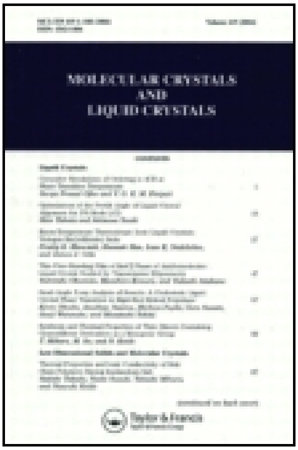

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New Measurement Method of Polar Anchoring Energy of Nematic Liquid Crystals

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New Measurement Method of Polar Anchoring Energy of Nematic Liquid Crystals

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On the basis of the concept used in the high-electric-field method reported by Yokoyama, we have developed a new measurement method of the polar anchoring energy of nematic liquid crystals. This method can derive the polar anchoring energy only by measuring the capacitance change against the applied voltage of a LC sample, and thus the method can be easily applied to measuring the polar anchoring energy of homeotropically-aligned samples. This paper presents the results of the computer simulation for verifying the developed method and also some experimental results of the polar anchoring energy for homeotropically-aligned samples.

Keywords: Nematic Liquid Crystal; Polar Anchoring Energy; Homeotropic Alignment

1. INTRODUCTION

Surface anchoring of nematic liquid crystals (LCs) on polymer films is one of the key issues for determining the electrooptical performance of LC devices, and thus many works on this subject have been done to clarify the alignment mechanisms of LCs on various substrate surfaces [1–5]. For these investigations, various methods to evaluate the surface anchoring energy were used. These methods may be classified into two groups according to the principle of deforming a LC medium [4]: one is a geometry type that uses conflicting surface LC alignment treatments for two substrate surfaces, and the other is an external-field type that utilizes an external field (electric, magnetic, and mechanical torque) to give a curvature stress to a LC medium. In most of these methods, the optical and/or

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electrical responses of a LC medium to a well-controlled external stress are measured, and the resulting data are analyzed by using a theoretical fit. This fitting procedure usually utilizes many material parameters, and the reliability of the obtained anchoring energy may depend strongly on the accuracy of the parameters used.

Yokoyama et al. proposed a new experimental method for estimating the polar anchoring energy of planar-aligned LC samples using a high electric field [3,4]. Since this high-electric-field (HEF) method does not use any theoretical fit and the procedure to derive the polar anchoring energy is very straightforward, this method can be considered to be more reliable than other methods. As described in their paper [3,4], the polar anchoring energy must be evaluated by the simultaneous measurements of the optical retardation and the capacitance of a LC sample as a function of the applied voltage, and thus the method is a little complicated and can not be applied to obtaining the polar anchoring energy of homeotropically-aligned samples [6].

In this paper, we present a new method (referred to as modified high-electric-field method) to measure the polar anchoring energy of LC samples, which is simpler than the original HEF method and is also applied to both for planar- and homeotropically-aligned LC samples.

2. THEORETICAL CONSIDERATIONS

Here we assume a homeotropically-aligned LC sample with zero pretilt angle and no twist deformation. The coordinate system used is shown in Fig. 1. The free energy per unit area of the LC medium between two identical substrate surfaces (gap:d and area:S) is written as

$$F = \frac{1}{2} \int_0^d \left[(K_1 \sin^2\theta + K_3 \cos^2\theta) \left(\frac{d\theta}{dz}\right)^2 + \frac{D_z^2}{\varepsilon_0(\varepsilon_1 \sin^2\theta + \varepsilon_2 \cos^2\theta)} \right] dz + 2f_s(\theta_s, \theta_p), \tag{1}$$

under the application of the electric field in the z direction, where K_1 and K_3 are Frank's elastic constants, ε_1 and ε_2, respectively, are the relative dielectric constants perpendicular and parallel to the director. θ represents the bulk tilt angle measured from the z-axis and depends only on the z coordinate. $f_s(\theta_s)$ is the surface-free energy density represented by the Rapini-Papoular-type formula, with

