Research Article

Calculation of the Dielectric Constant as a Function of Temperature Close to the Smectic A-Smectic B Transition in B5 Using the Mean Field Model

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The temperature dependence of the static dielectric constant (ϵ) is calculated close to the smectic A-smectic B (S_A - S_B) transition ($T_c = 71.3^\circ\text{C}$) for the liquid crystal compound B5. By expanding the free energy in terms of the order parameter in the mean field theory, the expression for the dielectric susceptibility (dielectric constant) is derived and is fitted to the experimental data for ϵ which was obtained at the field strengths of 0 and 67 kV/cm from literature. Coefficients in the free energy expansion are determined from our fit for the S_A - S_B transition of B5. Our results show that the observed behaviour of the dielectric constant ϵ close to the S_A - S_B transition in B5 can be described satisfactorily by our mean field model.

1. Introduction

Various smectic phases which occur in ferroelectric liquid crystals are of interest to study close to the phase transitions. In the smectic A phase, the long axes of the liquid crystal molecules are parallel to the director which is perpendicular to the smectic layers. In the smectic C (or C^*) phase, those molecules are tilted (a tilt angle θ between the long axis and the director) and in the presence of the chiral molecules, the AC (or AC^*) transition becomes more interesting to study in ferroelectric liquid crystals. As in the smectic C (or C^*) phase, the molecules are tilted in the smectic G phase and it has been observed experimentally [1] that the transitions between the ferroelectric phases (smectic A-C, smectic A-G and smectic C-G) are influenced by an applied electric field. However, it has also been observed [1] that transitions between the nonferroelectric phases (smectic A-B, smectic B-E) are not influenced by an applied electric field. This has been demonstrated experimentally [1] for the nonferroelectric phases of smectic A, B, and E of compound B5 by measuring the temperature dependence of the dielectric constant at fixed field strengths.

Some theoretical models have been given in the literature to explain the transitions between the smectic phases. The mean field models where the free energy is expanded in terms of the order parameters with the coupling terms, have been used to analyze the experimental data. Regarding the spontaneous polarization P and the tilt angle θ , a bilinear coupling ($P\theta$) [1, 2] and biquadratic coupling ($P^2\theta^2$) [3–5] in the free energy expansion have been used in the mean field models for the smectic AC (or AC^*) transitions. In our earlier studies [6–10], we have also studied the mean field models with the $P^2\theta^2$ and $P\theta$ couplings for the AC (or AC^*) transitions in ferroelectric liquid crystals.

In this study, we focus on the smectic A-B transition in compound B5 and we analyze the experimental data [1] for the temperature dependence of the dielectric constant ϵ for constant electric fields of 0 and 67 kV/cm. For this analysis, we use our mean field model [6] with the biquadratic coupling between the order parameters (polarization P) and a long-range bond-orientational order [11] for the smectic A-smectic B transition in B5.

Below, in Section 2 we give our mean field model for the smectic A-B transition. In Section 3, our calculations and

results are given. We discuss our results in Section 4 and finally, conclusions are given in Section 5.

2. Theory

The smectic A-smectic B transition can be described by the free energy expanded in terms of the two-order parameters, namely, polarization P (smectic A and B phases) and a long-range bond-orientational order ψ (smectic B phase only) under an external electric field. Thus, the free energy can be written as

$$g = \frac{1}{2}\alpha\psi^2 + \frac{1}{4}b\psi^4 + \frac{1}{6}c\psi^6 + \frac{1}{2\chi_0\epsilon_0}P^2 - DP^2\psi^2 + \frac{1}{4}eP^4. \quad (1)$$

Here, $\alpha = a(T - T_c)$ where T_c is the transition temperature between the smectic A and B phases, χ_0 is a constant dielectric susceptibility, and ϵ_0 is the permittivity. a , b , c , and e are constants and D is the coupling constant in (1).

