Statistical Modeling of Pretilt Angle in NLC on the Polyimide Surface

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Abstract

In this paper, the response surface modeling of the pretilt angle control in the nematic liquid crystal (NLC) on the homogeneous polyimide surface with different surface treatment is investigated The rubbing strength and the hard baking temperature are considered as input factors. After the design of experiments is performed, the process model is then explored using the response surface methodology. The analysis of variance is used to analyze the statistical significance and the effect plots are also investigated to examine the relationship between the process parameters and the response.

1. Introduction

LCDs require the monodomain alignment and the proper pretilt angle. The pretilt angle prevents the creation of the reverse tilted disclination in the twisted nematic (TN) mode. The uniform director orientation of the liquid crystal (LC) molecules and the control of the pretilt angle on the substrate surfaces are the most important task to improve the performance of LCDs. However, the statistical modeling of the control of the pretilt angle in NLC on the rubbed PI surface for the homogeneous alignment is not reported yet. The statistical modeling of the control of the pretilt angle is very useful and gives reliability to predict the pretilt angle. That is the reason why the statistical modeling in the pretilt angle research is important.

The methodology to characterize process using the response surface model with the design of experiments (DOE) has been applied to various fields. As an example, May *et al.* investigated the statistical experimental design in plasma etch modeling[1]. Garling *et al.* presented enhancing the analysis of variance (ANOVA) technique to wafer processing[2]. Lau *et al.* reported Taguchi design of experiment for wafer bumping by stencil printing[3]. Hu *et al.* optimized the hydrogen evolution activity on zinc-nickel deposition using experimental strategies by statistical methodology[4].

2. Experimental

The glass substrates are prepared at room temperature (22℃). The polymer (JSRJALS-1371-R1) is used as a homogeneous alignment layer and coated uniformly on the indium-tin-oxide (ITO) electrodes by a spin-coating machine[5]. The thickness of the PI film is set at 500 Å. The PI substrates are pre-baked at 80℃ for 10 minutes. The PI substrates are imidized at 180℃, 215℃ and 250℃ for 1 hour, again. These substrates are cooled at room temperature. After that, the substrate surfaces are rubbed by the rubbing machine with the nylon roller. The rubbing strength has been defined in some previous works[6].

We use three kinds of the rubbing strengths to make different pretilt angle such as 0.3mm, 0.5mm and 0.7mm. These numerical values represent the rubbing depth closely related to the rubbing strength. The substrates are arranged as a sandwich type for the pretilt angle measurement, and the cell gap is 60㎛. The fabricated cell is filled with a NLC (T_C=72℃, $\Delta\varepsilon$=8.2, from Merck Co.). In addition, the pretilt angle is measured using the crystal rotation method at room temperature (22℃) with TBA-701.

3. Modeling scheme

Two input factors are explored via D-optimal Design with 13 runs to minimize the variance associated with the coefficient estimates for the model. This design tends to put most design points on the edges of the design space. All experimental runs are made in random order. The experimental design matrix of input factors used in each run is summarized in Table 1. Quadratic model is used as basic model. The Quadratic model having intercept, two main effects, two square effects, and one two-factor interaction is defined as the following:

$$Y=\beta_0+\beta_1X_1+\beta_2X_2+\beta_3X_1^2+\beta_4X_2^2+\beta_5X_1X_2 \qquad (1)$$

Where, Y is the response value, β_i s are the model coefficients, and X_i s are the process factor values.

Table 1. The D-optimal design matrix.

