Critical behavior of the size of a drop facet in the nematic-smectic *A* phase transition

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The critical behavior of the radius of a facet of a smectic *A* drop near the nematic-smectic *A* phase transition and near the liquid-smectic *A* phase transition is examined theoretically. Near the nematic-smectic *A* phase transition, the drop radius has a behavior $R \sim \tau^{\nu_\perp}$, where τ is proportional to the deviation of the temperature from the transition temperature, and $\nu_\perp$ is the critical exponent of the transverse correlation radius. The critical exponent for the facet radius is the same as that for the elastic modulus *B* only in the case of isotropic scaling. Near the liquid-smectic *A* phase transition point, the facet radius has a behavior $R \sim \Delta^{5/4}$, where Δ is the size of the gap in the correlation function of the short-wave density field.

INTRODUCTION

The nematic-smectic *A* phase transition is one of the most interesting from the theoretical standpoint, since fluctuations of the director play an important role along with fluctuations of the order parameter near this transition. The director fluctuations are analogous in many ways to fluctuations of the electromagnetic field near a superconducting phase transition.[1–8] The consequences of an influence of director fluctuations have not been clarified theoretically. It is essentially impossible to study the de Gennes model,[1] which describes this phase transition on the basis of an ε expansion, since the term of second order in ε is numerically larger than the first in the renormalization-group equations.[3] In other words, there is no hope that the first terms of an ε expansion of the renormalization-group equations will give a valid description of the situation.

It thus become necessary to consider all situations which are possible in principle:

1. The fluctuations of the director convert the transition into a first-order phase transition.[3]

2a. The phase transition is a second-order phase transition with distinctive natural exponents.[8]

2b. The phase transition is a second-order phase transition characterized by an anisotropic scaling.[4]

The calorimetric data which are available on the vicinity of the triple point[9] speak in favor of the first of these possibilities, although a continuous transition has been observed in most studies, at the experimental accuracy. Recent measurements put the heat-capacity index close to the helium value.[10–14]

There are two possible ways to explain this phenomenon. First, the behavior of this system may depend strongly on the seed values of the parameters, and either scenario 1 or scenario 2 will be realized, depending on the relation among these seed values. If it is scenario 2, the heat-capacity exponent turns out by chance to be close to the helium value (the exponent of the *X*–*Y* model). The second possibility is that scenario 1 is ultimately realized in all cases, but near the transition there is a significant intermediate temperature interval in which the director fluctuations do not play an important role, so the system exhibits helium behavior.

Further experimental data are required in order to choose between these two possibilities. Corresponding data can be extracted from experiments on the critical behavior of the dimensions of the facets on drops of a smectic phase near the nematic-smectic *A* transition.[15] As we show below, the corresponding exponent can be expressed in terms of the basic independent exponents characterizing the phase transition. A comparison of the result found for a helium transition (the exponents for the *X*–*Y* model are well known) with experimental data can thus answer our question. The results of a comparison of this sort are presented in the Conclusion to this paper.

SHAPE OF A DROP

Let us consider the equilibrium shape of a drop of smectic *A*. Like ordinary crystals,[16] a smectic must have a flat face (a facet) parallel to the smectic layers. In contrast with ordinary crystals, however, the facet of the smectic is circular, because of the isotropy of the smectic layer. The facet of a drop of smectic *A* is thus characterized exclusively by its radius *R*, and it is the critical behavior of this radius in which we are interested here. Yet another important distinction between a smectic and an ordinary crystal is that the equilibrium shape is reached quickly. This speed is of assistance in experiments on smectics.

Landau has shown[17] that, from the theoretical standpoint, the presence of facets on the surface of a crystal stems from a singular behavior of the surface tension of the facet as a function of the orientation of the plane of this facet. The dependence is in turn a consequence of the pres-

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ence of steps on the surface of the crystal. The same arguments apply to a facet on the surface of a smectic, so we will use Landau's ideas below.