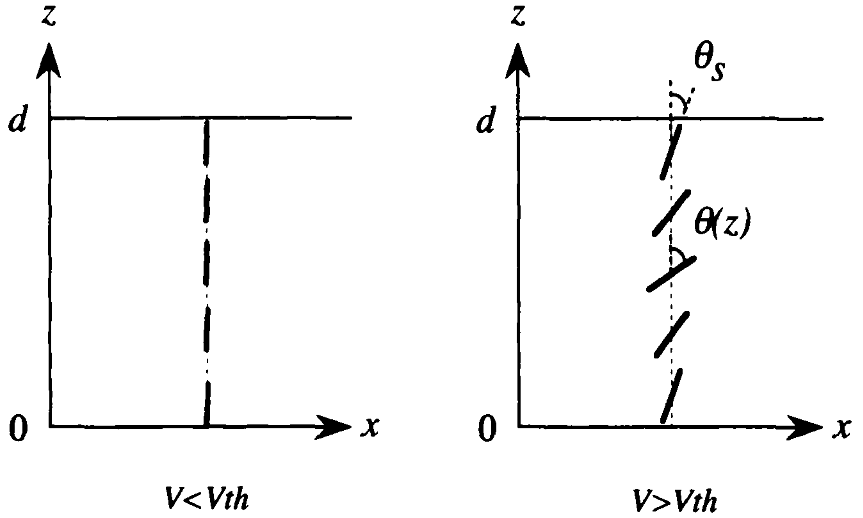

FIGURE 1 The coordinate system used in theoretical considerations. Vth is the threshold voltage, above which the deformation of a LC medium occurs

θ_S of the surface tilt angle. Other symbols used in Eq.(1) have conventional meaning. If θ_S is small, $f_S(\theta_S)$ may be well approximated by

$$f_s(\theta_s) = \frac{1}{2}A_\theta(\theta_s)^2, \tag{2}$$

where A_θ is known as the polar anchoring energy. Minimizing the free energy of Eq.(1) taking into account the finite anchoring conditions at the two substrate surfaces, the following two torque balance equations for the bulk and the surface are obtained

$$\frac{d}{dz}\left[(K_1\sin^2\theta + K_3\cos^2\theta)\left(\frac{d\theta}{dz}\right)^2 - \frac{D_z}{\varepsilon_z(\theta)}\right] = 0, \tag{3}$$

$$\frac{df_s(\theta_s)}{d\theta_s} = (K_1\sin^2\theta + K_3\cos^2\theta_s)\left.\frac{d\theta}{dz}\right|_{z=0}, \tag{4}$$

where $\varepsilon_z(\theta)$ is defined as $\varepsilon_0(\varepsilon_1\sin^2\theta+\varepsilon_2\cos^2\theta)$. By considering the symmetric director profile at a midplane (z=d/2) of the sample, Eq.(3) is rewritten as

$$\left(\frac{d\theta}{dz}\right)^2 = \frac{D_z^2\Delta\varepsilon}{K_3\varepsilon_0\varepsilon_2^2}\frac{\sin^2\theta_m - \sin^2\theta}{(1+\alpha\sin^2\theta_m)(1+\alpha\sin^2\theta)(1+\beta\sin^2\theta)}, \tag{5}$$

using the conditions of $\theta(d/2)=\theta_m$ and $d\theta/dz=0$ at $z=d/2$. Here $\Delta\varepsilon$, α and β are represented by $(\varepsilon_1-\varepsilon_2)$, $\Delta\varepsilon/\varepsilon_2$, and $(K_1-K_3)/K_3$, respectively. By combining Eqs.(4) and (5), the following equation is obtained

$$\frac{\mathrm{d}f_s(\theta_s)}{\mathrm{d}\theta_s}=\frac{K_3}{d_c}\sqrt{\frac{\cos^2\theta_s(1+\beta\sin^2\theta_s)}{(1+\alpha\sin^2\theta_m)(1+\alpha\sin^2\theta_s)}}, \qquad (6)$$