Run	Rubbing strength (mm)	Hard baking temperature (℃)
1	0.3	180
2	0.3	180
3	0.5	250
4	0.5	215
5	0.3	250
6	0.7	180
7	0.3	250
8	0.7	250
9	0.5	180
10	0.7	215
11	0.5	215
12	0.3	215
13	0.7	250

In order to build the model, the insignificant effects in this study are eliminated backward elimination method under the statistical significance level is 0.01 (α= 0.01). The backward elimination method starts with the equation in which all effects are included and the insignificant effects in the model are eliminated one at a time. At any step, the variable with largest p-value, as computed from the current regression, is eliminated if this p-value exceeds a specified value[7]. The square effect for the rubbing strength is eliminated from the model, because of its significance (P-value = 0.353) in the full quadratic model. The selected significant effects are summarized in Table 2. The analysis of variance for the response is summarized in Table 3. P-value of the main effects, the square effect and the two-factor interaction are 0.001, 0.008 and 0.007, respectively. It indicates that all the effects are significant in this model for the pretilt angle. The adjusted R-squared value is 0.971 in Table 4. It means that 97.1% of variation is being explained by the model.

Table 2. The summary of the statistical significance.

Response	Effect	p-value
Pretilt angle	RS	< 0.0001
	HBT	< 0.0001
	HBT * HBT	0.0080
	RS * HBT	0.0071

The regression model for the pretilt angle is the following expression:

Pretilt Angle = - 3.655748891 - 32.74291925 * RS + 0.262209494 * HBT - 0.000871074 * HBT*HBT + 0.100279503 * RS * HBT (2)

Where, the RS is the rubbing strength and the HBT is the hard baking temperature.

Table 3. The ANOVA for the pretilt angle.

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Regression	4	103.406	103.406	25.85149	102.6	0
Linear	2	97.602	8.65716	4.32858	17.18	0.001
Square	1	2.566	3.09922	3.09922	12.3	0.008
Interaction	1	3.238	3.23803	3.23803	12.85	0.007
Residual Error	8	2.016	2.01568	0.25196		
Lack-of-Fit	4	2.013	2.01303	0.50326	759.64	0
Pure Error	4	0.003	0.00265	0.00066		
Total	12	105.422				

Table 4. The summary of statistics

Std. Dev.	0.501957	R-Squared	0.98088
Mean	6.182308	Adj R-Squared	0.97132
C.V.	8.119245	Pred R-Squared	0.953642
PRESS	4.88714	Adeq Precision	28.35847

The modeling result exhibit a good agreement with the values between the predicted and the measured response as shown in Fig. 1.

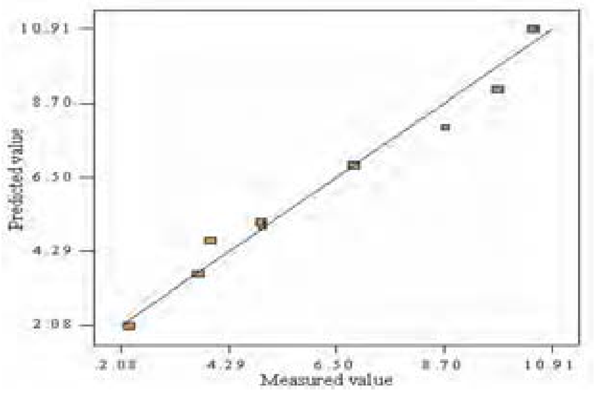


Fig. 1. The modeling result with the values between the predicted and the measured response.

There are three assumptions to use ANOVA, which is independence, normally distributed, and homogeneity of variance. First assumption is that each of the group is independent. Second assumption is that the values in each group of the design are normally distributed.

Last assumption is that the variances in each of the group are not different from each other. Those assumptions can be verified using the residual analysis. A check of the normality assumption may be made by constructing a normal probability plot of the residuals. The normal probability plot of the residuals is illustrated in Fig. 2. If the residuals plot approximately along a straight line, then the normality assumption is satisfied[8].

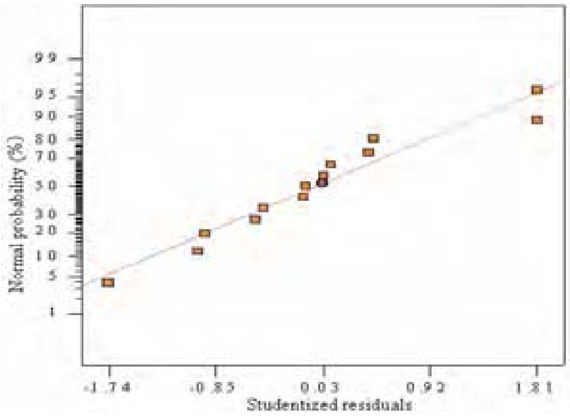


Fig. 2. The normal plot of residuals.

