Rational Analysis of Self-Alignment Force of Reactive Additive Monomer with Multiple Methods

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Abstract. Analysis self-alignment force (SAF) of reactive self-assembly additive monomer is highly valuable in self-alignment vertical alignment mode (SAVA), because this force directly influences performance of optoelectronics device. In this work, SAF has been studied by multiple methods, such as atomic force microscopy, Mueller matrix imaging polarimeter. Reactive additive monomer and LC molecular were immobilized on the surface of an AFM probe and ITO, respectively. Due to the complexity of the additive monomer-hydroxy, additive monomer-LC molecular interaction, parallel experiments were designed to discriminate specific interactions. The difference of pretilt angle between TFT side and CF side also reveals the difference of SAF at various structure cell. The additive with strong SAF showed well alignment state after forming into optoelectronic device.

1. Introduction

In recent years, the profound impact of alignment layers in liquid crystal (LC) cell on the improvement of LC display (LCD) applications has attracted enormous attention[1-3]. Thus, alignment of LC molecular along a preferred direction plays an important role in the fabrication of LC cell[4]. Controlling LC alignment by regulating interfacial properties becomes significant in both academic field and engineering application. At present, the most conventional methods is mechanical rubbing on the substrate, the other is using polyimide (PI) material as alignment layer[5-7]. However, PI alignment film always requires time-consuming fabrication with uncertain side defect. It has hindered the development of new technologies, such as narrow frame design. Therefore, it is necessary to develop a new self-alignment technology in LCD to avoid side defect risk, cost down, enhance performance and promote the development of new technologies.

Recently, many researches reported various types of additive adding into LC molecular as self-alignment additive to replace conventional PI layers, such as nanoparticles (POSS), polymer monomer, etc[8-10]. However, there is less report on additive alignment force, so far. Additive alignment force can only be tested after fabricating in cell. Therefore, it is necessary to develop a rapid and efficient route for analysing of additive alignment force.

In this report, we developed multiple methods to analysis self-alignment force of reactive additive monomer. The interaction between additive and ITO substrate was investigated using AFM. Through chemical modification, we immobilized additive monomer by covalent bonds on the surface of AFM probe. We designed parallel experiments to discriminate specific interactions among the complex additive-substrate/additive-LC interactions. We derived nonspecific interaction values from the observed force curves. Furthermore, the properties of different types of additive monomer were compared by measuring pretilt angle of TFT side and CF side, respectively. The additive with strong alignment force also showed well alignment state after forming into optoelectronic device.
2. Results and discussion

As figure 1a shown, a schematic diagrams of the difference structure between PSVA and SAVA mode. The additive monomer plays a role in SAVA mode to replace PI alignment layer in PSVA mode. To further analysis additive’s alignment force, a schematic diagram of self-alignment additive molecules’ interfacial action between ITO substrate and LC molecules, as shown as figure 1b. The alignment force of reaction additive monomer contains intermolecular force between LC molecule and additive monomer, hydrogen bonding force between ITO substrate and additive monomer.

![Figure 1](image)

Figure 1  a, schematic diagrams of the difference between PSVA mode and SAVA mode; b, a schematic diagram of self-alignment additive molecules’ interfacial action between ITO substrate and LC.

To evaluate the influence of the parameters to self-alignment force, a series of analytic strategies were employed, as shown as Figure 2. The road-map of analytic self-alignment force contains analytic factor, analytic strategy, analytic scheme. In this report, AFM was employed to test intermolecular force between additive and different substrate (ITO substrate, LC modified substrate). The pretilt angle of TFT side and CF side will be different at one side using PI alignment layer and the others using additive self-alignment layer. Self-alignment force of different types additive was also characterization analysis by pretilt angle due to the difference between PI layer and additive self-alignment layer. Meanwhile, hydrogen bond energy between additive monomer and hydroxy was calculated by simulating computation. The optical images reveal additive alignment force by observering alignment state of different types of additive monomer formed optoelectronic device.