where d_c is the electric coherence length defined by $\varepsilon_2(\varepsilon_0 K_3/\Delta\varepsilon)^{1/2}/D_z$, and we only consider the LC deformation in the lower half region $(0<z<d/2)$. If θ_s is small, Eq.(6) may be rewritten using Eq.(2) as

$$\theta_s=\frac{d_e}{d_c}\frac{1}{\sqrt{(1+\alpha\sin^2\theta_m)}}. \qquad (7)$$

Here d_e is known as the extrapolation length and is defined by K_3/A_θ.

Gruler et. al. reported the relationship between the applied voltage V and the capacitance C of a LC sample assuming strong anchoring conditions [7,8]. In the case of the finite anchoring, the surface tilt angle θ_s is varied as the applied voltage V is changed. Therefore, the applied voltage and the capacitance of the sample may be governed by the following two equations;

$$\frac{V}{V_{th}}=\frac{2}{\pi}\sqrt{1+\alpha\sin^2\theta_m}\cdot\int_{\theta_s}^{\theta_m}\sqrt{\frac{1+\beta\sin^2\theta}{(1+\alpha\sin^2\theta)(\sin^2\theta_m-\sin^2\theta)}}\mathrm{d}\theta, \qquad (8)$$

$$\frac{C}{C_0}=(1+\alpha)-\alpha.\frac{\int_{\theta_s}^{\theta_m}\sqrt{\frac{(1+\alpha\sin^2\theta)(1+\beta\sin^2\theta)}{(\sin^2\theta_m-\sin^2\theta)}}\cos^2\theta\mathrm{d}\theta}{\int_{\theta_s}^{\theta_m}\sqrt{\frac{1+\beta\sin^2\theta}{(1+\alpha\sin^2\theta)(\sin^2\theta_m-\sin^2\theta)}}\mathrm{d}\theta}, \qquad (9)$$

where $V_{th}=\pi(K_3/\varepsilon_0\Delta\varepsilon)^{1/2}$, and C_0 stands for the capacitance without the external field.

Let us now consider the case in which the applied voltage *V* is so high that θ_m is well approximated by $\pi/2$ but weak enough to assure $\theta_s\ll 1$. As discussed by Yokoyama [3,4], this situation is satisfied in the case of $d\gg d_c\gg d_e$, so Eq.(9) may become

$$\frac{C}{C_0}=(1+\alpha)-\frac{2\alpha\sqrt{1+\alpha}}{\pi}\frac{V_{th}}{V}[I(\alpha,\beta,0)-\theta_s], \qquad (10)$$

using Eq.(8). Here $I(\alpha,\beta,0)$ is represented by

$$I(\alpha,\beta,0)=\int_0^{\pi/2}\sqrt{\frac{1+\beta\sin^2\theta}{1+\alpha\sin^2\theta}}\cos^2\theta\mathrm{d}\theta,$$

which depends only on the LC material parameters. After some rearrangements of Eq.(10) using Eq.(7) and the relations of $SD_z=CV$ and $C_0=\varepsilon_0\varepsilon_2 S/d$, we finally get the following equation

$$\frac{C_0}{C} = \gamma I(\alpha,\beta,0)\frac{C_0}{CV} + \left(\frac{1}{1+\alpha} - 2\frac{\alpha}{1+\alpha}\frac{d_e}{d}\right), \tag{11}$$

where $\gamma=(2\alpha V_{th}/\pi)/(1+\alpha)^{1/2}$. Equation (11) tells us that, if the voltage range applied to a LC sample satisfies the conditions of $\theta_s \ll 1$ and $\theta_m \approx \pi/2$, the C_0/C vs. C_0/CV plot shows a linear relationship. And if the straight line with the slope $\gamma I(\alpha,\beta,0)$ is extrapolated to the C_0/C axis, the extrapolating value gives the extrapolation length d_e when the parameters of α and d are known. Note that this equation can be also applied to planar samples by exchanging ε_1 and ε_2, so the equation is more useful to obtain the polar anchoring energy of LC samples than the HEF method proposed by Yokoyama et al [3,4].

