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Ellipsometry Studies of 3D Orientational Structures in Thin Liquid Crystal Layers

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We studied the director configuration in thin liquid crystalline layers of 5 CB using a null ellipsometry technique. Liquid crystal (LC) material was spin- coated on polyimide (PI) substrates. The influence of different treatment of PI substrates on the director configuration was investigated. The PI substrates without additional treatment provide homeotropic LC alignment. The UV irradiated substrates provide the formation of biaxial (fan-like) LC structure that is symmetric with respect to the film normal. The rubbed PI substrates provide the splayed optic axis distribution with the average tilt angle of 25° with respect to the film normal.

Keywords: liquid crystal; director distribution; ellipsometry

INTRODUCTION

The studies of orientational structure of LC layers are very important for their application in modern liquid crystal displays (LCD). The structure of thin liquid crystalline films can be described if one considers a 3 dimensional molecular distribution. However, only few experimental techniques can provide the information about the distribution of the liquid crystal director or optic axis within the film thickness. They are associated with absorption [1-3] and birefringence [4] measurements of the ordered films.

In this work we applied a transmission ellipsometry technique that was previously used by us for studies of polymer films [5,6]. As the objects of investigation we used thin LC layers coated on PI alignment substrates. One of the possible applications of these films is for alignment layers [7], thus, the knowledge of the film structure is very important.

EXPERIMENTAL

Samples

The nematic LC 4-pentyl-4'-cyanobiphenyl (5CB) was dissolved in hexane at the concentration of 0.5% by weight. The solution was spin coated on glass slabs covered with PI 3510 polyimide by Dupont Inc. The centrifuging velocity and time were 2500 rpm and 30 s, respectively.

We used three types of PI substrates:

1) PI substrates without additional treatment;
2) PI substrates rubbed uniformly;
3) PI substrates irradiated with polarized UV light. (For irradiation we used a Xe lamp and a dichroic UV polarizer, both from Oriel Inc.).

Method

We used the null ellipsometry technique with the fixed orientation of the polarizer at 45° to horizontal and a quarter wave plate in the analyzing part of the ellipsometer that has its optic axis parallel to the transmission axis of the polarizer (Fig.1). When the birefringent sample is in the system, the minimum light leakage is observed at a certain analyzer angle φ. The value of φ was measured for different incidence angles θ of the testing beam of He-Ne laser (λ=630 nm). The measurements were carried out for both horizontal and vertical position of the easy axis of LC.

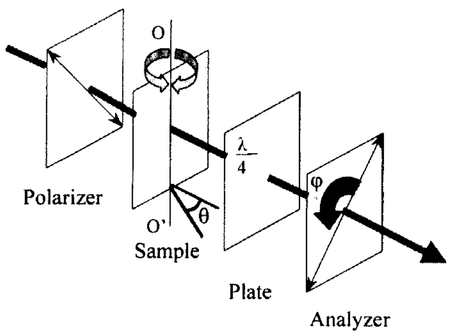

FIGURE 1 Scheme of null ellipsometry set up

The experimental φ versus θ curves were compared with the results of modeling for which φ was calculated from the Maxwell's equations for light propagation through a multi-layered medium. We modeled 3 types of birefringent media: biaxial, with two principal dielectric axes coinciding with the plane of the film; uniaxial, with arbitrary tilt angle for optic axis; and layers with splayed optic axis. The comparison between the measurement and the model provided information about the relationship between three principal refractive indices and the distribution of the optic axis. Knowing the optic axis distribution within the film, one can determine the average director distribution, i.e. planar, homeotropic, or splayed. Details of the method can be found in our previous publication [5].

RESULTS AND DISCUSSION

In order to separate birefringence effects from the LC layer and the alignment layer, we measured phase retardation of PI films before covering with LC. Results of these measurements are presented in Fig.2. All types of used PI substrates are isotropic. Thus, the birefringence effects originate from ordered LC layers.

The φ versus θ curves obtained for the LC layer coated on the non-treated PI substrate are presented in Fig.2. The results of modeling show that the film is a positive birefringent medium with the optic axis along the film normal. The value of birefringence is about $(n_e-n_o)d$=20nm. Thus, the LC molecules on the untreated PI substrates form homeotropic structures on average. Using the birefringence value for 5CB n_e-n_o=0.2 [8] and assuming the same order parameter for the film as for the bulk 5CB, one can estimate the thickness of the film which is about 100 nm in our case.

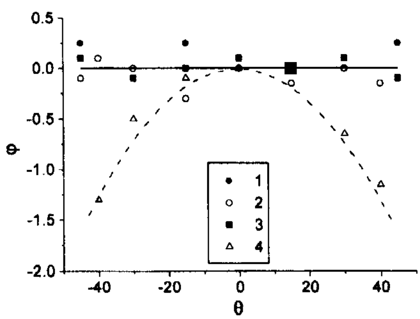

FIGURE 2 Curves φ vs θ; 1-not-treated PI film; 2- rubbed PI film; 3-irradiated PI film; 4 -5CB layer coated on the non-treated PI film.