Intermolecular force between additive molecular and different substrate surface can be measured by AFM. In this experiment, additive molecular was modified on the surface of AFM probe by following actions as shown as scheme 1. Firstly, AFM probes were cleaned surface by EUV exposing (313 nm). After EUV treatment, the surface of probes were rich in hydroxyl groups. Secondly, put the treated probes in additive solution and exposed by UV light (365 nm). The reactive additive molecular were reacted with hydroxyl groups to modify on the surface of probes. Finally, removed excess solution and dried in N2 atmosphere.
Figure 2 The road-map of analytic factors, analytic strategys, analytic shceme diagrams of self-alignment force.

Scheme 1 Synthetic route for modified AFM probes for testing intermolecular forces, involving AFM probe’s surface treatment with EUV light, further interface additive molecular aggregation on the surface of AFM probes, finally removal of solvent via drying in N2.

Figure 3 shows typical force curves when additive molecular retracted from the ITO substrate or LC-immobilized ITO substrate by withdrawal of additive molecular-immobilized AFM probes, scheme as figure 3a,b shown. Two different kinds of additive molecular were employed to immobilize AFM probes, respectively. The modified AFM probes with spring constant 2 N/m in the measurements. The intermolecular force of different test conditions were measured by AFM, shown in figure 3c. The intermolecular force of additive 1 was stronger than additive 2 at same conditions. Therefore, we inferred the alignment force of additive 1 were stronger than additive 2. Additive 1 will help LC to complete well alignment in real panel.
Figure 3 Mechanism diagrams for hydrogen bonding force between additive molecular with hydroxide radical (a), intermolecular force between additive molecular with LC molecular (b). c, typical force curves of the interaction between ITO substrate with additive1 molecular and additive2 molecular, and typical force curves of the interaction between RM1/2 modified substrate and additive1/2 molecular.

Figure 4 The pretilt angle of TFT side is different from CF side due to self-alignment force difference in SAVA. a, schematic diagram of self-alignment cell structure without PI layers on both TFT and CF sides; b, schematic diagram of self-alignment cell structure with PI layer on CF side and no PI layers on TFT side; c, schematic diagram structure of self-alignment cell with PI layer on TFT side and no PI layer on CF side; At the same cell structure a, the Δpretilt angles are different among additive 1, 2, and 3 (d); At the same cell structure b, the Δpretilt angles are increasing with PI layer thickness increased (e); At different cell structure b and c, Δpretilt angle is bigger at b structure than c structure.

By compared with PI layer, the alignment force of additive was weak because of the thickness of
additive polymer layer. When the device chose one side used PI layer as alignment layer, the other side chose additive layer as alignment layer, the pretilt angle of each side will be exist quite difference. There are three conditions in this study, one is self-alignment cell structure without PI layers on both TFT and CF sides (Figure 4a, d), one is self-alignment structure with PI layer on CF side and additive polymer layer (no PI layer) on TFT side (Figure 4b,e), the last one is self-alignment structure with additive polymer layer (no PI layer) on CF side and PI layer on TFT side (Figure 4c).

![Figure 5 The optical images of different cells using additive 1 and additive 2. At dark and 3.0 V state images, alignment states which cell used additive 1 are better than cell used additive 2.](image)

Though AFM measured and pretilt angle compared, the additive 1 exhibits stronger alignment force. To further proof the alignment force of additive, additive 1 and additive 2 were adding into the same host LC, respectively. And these two kinds of self-alignment LC were chosen to form optoelectronic device, as figure 5 shown. The self-alignment LC with additive 1 exhibits well alignment state than self-alignment LC with additive 2. The real device results are consistent with AFM intermolecular force and pretilt angle.

3. Conclusion
In conclusion, multiple methods were employed to analysis self-alignment force of reactive additive monomer. The intermolecular force between additive and ITO substrate or ITO-LC substrate was investigated using AFM. Through chemical modification, we immobilized additive monomer by covalent bonds on the surface of AFM probe. The parallel experiments were carried out to discriminate specific interactions among the complex additive-substrate/additive-LC interactions. We derived nonspecific interaction values from the observed force curves. Furthermore, the properties of different types of additive monomer were compared by measuring pretilt angle of TFT side and CF side, respectively. After AFM measured and pretilt angle compared, the alignment force of different types of additive can be selected. The additive with strong alignment force also showed well alignment state after forming into optoelectronic device. Therefore, the AFM force tested, pretilt angle compared, and alignment state observed can help set up a rapid detection technology to distinguish alignment force of additive. It will facilitate the development of self-alignment mode.

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