3. RESULTS AND DISCUSSION

Computer simulation is carried out for homeotropically-aligned samples to verify the developed method. The cell parameters used are shown in Table I.

TABLE I Cell parameters used in the simulation

Parameters	*Value*
Relative Dielectric Constant	$\varepsilon_1=9$
	$\varepsilon_2=4$
Elastic Constant (J/m)	$K_1=13.0\times10^{-12}$
	$K_3=15.0\times10^{-12}$
Pretilt Angle (deg.)	$\theta_p=0$
Cell Thickness (μm)	20, 60
Extrapolation Length (nm)	0, 50, 100, 200

In Fig. 2, the applied voltage dependences of the tilt angle at a midplane of the LC medium and the surface tilt angle are shown, where the cell thickness of 60 μm and the extrapolation length of 50 nm were assumed. In a high electric field region ($V>4V_{th}$), the tilt angle is almost equal to 90 deg. (parallel to the substrate surface), and the surface tilt angle is enough to satisfy the condition of $\theta_s \ll 1$, so the voltage range of 8V~25V can be used to derive the polar anchoring energy of this simulated sample.

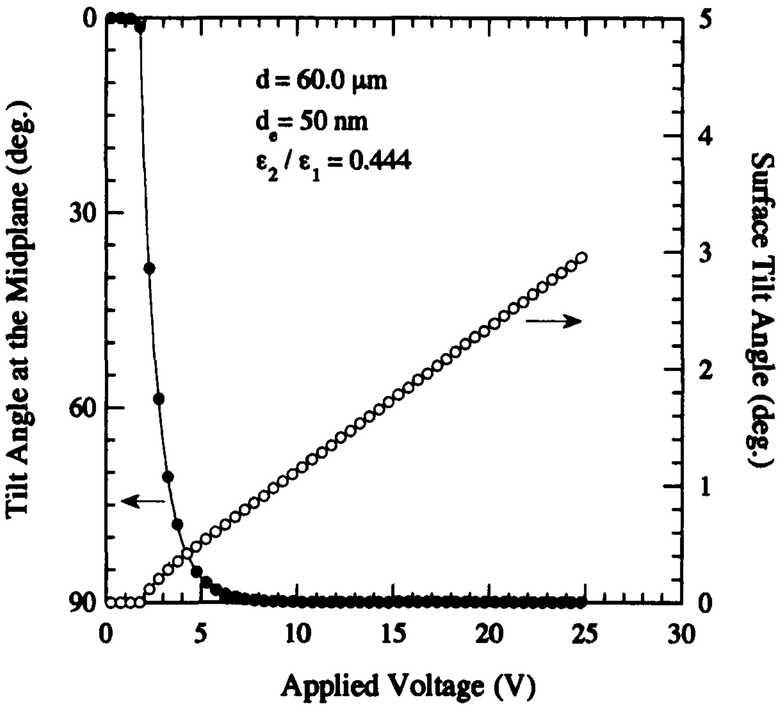

FIGURE 2 Variations of the tilt angle at a midplane (closed circle) and the surface tilt angle (open circle) of a LC medium are calculated as a function of the applied voltage

We then simulated the C_0/C vs. C_0/CV characteristics varying the extrapolation lengths of 0, 50 and 200 nm by keeping the cell thickness of 20 μm. As seen in Fig. 3, an excellent linearity of the plots is observed and a decrease in the extrapolation length shifts the extrapolating point to a higher value. This upward shift of the plot with decreasing the extrapolation length is easily understood by seeing Eq.(11). From these extrapolating values, we derived the extrapolation length for each simulated result. The obtained extrapolation lengths are 0, 49.5 and 185 nm, which are within a 10% error of those used in the simulation (0, 50, and 200 nm).