The experimental φ versus θ curves for LC layer coated on the photo-irradiated PI substrate are presented in Fig.3 (curves 1 and 1'). The indexes 1 and 1' correspond to horizontal and vertical position of the easy axis of LC, respectively. Curve fitting gives a biaxial medium with the following relationship between three principal refractive indices: $(n_y-n_x)d=2$ nm, $(n_z-n_x)d=20$ nm, $n_x<n_y<n_z$.. The highest index is observed along the film normal, thus, indicating the preferential out-of-plane molecular alignment. The film possesses small in-plane birefringence. Thus, some molecules are slightly tilted out of the normal direction. The higher in-plane index was found in the direction that is perpendicular to the polarization direction of the actinic UV light E_{exc}. The possible molecular structure is presented in Fig.4a. We suggest a fan-like molecule distribution with preferential out-of-plane alignment. The structure is symmetric with respect to the film normal.

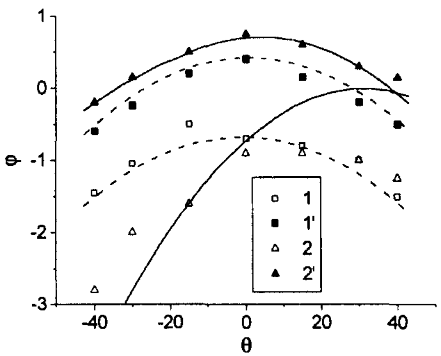

FIGURE 3 Curves φ vs θ for LC layers coated on PI substrates of different treatment. 1 and 1'-photoirradiated PI substrate; 2 and 2' -rubbed PI substrates.

The measured φ versus θ curves for LC layer coated on the rubbed PI substrate are presented in Fig.3 (curves 2 and 2'). The direction of higher in-plane index is along the rubbing direction. Curve asymmetry could be associated with a molecular distribution that provides tilted optic axis or biaxial structures that have principal dielectic axes at some angle to the film substrate. The latter case could not be modeled with

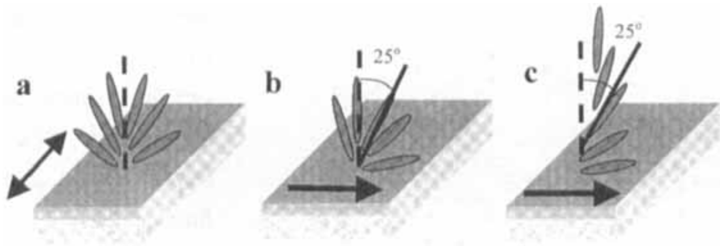

FIGURE 4. Possible distribution of LC director in LC layers coated on UV irradiated (a) and rubbed (b and c) PI substrates.

our existing simulation program. However, the modeling of the film as a uniaxial medium with tilted optic axis gives qualitatively reasonable results (Fig.3). The fitting gives $(n_e-n_o)d=23$ nm and the tilt angle for the optic of 25° from the film normal. The similarity between the 2 cases of LC alignment by rubbed and UV irradiated PI substrates suggests the molecular distribution presented in Fig.4b. The results of UV absorption measurements also confirm these results [3]. However, very similar phase shifts can be obtained for the splayed films with the average tilt angle of 25 deg shown in Fig. 4c. The splay can be induced by different anchoring at the film boundaries. We measured the pretilt angle generated by PI by measuring the pretilt in a 20 μm thick cell fabricated with the same PI substrates as we used for the films. For the measurements, we used the crystal rotation method described in [9]. We found that the rubbed PI provides 2^0 pretilt angle for 5CB. The irradiated PI provides a smaller pretilt angle of 0.5°. Thus, both substrates provided planar boundary conditions. Contrarily, air provides homeotropic alignment of thick 5CB layers [10].

The resultant director configuration in the film will be influenced by the boundary conditions at the film-PI and film-air interfaces. All the studied films demonstrate preferable out-of-plane alignment that can be associated with strong air anchoring. Weak anchoring of the UV irradiated PI provides some rotation of the LC molecules in the plane that is perpendicular to the polarization direction of UV light. This effect gives rise to small in-plane birefringence. The stronger anchoring of rubbed PI substrate provides possible director tilt or splay in the plane along the rubbing direction. The angle for the average optic axis is about 25^0 calculated from the film normal.

CONCLUSION

We studied the director distribution in thin LC layers coated on various PI substrates by using the null ellipsometry technique. We found that the structure of the LC layers coated on PI substrates strongly depends on the treatment of the PI. Untreated PI substrates provide weak and, possibly, degenerate in-plane alignment. The resultant LC structures on untreated PI feature homeotropic alignment. Photo-irradiated polyimide substrates also provide almost homeotropic molecular alignment. However, the irradiation of the substrate provides a favorable direction in the plane of the film, giving rise to some small in-plane retardation. The resultant structure may be pictured like an unopened fan with the axis of symmetry along the film normal. Rubbed polyimide substrates provide tilted alignment on average. However, taking into account strong air anchoring and relatively strong anchoring provided by rubbed PI, the most probable is the splayed director distribution with the average tilt angle of 25 degrees.

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