4. Result and discussion

The pretilt angle is measured by the crystal rotation method such as Fig. 3. Figure 3 shows the pretilt angle at 0.5mm of the rubbing strength. The error rate of the result is approximately 0.002.

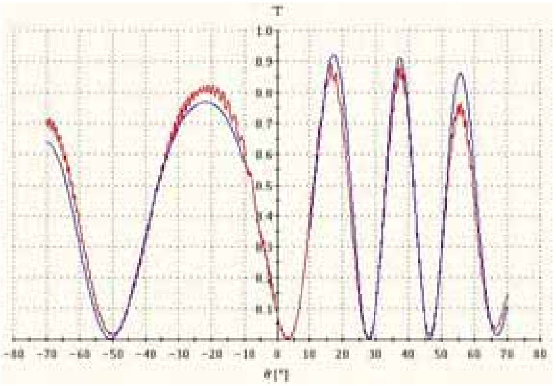
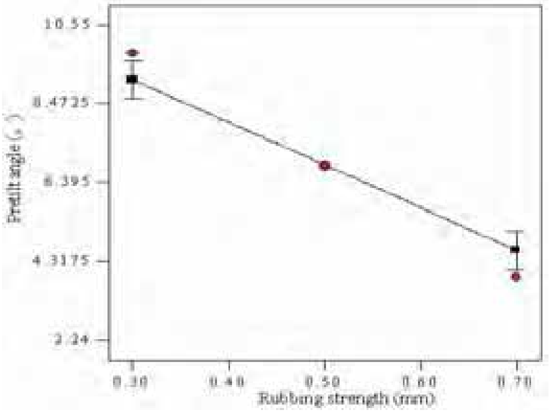
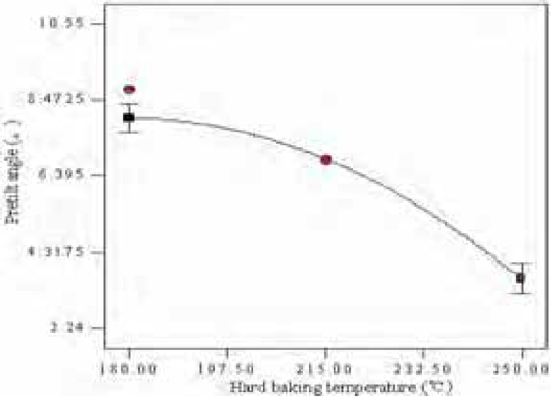


Fig. 3. The pretilt angle at RS =0.5mm

The main effect plots for the response are illustrated in Fig. 4. The square dots are predicted response and the circular dots are measured response. They are alike in response. When the hard baking temperature factor is fixed in middle point, the effect of the rubbing strength plots for the pretilt angle is illustrated in Fig. 4(a). Figure 4(a) shows that the pretilt angle on the PI surface in the middle hard baking temperature tends to increase as the rubbing strength increases. The rubbing treatment generates the obliquely inclined force on the alignment layer. Therefore, It seems quiet probable that the generation of the pretilt angle caused by a micro-asymmetrical triangular structure of the PI.



(a) The rubbing strength.



(b) The hard baking temperature.

Fig. 4. The main effect plots for the pretilt angle generation.

When the rubbing strength factor is fixed in middle point, the effect of the hard baking temperature plots for the pretilt angle is illustrated in Fig. 4(b). It shows that the pretilt angle on the PI surface in the middle rubbing strength tends to increase as the hard baking temperature increases. In the cases of the hard baking temperature at 180℃, 220℃ and 250℃, PI exhibited imidization rates of 20%, 68% and 100% in the previous work[9]. In order to explain the pretilt angle as a function of hard baking temperature, we must refer to the imidization ratio. As the hard baking temperature is increased, the imidization ratio is increased. Added to this, the pretilt angle is stabilized. In other words, this result implies that the imidization ratio is a potent influence on the generation of the pretilt angle.