Figure 4 shows the cell thickness dependence of the C_0/C vs. C_0/CV characteristics with the extrapolation length of 100 nm. With increasing the cell thickness from 20 μm to 60 μm, the C_0/C vs. C_0/CV plot shifts upward, which means that a thicker sample behaves like a stronger anchoring sample than a thinner one even if both samples have the same anchoring energy. This behavior is also predicted by Eq.(11).

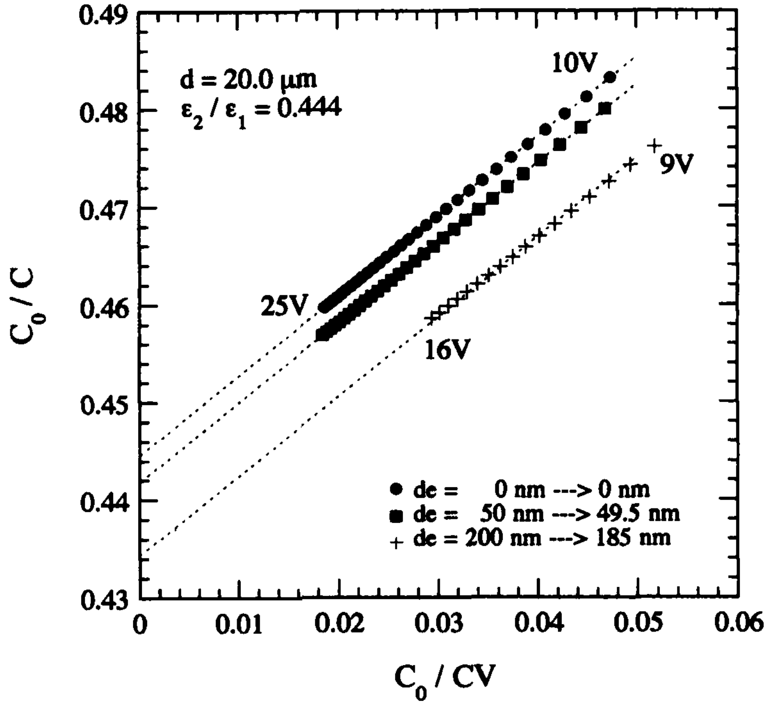

FIGURE 3 Simulated C_0/C vs. C_0/CV plots for the samples with various extrapolation lengths. The cell thickness of 20 μm is assumed

From these simulated results, we can verify that Eq.(11) is very reliable and useful to measure the polar anchoring energy of LC samples.

In order to measure the polar anchoring energy of homeotropically-aligned LC samples using Eq.(11), we fabricated sandwich-type LC cells, in which, for promoting homeotropic LC alignment, the ITO-coated glass-substrate surfaces were coated with 40nm-thick JALS-204-R55 (JSR) treated thermally at 180 °C for 1 hour. The liquid crystal used was MLC-2038 (Merck) with negative dielectric anisotropy (ε_2-ε_1<0), and it was injected into the empty cell via a capillary action in the isotropic phase.

The thickness of the sample was estimated using the interference spectroscopy, and then the capacitance was measured by a capacitance meter (HP-4284A) using a sinusoidal voltage of 10 KHz. From this capacitance measurement, the temperature dependence of the polar anchoring energy of the sample was estimated using Eq.(11); we used two samples with identical surface treatments but