The temperature dependence of the polarization P and the bond-orientational order ψ can be obtained from the minimization of the free energy (1) with respect to P and ψ , which gives

$$\alpha + b\psi^2 + c\psi^4 - 2DP^2 = 0, \quad (2)$$

$$\frac{1}{\chi_0\epsilon_0} - 2D\psi^2 + eP^2 = 0, \quad (3)$$

respectively. Substituting (3) for P^2 into (2) then gives the free energy g in terms of the bond-orientational order parameter ψ only,

$$g = \frac{1}{2}\alpha'\psi^2 + \frac{1}{4}b'\psi^4 + \frac{1}{6}c'\psi^6 \quad (4)$$

with the new variables

$$\alpha' = \alpha + \frac{2D}{e\chi_0\epsilon_0}, \quad b' = b - \frac{4D^2}{e}, \quad c' = c. \quad (5)$$

Since (4) gives the free energy of the smectic B phase (in terms of the bond-orientational order parameter in this phase), the dielectric susceptibility χ_ψ can be obtained as a function of temperature by taking the second derivative of g with respect to the ψ , which gives

$$\chi_\psi^{-1} = a(T - T_c) + \frac{2D}{e\chi_0\epsilon_0} + a_1\psi^2 + a_2\psi^4, \quad (6)$$

where $a_1 = 3b'$ (5) and $a_2 = 5c'$.

In order to predict the temperature dependence of the reciprocal dielectric susceptibility χ_ψ^{-1} (6), a functional form of ψ is needed, which can be adopted from the molecular field theory [12] as follows:

$$\begin{aligned} \psi &\approx 1 - 2 \exp\left(-\frac{2T_c}{T}\right), \quad T \ll T_c, \\ \psi &\approx \left[3\left(1 - \frac{T}{T_c}\right)\right]^{1/2}, \quad 0 < T_c - T \ll T_c, \\ \psi &\approx 0, \quad T_c < T \end{aligned} \quad (7)$$

FIGURE 1: The dielectric constant ϵ calculated from (6) as a function of temperature for the smectic A-smectic B transition under the dielectric fields of 0 and 67 kV/cm for compound B5. The observed data [1] is also shown here.

for the long-range bond-orientational order parameter in the smectic B phase. Close to the smectic A-smectic B transition, a power law formula is valid, as given in (7).

3. Calculations and Results

We analyzed the temperature dependence of the dielectric susceptibility according to (6) which was fitted to the experimental data for the dielectric constant ϵ [1] ($\chi = \epsilon - 1$) close to the smectic A-smectic B transition in B5. In (6), we first calculated the temperature dependence of the order parameter ψ using the power-law formula (7) where the temperature for the smectic A-smectic B transition was taken as $T_c = 71.3^\circ\text{C}$ at zero electric field ($E = 0$) in B5. By fitting (6) to the experimental ϵ data [1], the fitted parameters a , a_1 and a_2 below T_c were obtained ($E = 0$), as given in Table 1. Similarly, (6) was fitted to the experimental ϵ data [1] for the electric field of 67 kV/cm close to the smectic A-smectic B transition with the fitted parameters (Table 1). Values of $2D/e\chi_0\epsilon_0$ were deduced from the experimental ϵ data [1] when $\psi = 0$ at $T = T_c$ (6). Since the transition temperatures are not induced by the external electric field for nonferroelectric phases [1], we took the same transition temperature ($T_c = 71.3^\circ\text{C}$) for 67 kV/cm in B5, as shown in Figure 1. Thus, we get the same fits (6) for the fixed bias field strengths of 0 and 67 kV/cm for the smectic A-smectic B transition in B5 (Figure 1). In the same manner, we analyzed the experimental data for the dielectric constant ϵ [1] according to (1) with $\psi = 0$ for $T > T_c$ using the fixed electric fields of 0 and 67 kV/cm. Values of the fitted parameter a are given within the temperature intervals in Table 2. This data is also plotted in Figure 1 with the observed data [1].

