Rubbing-free Planar Alignment of Nematic Liquid Crystal on Organic Single Crystal Rubrene

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Keywords: Rubbing-free, Liquid crystals, Single-crystal rubrene, π - π electron stacking, Van der Waals.

ABSTRACT

High-quality LC alignment on organic SCR has been examined and used to manufacture rubbing-free LC devices. Here, the first contact geometry of the LCs in the SCR determines LC orientation. SCR cell performs wider thermal tolerance, better electrical stability, Higher VHR, faster switching time, and lower operating voltage.

1 Introduction

Liquid crystals (LCs) are essential in today's communication and photonic technology. However, high-quality alignment control of LCs for ultrahigh-definition large-sized displays is a difficult challenge. A traditional rubbing approach has clear difficulties producing large displays with small pixel sizes and an uneven inner surface, dust particles, and electrostatic charges.

Organic single-crystal rubrene (SCR), as a typical ptype organic semiconductor material, held high field-effect mobility (20 cm²/V s) [1], thus enabling organic molecules to assemble into well-ordered structures via van-der Waals (vdW) interactions. At the same time, random heterogeneous nucleation processes are minimized [2]. The present article reports the LC orientation on organic SCR-based LC cells. LC alignment on SCR can be determined with contact geometry while the LC molecule first contacts with SCR. For SCR-based LC cells, rubbingfree treatment shields the cell from electrostatic charges, dust contamination, and surface degradation. Thermal stability and electric field recovery test of the SCR-based LC cell has been established by polarized optical microscope (POM) and voltage vs. transmission (V-T). The advantages of SCR-based LC cell include excellent thermal and electrical stabilities, lower operation voltage, lower voltage holding ratio (VHR), and fast response time. Furthermore, unlike conductor Graphene, semiconductor SCR simultaneously can act as alignment and high resistivity layers, particularly for modal LC lens application.

2. Experimental procedure

In this work, 5,6,11,12-tetraphenylnaphthacene (rubrene) powder was dissolved in toluene. The rubrene solution was spin-coated on the ITO glass substrate. Immediately the substrates were placed on the hot plate

at 170 °C for 1 minute; an amorphous rubrene film was instantaneously changed into a highly ordered SCR thin film by an abrupt heating method. In this experiment nematic LC was used. A 3-µm-thick empty cell was prepared with two ITO substrates deposited with SCR (or polyimide (PI)).

3. Results and discussion

Fig 1a shows that after annealing, the highly crystalline nature of the SCR had an orthorhombic structure with unit cell parameters of a = 26.43, b = 7.08, and c = 14.18 Å [1]. Moreover, the X-ray diffraction (XRD) pattern of orthorhombic SCR was calculated using the Vienna Ab Initio Simulation Package (VASP), which is consistent with the measured XRD pattern. Furthermore, orientation geometry reveals that the distance between LC molecule and rubrene was ~5 Å calculated by VASP (Fig 1b). The small distance maximizes the π - π electron stacking and vdW interactions. The vdW interaction is caused by the rubrene tetracene (*ortho* and *para* positions in Fig 1b) undergoing a nucleophilic aromatic substitution on the cyanide group of the LC.



Fig.1. (a) XRD pattern of SCR film; (b) calculated geometry between the LC molecule and rubrene.

LC molecules can be oriented macroscopically in the SCR LC cell through capillary flow. As shown in Fig 2a-c, the POM images demonstrate the LC alignment with different capillary flow directions. Opaque (Bright) images appear when the capillary flow is perpendicular or parallel (45°) to the transmission axis of the polarizer. Confirming that LC molecules are aligned along the LC capillary flow directions (i.e., flow direction when they first contact with SCR) [3]. According to Fig. 2d, which depicts a change in intensity from bright to dark (or dark to bright) every 45°, SCR causes a planar LC alignment due to the capillary flow and the strong interactions between the LC molecule and rubrene.



Fig. 2. (a-c) POM textures of LC alignments in the 0.5wt% SCR LC cells are obtained with various directions of capillary flow. (d) The intensity of the POM image as a function of the sample rotation angle. Polarizer (P), analyzer (A), and capillary injection (I).

To examine the thermal tolerance of the LC orientation the SCR and PI LC cells were heated to a maximum temperature (T_{max}) and cooled to room temperature. T_{max} was higher than the clearing point T_{NI} (64 $^\circ C). As shown in$ Fig 3(a and b), when T_{max} was 180°C, the initial alignment was ideally recovered. Though, when T_{max} was increased to 200°C, the memory effect gradually weakened. Finally, the T_{max} reached 220°C the initial alignment of the PI cell was almost eliminated. In contrast, when the cell is rotated from 45° to 90°, the POM image of the SCR LC cell still undergoes a transition from bright to dark, despite the defect domains appearing at 220°C, which implies the strong anchoring nature of LCs on SCR by the vdW and π - π electron stacking interactions between the LC molecule and rubrene. The polar anchoring energy of LCs on SCR and PI were measured as 3.3 and 1.7 \times 10⁻⁴ J/m², respectively. As a result, the LCs on SCR may be thought of as strong anchoring than rubbed PI layer, and it can clarify the LC orientation conserved in the heating test up to 220°C [3]. Even after several months, LC alignment on SCR remains unchanged, indicating the durability of LC alignment on SCR.



Fig. 3. Thermal tolerance tests of (a) PI, (b), 0.5wt% SCR LC cells: Rubbing direction(R), capillary injection (I).

The electro-optical properties of the PI and SCR LC cell (Fig 4a). The V-T curve of the SCR LC cells shifts toward the low-voltage side, indicating that rubrene coating reduces the operating voltage of the cell. Moreover, after applying several voltage cycles, the LC alignment on SCR keeps identical. Fig 4b shows that the 0.5wt% SCR cell offers a high VHR due to the free-ions trapping by the SCR substrate. The fall time of the PI (2 wt.% SCR) cell has 6.94 ms (4.3ms) because SCR cells decrease in rotational viscosity of the LC mixture. Furthermore, the resistivities of ITO electrodes deposited with PI, 2 wt% SCR, were measured at ~ 10 and 4 Ω m, respectively.



Fig. 4. (a) V-T curve and (b) VHR of PI and SCR LC cells.

4. Conclusions

The LC alignment on SCR is determined with the capillary flow by π – π electron stacking and vdW interactions. The SCR LC cell has excellent thermal and electrical stabilities, faster switching, lower operation voltage, and higher VHR. These exciting and unique aspects of LCs on SCR offer a novel possibility for rubbing-free LC devices. SCR-based modal LC lens has been studied in progress.

5. Acknowledgments

The funding was supported by MOST-110-2112-M-018-009 and MOST-111-2811-M-029-008 Taiwan.

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