d)(l-x)}\right|\right.\\ &\quad\left.-\operatorname{arccosh}\left|\frac{(l+d)^2+lx}{(l+d)(l+x)}\right|\right],\end{aligned} \tag{9}$$

(the details of the mathematical calculation are quite lengthy and are omitted here), in which $\mathrm{i}=\sqrt{-1}$, and G is defined by Eq. (7). Because the dislocation density $f(x)$ should be a real function, the factor multiplied by the imaginary number i in the first term on the right-hand side of Eq. (9) must be zero, which leads to

$$2\tau_c\arccos\left(\frac{l}{l+d}\right)-\tau^{(\infty)}\pi=0,$$

that is,

$$d=l\left[\sec\left(\frac{\pi\tau^{(\infty)}}{2\tau_c}\right)-1\right]. \tag{10}$$

This determines the plastic zone size.

From solution (9), we evaluate the number of dislocations $N(x)$ as follows:

$$N(x)=\int_0^x f(\xi)\,\mathrm{d}\xi. \tag{11}$$

By substituting solution (9) (coupled with Eq. (10)) into Eq. (11) we can obtain the values of $N(l+d)$ and $N(l)$, so the quantity of dislocation motion is

$$\begin{aligned}\delta &= b[N(l+d)-N(l)]=\frac{2bl\tau_c}{\pi^2G}\left(\ln\frac{l+d}{l}\right)\\ &= \frac{2\tau_cl}{\pi\rho_0B'}\ln\sec\left(\frac{\pi\tau^{(\infty)}}{2\tau_c}\right).\end{aligned} \tag{12}$$

This is the crack tip opening (tearing) displacement, which is an important parameter

3. Rupture criterion

We suggest the following rupture criterion:

$$\delta=\delta_c, \tag{13}$$

which can be used for determining the thermodynamic stability/instability of the material. Here, δ_c is the critical value of the crack tip sliding displacement, which can be measured experimentally, and is a material constant of the liquid crystal. Equation (13) describes a critical state of equilibrium of the plastic crack. When $\delta<\delta_c$, the crack does not propagate but when $\delta>\delta_c$ the crack will propagate. By using this criterion, the limit value of the applied stress $\tau^{(\infty)}$ or the limit value of the crack size l can be determined.

The above treatment is a macro-description (or the continuum model), a micro-description (or a micro-mechanism) can be given below.

By introducing the de Gennes theory (refer to Ref. [1]), the yield stress is

$$\tau_c\sim\frac{\pi\gamma_0^2}{a_0k_BT\ln(v_0/v_1)}, \tag{14}$$

where

$$\begin{aligned}&\gamma_0\approx\frac{1}{2}\sqrt{K_1B}a_0^2/\eta,\quad \eta\sim\sqrt{\frac{K_1}{B}},\\ &v_0=10^{33}\ \mathrm{s}^{-1}\cdot\mathrm{cm}^{-3},\quad v_1=1\ \mathrm{s}^{-1}\cdot\mathrm{cm}^{-3},\end{aligned} \tag{15}$$

and a_0 represents the thickness of the layer of the smectic, whose value is almost equivalent to the magnitude of a Burgers vector, k_B is the Boltzmann constant, T the absolute temperature, v_0 and v_1 are the fluctuation frequencies, respectively.

Substituting expression (14) into Eqs. (10) and (12) respectively, one reveals the physical meanings of the plastic zone size (or dislocation sliding width) and crack tip sliding displacement (or amount of dislocation motion) in-depth. Owing to the limitation of space, a detailed discussion is not given here.

4. Conclusions

Cracks and plasticities are difficult topics in liquid crystals. One of the reasons for this lies in the lack of a theory of

plasticity, at least, no macroscopic plastic constitutive equation has been available so far. Here, we adopt a phenomenological model to discuss the said problem. In this way, we obtain some physical quantities for describing the coupling between fracture and plasticity. In particular, the solution given in this study exactly satisfies the Peach–Koehler force rule. The method developed here is generally effective for other problems in smectics and other kinds of liquid crystals.

References

[1] de Gennes P G and Prost J 1993 *The Physics of Liquid Crystals* (London: Clarendon) pp. 490, 493, 499

[2] Kleman M and Oswald P 1982 *J. Physique* **43** 655

[3] Oswald P and Pieranski P 2006 *Smectic and Columnar Liquid Crystals* (London: Taylor & Francis) p. 123

[4] Landau L D and Lifshitz E M 1986 *Theory of Elasticity*, 3rd edn. (Oxford: Pergamon) pp. 177, 181

[5] Fujii S, Komura S, Ishii Y and Lu C Y D 2011 *J. Phys.: Condens Matter* **23** 235105

[6] Brostow W, Cunha A M, Quintanila J and Simoes R 2002 *Macromol. Theory Simul.* **11** 308

[7] Samulski E T 1985 *Faraday Discuss. Chem. Soc.* **79** 7

[8] Brostow W 1990 *Polymer* **31** 979

[9] Hess M 2000 *High Performance Polymers* in *Performance of Plastics* (Munich-Cincinnati: Hanser), ed. Brostow W, Chap. 21, p. 519

[10] Fan T Y 2012 *Phil. Mag. Lett.* **92** 153

[11] de Gennes P G and Kleman M 1974 *Liquid Crystals and Plastic Crystals* **1** 92

[12] Fan T Y 2014 "Displacement Potentials and Elliptic Disk-shaped Crack in Three-dimensional Smectic B Liquid Crystals", submitted

[13] Bilby B A, Cottrell A H and Swinden K H 1963 *Proc. R. Soc. A* **272** 304

[14] Bilby B A, Cottrell A H, Smith E and Swinden K H 1964 *Proc. R. Soc. A* **279** 1

[15] Fan T Y, Trebin H R, Messerschmidt U and Mai Y W 2004 *J. Phys.: Condens. Matter* **16** 5229

[16] Fan T Y 2010 *Mathematical Theory of Elasticity of Quasicrystals and Its Applications* (Heidelberg: Springer-Verlag) p. 307

[17] Kleman M 1974 *J. Physique* **35** 595

[18] Pershan P S 1974 *J. Appl. Phys* **45** 1590

[19] Fan T Y and Li X F 2014 *Chin. Phys. B* **23** 046102

[20] Muskhelishvili N I 1956 *Singular Integral Equations* (Gnoningen: Noordhoff) p. 251