TABLE 1: Values of the coefficients according to (6) for the smectic A-smectic B transition below T_c within the temperature interval under the electric fields indicated for compound B5.

E (kV/cm)	T_c (°C)	a (°C ⁻¹)	a_1	a_2	$2D/e\chi_o\epsilon_o$	Temperature interval (°C)
0	71.3	0.056	1.16	1.70	0.172	70.14 < T < 71.24
67	71.3	0.057	1.13	2.53	0.173	70.06 < T < 71.29

TABLE 2: Values of the coefficients according to (6) for the smectic A-smectic B transition above T_c within the temperature interval under the electric fields indicated for compound B5.

E (kV/cm)	T_c (°C)	a (°C ⁻¹)	$2D/e\chi_o\epsilon_o$	Temperature interval (°C)
0	71.3	0.065	0.170	71.39 < T < 71.70
67	71.3	0.059	0.171	71.34 < T < 71.77

4. Discussion

We analyzed here the temperature dependence of the dielectric constant ϵ through the reciprocal dielectric susceptibility χ^{-1} (6) in our mean field model with the biquadratic ($P^2\psi^2$) coupling for the smectic A-smectic B transition in B5. As pointed out previously, transition temperatures are not shifted for the external electric fields of 0 and 67 kV/cm (Figure 1) due to the fact that the smectic A and smectic B phases are nonferroelectric of compound B5. For the ferroelectric transitions of smectic A-smectic C, smectic A-smectic G and smectic C-smectic G of compound A6, it has been observed experimentally [1] that the transition temperatures are shifted under various fixed field strengths. It has also been observed [1] that nonferroelectric phases (smectic B-smectic E) are not influenced by an electric field for this compound B5 studied here. Regarding nonferroelectric phases, in fact the smectic A phase at high temperatures occurs at zero electric field only since the external electric field induces a tilt angle which exists in the smectic C phase. The tilted smectic phase possesses a spontaneous electric polarization P_s if the molecules have a permanent dipole moment and they are chiral [13].

As shown in Figure 1, dielectric constant ϵ increases abruptly with the decreasing temperature near the smectic A-smectic B transition ($T_c = 71.3^\circ\text{C}$) of compound B5. This is due to the larger electroclinic effect in the smectic B phase [1].

As we pointed out previously, the dielectric constant (or dielectric susceptibility) was calculated as a function of temperature (6) from our mean field model with the biquadratic $P^2\psi^2$ coupling (1) for the smectic A-smectic B transition of compound B5 (Figure 1). In this model, the long-range bond-orientational order parameter ψ was considered as the primary order parameter and the polarization P as the secondary order parameter in the free energy expansion (1). With the biquadratic coupling ($P^2\psi^2$), quadrupolar interactions between the molecules are attributed to the mechanism of the smectic A-smectic B transition of compound B5 in our mean field model. Regarding the temperature dependence of the dielectric constant ϵ calculated from (6) which was fitted to the experimental data [1] as stated above, our mean field model describes the observed behaviour of ϵ satisfactorily for the smectic A-smectic B transition of compound B5.

This indicates that the main mechanism for this transition is due to quadrupole-quadrupole interactions which involve a long-range bond-orientational ordering in B5.

5. Conclusions

The dielectric constant ϵ was predicted using our mean field model with the biquadratic coupling $P^2\psi^2$ (P is the polarization and the ψ is the long-range bond-orientational order parameter) for the smectic A-smectic B transition for constant electric fields in compound B5. The predicted ϵ was fitted to the experimental data from the literature and the fitted parameters were determined for the smectic A-smectic B transition of compound B5. It was shown here that our mean field model describes the observed behaviour of the dielectric constant adequately for this transition of the liquid crystalline material studied here. The observed data also shows that the transition temperatures are not shifted under the electric field for this nonferroelectric transition.

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