For small values of the angle θ, between the plane of the facet and the smectic layers, the surface tension can be written as

$$\sigma=\sigma_0+bn. \tag{1}$$

Here n is the number of steps per unit length, which for small angles is given by

$$n=|\theta|/d,$$

where d is the distance between layers. The parameter b in (1) determines the excess energy associated with the presence of one step on the surface of the drop. The corrections to (1) for the interaction of steps at small values of θ, i.e., at a low step density n, can be ignored.

It follows from (1) that the value $\theta=0$ corresponds to a point at which the derivative of the function $\sigma(\theta)$ is discontinuous. We know that the linear size of a facet is directly proportional to the jump in the derivative $d\sigma/d\theta$, i.e., to the value of b/d (Refs. 17 and 18).

$$R\propto b/d. \tag{2}$$

Since the distance between layers in a smectic, d, is basically insensitive to the proximity to the transition point, the critical behavior of R is determined primarily by the critical dependence of the step energy b.

It is easy to see that an estimate of the quantity b will be the same as an estimate of the energy of an edge dislocation in the interior of a smectic, so a step may be thought of as an edge dislocation emerging at the surface. The energy of the dislocation, on the other hand, can be expressed in terms of the smectic's elastic moduli B and K (Ref. 19), which have a known critical behavior. The elastic energy of a smectic is

$$F_{el}=\int dV[\tfrac{1}{2}B(\nabla_{\parallel}u)^2+\tfrac{1}{2}K(\nabla_{\perp}^2u)^2]. \tag{3}$$

The subscripts $\parallel$ and $\perp$ in (3) mean the directions parallel and perpendicular to the director $\mathbf{n}$.

To calculate the energy of the dislocation we need to specify boundary conditions [e.g., $u(x\to-\infty)=0$, $u(x\to\infty)=d$] and to determine the distribution $u(\mathbf{r})$ corresponding to an extremum of the elastic energy. For our purposes it is sufficient to derive an estimate of the dislocation from dimensional considerations. The energy of a dislocation per unit length of the dislocation, f_{disl}, can evidently be estimated from

$$f_{disl}\sim\left(B\frac{u^2}{l_{\parallel}^2}+K\frac{u^2}{l_{\perp}^4}\right)l_{\perp}l_{\parallel}. \tag{4}$$

Using

$$Bl_{\perp}^4\sim Kl_{\parallel}^2,\quad u\sim d,$$

we easily find the following estimate of the radius of the facet:

$$R\sim\frac{b}{d}\sim\frac{f_{disl}}{d}\sim Bdl_{\perp}/l_{\parallel}. \tag{5}$$

The parameters $l_{\parallel}$ and $l_{\perp}$ in (5) can be estimated as the correlation radii

$$l_{\parallel}\sim r_{c\parallel},\quad l_{\perp}\sim r_{c\perp}.$$

If the nematic-smectic A phase transition is a second-order transition, the quantities B, $r_{c\parallel}$, and $r_{c\perp}$ have the following behavior near the transition point:

$$B\sim\tau^{\varphi},\quad r_{c\parallel}\sim\tau^{-\nu_{\parallel}},\quad r_{c\perp}\sim\tau^{-\nu_{\perp}}, \tag{6}$$

where $\tau=1-T/T_{N-A}$. Using

$$Bu^2/l_{\parallel}^2\sim\tau^{2-\alpha}\sim\tau^{2\nu_{\perp}+\nu_{\parallel}},$$

we find $\varphi=2\nu_{\perp}-\nu_{\parallel}$ for the critical exponent of the elastic modulus B. For the facet radius R we thus find the asymptotic behavior

$$R\sim\tau^{\nu_{\perp}}. \tag{7}$$

CONCLUSION

The experimental data indicate that the critical exponents for the nematic-smectic A transition often have the standard values for the universality class of the X–Y model.[14] We then find the following value of the critical exponent for R:

$$R\sim\tau^{\nu},\quad \nu\simeq0.67. \tag{8}$$

The value 0.45 ± 0.1 was found for the critical exponent of a facet radius by Bechhoefer *et al.*[15] They mentioned that this value is close in magnitude to the critical exponent for the elastic modulus B. As can be seen from (7), the critical exponents for the elastic modulus B and the face radius R are the same only in the case of isotropic scaling. The specific value found for the exponent in Ref. 15 is apparently not very accurate, since there were only a few experimental points, and they were scattered over an interval of 20°. If an anisotropic scaling prevails in the system, the exponent of the facet radius will no longer be universal, and it will depend on the values of the exponents for the correlation radii (Ref. 20, for example).