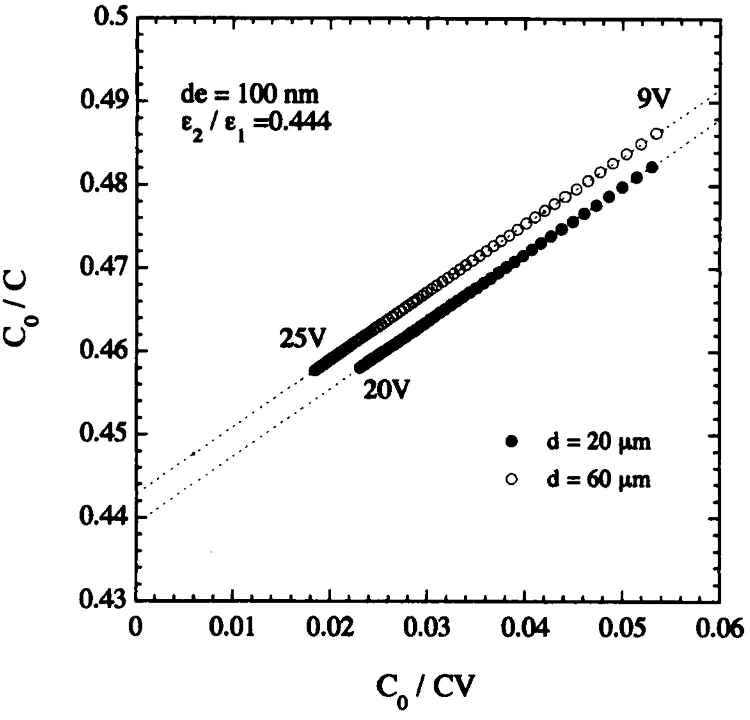

FIGURE 4 Simulated C_0/C vs. C_0/CV plots for samples with different thicknesses of 20 μm (closed circle) and 60 μm (open circle). The extrapolation length is assumed to be 100 nm

with different cell thicknesses of about 14 μm and 60 μm, and the resulting two extrapolating values obtained from the two samples were utilized for deriving the extrapolation length d_e and $\alpha=\Delta\varepsilon/\varepsilon_2$. The polar anchoring energy $A_\theta=K_3/d_e$ was then calculated by using the elastic constant K_3 estimated from the threshold voltage.

Figure 5 shows the C_0/C vs. C_0/CV plots for the two homeotropically-aligned samples at the temperature of −50 °C from the clearing point (80 °C). As seen in this figure, these two plots show an excellent linearity with the same slopes, and the plot for the thicker sample shifts upward with respect to that for the thinner one, which is consistent with the simulated result (Fig. 4). The extrapolating values obtained for the two samples were 0.4749 (60.4 μm) and 0.4659 (14.2 μm), and thus the resulting extrapolation length can be calculated to be 160 nm. By using the elastic constant $K_3$of $1.482\text{x}10^{-11}$ J/m estimated from the threshold voltage, the polar anchoring energy of $9.3\text{x}10^{-5}$ J/m^2 is obtained.