The interaction effect plot between the rubbing strength and the hard baking temperature for the pretilt angle is illustrated in Fig. 5. It shows that the generation of the pretilt angle in NLC on the rubbed PI surface with different baking temperatures (180~250℃) as a function of the rubbing strength. The upper straight line is a case of the low hard baking temperature and the under straight line is a case of the high hard baking temperature.

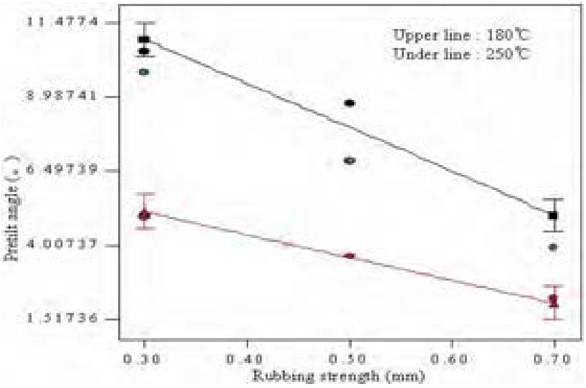


Fig. 5. The interaction effect plots for the pretilt angle.

The large difference between the effectiveness of one factor according to the other factor means that the interaction effect between the factors has a strong potential for the response. The rubbing strength is more effective for the pretilt angle when hard baking temperature is at the lower level than the higher level. It means that there is the difference of rubbing strength effect in accordance with the change of the hard baking temperature. This can be interpreted that the effect of the rubbing treatment is stronger when imidization rate is at the lower level. However, both the rubbing treatment and the hard baking temperature have a deep connection with the pretilt angle. The sum of the rubbing treatment and the hard baking temperature offers the key to the control of the pretilt angle.

The contour plot of the pretilt angle according to the change of the rubbing strength and the hard baking temperature is illustrated in Fig. 6. The smallest pretilt angle is generated applying the largest rubbing strength and highest hard baking temperature on the PI surfaces. In a similar fashion, the largest pretilt angle is generated applying the smallest rubbing strength and lowest hard baking temperature on the PI surfaces. As a consequence, it is very informative for the control of the pretilt angle. The contour plot of the pretilt angle according to the change of the rubbing strength and the hard baking temperature helps us to predict and realize the wanted pretilt angle. From the Fig. 2, we realize that contour plot can allow us to predict the pretilt angle with respect to the varying process conditions.

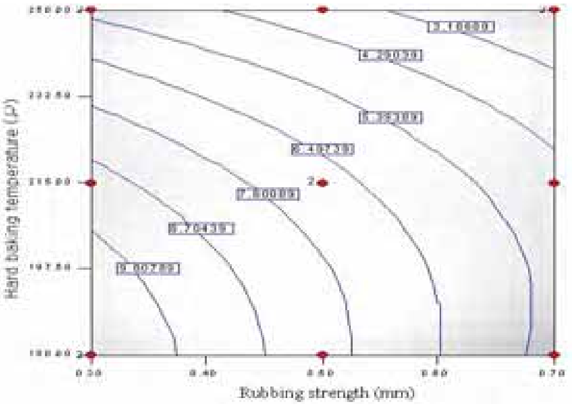


Fig. 6. The response surface plots for the pretilt angle.

5. Conclusion

The control of the pretilt angle in NLC on the PI surface as a function of the rubbing strength and the baking temperature is investigated via the response surface modeling. The statistical significance factors are determined by ANOVA and those effects are compared with that of the varying process conditions, and are analyzed by the effect plots. The response surface modeling is in an agreement with the experimental data and represents a comprehensive characterization of the pretilt angle. As a result, the statistical modeling of the control of the pretilt angle is very useful and gives reliability to predict the pretilt angle.

6. Acknowledgement

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