Expression (5) can be used to study a weak, first-order liquid-smectic phase transition; this transition was also studied in Ref. 15. For this transition the following estimates hold:

$$B\sim K\sim\langle\rho\rangle^2,\quad l_{\parallel}\sim\Delta^{-1/2}, \tag{9}$$

where Δ is the size of the gap in the correlation function of the short-wave density field, $\rho(\mathbf{r})=\Sigma_{\mathbf{q}}\rho(\mathbf{q})\exp(i\mathbf{qr})$,

$$\langle\rho(\mathbf{q})\rho(-\mathbf{q})\rangle=\frac{T}{\Delta+\alpha(q-q_0)^2}. \tag{10}$$

In the case of a weak first-order phase transition, the facet radius thus varies in accordance with

$$R\sim B^{3/4}K^{1/4}dl_{\parallel}^{-1/2}\sim\langle\rho\rangle^2\Delta^{1/4}\sim\Delta^{5/4}. \tag{11}$$

This result can be used to express the $R(\tau)$ dependence in terms of the $\Delta(\tau)$ dependence. The latter can be derived in weak-crystallization theory (for example) or extracted from x-ray measurements.

[1] P. G. de Gennes, Solid State Commun. **10**, 753 (1972).
[2] T. C. Lubensky, J. Chem. Phys. **80**, 31 (1983).
[3] B. I. Halperin and T. J. Lubensky, Solid State Commun. **14**, 997 (1974).
[4] T. C. Lubensky and J.-H. Chen, Phys. Rev. B **17**, 366 (1978).
[5] S. G. Dunn and T. C. Lubensky, J. Phys. (Paris) **42**, 1201 (1981).
[6] T. C. Lubensky, S. G. Dunn, and J. Isaakson, Phys. Rev. Lett. **47**, 1609 (1981).
[7] T. C. Lubensky and A. J. McKane, Phys. Rev. A **29**, 317 (1984).
[8] A. R. Day and T. C. Lubensky, Phys. Rev. A **30**, 481 (1984).
[9] M. A. Anisimov, V. P. Voronov, V. É. Podnek, and F. Kholmurodov, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 336 (1987) [JETP Lett. **45**, 425 (1987)].
[10] C. W. Garland, G. Nounesis, and K. J. Stine, Phys. Rev. A **39**, 4949 (1989).
[11] C. W. Garland, G. Nounesis, K. J. Stine, and G. Heppke, J. Phys. (Paris) **50**, 2291 (1989).
[12] P. Das, G. Nounesis, C. W. Garland, G. Sigaud, and N. H. Tinh, Liq. Cryst. **7**, 883 (1990).
[13] G. Nounesis, C. W. Garland, and R. Shashidhar, Phys. Rev. A **43**, 1849 (1991).
[14] X. Wen, C. W. Garland, and G. Heppke, Phys. Rev. A **44**, 5064 (1991).
[15] J. Bechhoefer, L. Lijcek, and P. Oswald, J. Phys. II **2**, 27 (1992).
[16] G. Wulf, Kristallografiya **34**, 449 (1901).
[17] L. D. Landau, *Collected Works* (ed. E. M. Lifshitz and I. M. Khalatnikov), Vol. 2, Nauka, Moscow, 1969, p. 119; L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Nauka, Moscow, 1976 (Pergamon, New York, 1980).
[18] M. Wortis, in *Chemistry and Physics of Solid Surfaces VII* (ed. R. Vanselow and R. Howe) Berlin, 1988, p. 367.
[19] P.-G. De Gennes, *Scaling Concepts in Polymer Physics*, Cornell U. Press, Ithaca, 1979.
[20] B. M. Ocko, R. J. Birgeneau, J. D. Litster, and M. E. Neubert, Phys. Rev. Lett. **52**, 208 (1984).

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