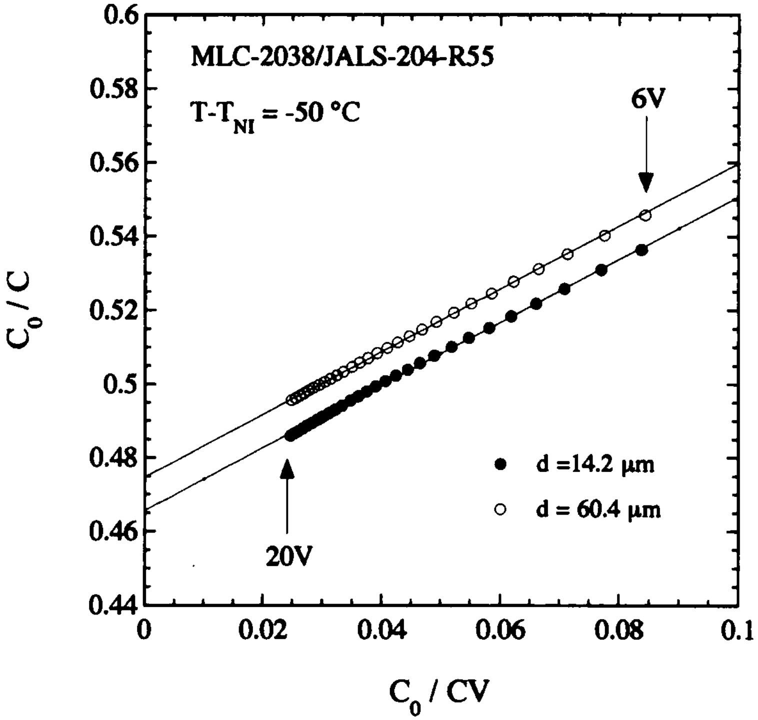

FIGURE 5 Measured C_0/C vs. $C_0/(CV)$ plots for two homeotropically-aligned samples with different thicknesses of about 14 μm (closed circle) and 60 μm (open circle)

In Fig. 6, we show the overall behavior of the temperature dependence of the polar anchoring energy for a homeotropically-aligned sample. The polar anchoring energy of the sample gradually decreases with increasing the sample temperature, and near the clearing point the anchoring energy becomes almost one order of magnitude lower than that at room temperature. The polar anchoring energy obtained in this study is almost the same order of magnitude as that reported in Yang's work [1] using a homeotropically-aligned sample but about one order of magnitude lower than conventionally rubbed polymer samples [5].

CONCLUSION

The modified high-electric-field method was developed and was examined by computer simulation for verifying the reliability of the method. The simulated

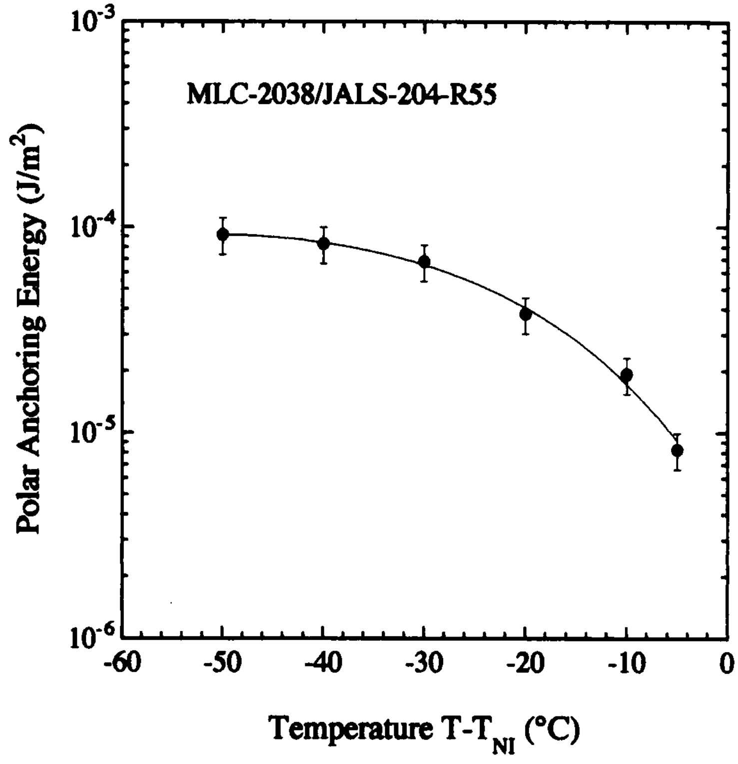

FIGURE 6 Temperature dependence of the polar anchoring energy of a homeotropically-aligned sample. The polar anchoring energy of the sample gradually decreases with increasing the sample temperature

results for homeotropically-aligned samples demonstrated that the present method was very useful for measuring the polar anchoring energy of LC samples. This method was then applied to the measurement of the polar anchoring energy of a homeotropically-aligned sample, and the polar anchoring energy obtained ranged from 10^{-4} J/m^2 to 10^{-5} J/m^2, which showed the negative dependence on the sample temperature.

From this study, it was demonstrated that the modified high-electric-field method is useful and reliable to measure the polar anchoring energy not only for homeotropically-aligned samples but also for planar-aligned samples.

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