

# Numerical Simulation Study of Cell Gap Dependence on Anisotropic Phase Separation

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## Abstract

Cell gap dependence on anisotropic phase separation was studied by numerical simulation. The numerical results showed that the morphology of phase separation depended on cell gap and material parameters. The well separated relation between material parameters and cell gap is suggested.

## 1. Introduction

Recently devices using photopolymerization induced phase separation (PIPS) of polymer and LC mixtures are widely studied. Among several kind of PIPS, phase separated composite organic film (PSCOF)[1] draw much attention because of its device application such as flexible LCDs[2-4] due to possibility of constructing microstructure. Unlike isotropic phase separation (e.g. polymer dispersed liquid crystal) PSCOF has layered structure. Figure 1 shows schematic diagram of PSCOF.

Qian, Et.al demonstrated essential parameters of well separating condition by experiments and numerical analysis. The relevant parameters are UV intensity, UV intensity gradient[5].

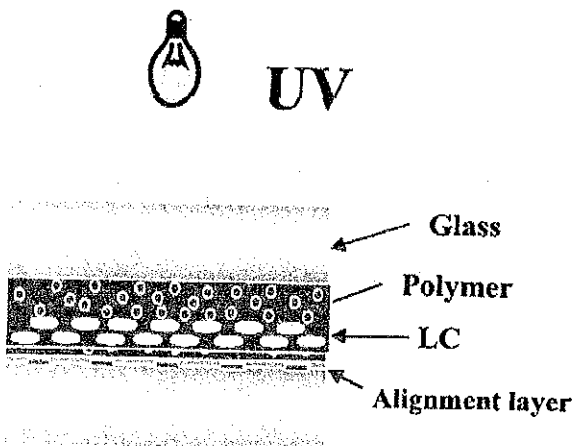


Figure 1 Schematic diagram of PSCOF

More recently, temperature and cell gap dependence on PSCOF morphology was reported.[6] And lower cell

gap show more good separation morphology. We here studied the gap dependence of morphology does not monotonically and rather optimal gap range by numerical simulation.

## 2. Numerical Simulation

The basic equation for PSCOF is same as that of diffusion of binary mixture. The equations for using numerical simulation is as follow[5]:

$$\frac{\partial \psi}{\partial t} = -\frac{\partial J_{\psi}}{\partial z}$$

$$\frac{\partial \phi}{\partial t} = -\frac{\partial J_{\phi}}{\partial z} - \frac{\partial \eta}{\partial t}$$

$$\frac{\partial \eta}{\partial t} = kI\phi(\phi + \eta)$$

$$J_{\phi} = D\left(-\psi \frac{\partial \phi}{\partial z} + \phi \frac{\partial \psi}{\partial z} - \chi\phi\psi \frac{\partial \psi}{\partial z}\right)$$

$$J_{\psi} = -J_{\phi}$$

$$\frac{\partial I}{\partial z} = -b\psi I$$

Where  $\psi$ ,  $\phi$  and  $\eta$  are concentration of LC, monomer and polymer, respectively.  $J_{\psi}$  and  $J_{\phi}$  are current density of LC and monomer. Polymers were assumed to be immobile due to cross-linking structure.  $D$  is the diffusion constant,  $I$  is the UV intensity and  $b$  is the absorption coefficient by LC. We here assumed the UV is absorbed predominantly by LC. From the above equations, when transformed to dimensionless coupled equations, there remain two essential bulk parameters  $R$  and  $L$ .

$R = kI_0d^2/D$ , related to polymerization, where  $k$  is polymerization rate,  $I_0$  is UV intensity at illuminated surface and  $d$  is cell gap. For larger  $R$ , the separation morphology becomes more polymer dispersive. Another parameter  $L = 1/bd$ , is related to UV intensity gradient. That means as shown in Fig.1, UV intensity is strongest at illuminated surface and due to absorption by LC

molecules, intensity shows exponentially decaying profile. We can see that the cell gap is related to both  $R$  and  $L$ . In numerical simulation, we adopted finite difference method.

### 3. Results and Discussion

Figure 2. shows the typical phase separation morphology of two kind. Fig.2(a) shows well separated texture and scanning electron microscopic(SEM) image. Whereas the Fig. 2(b) shows polymer dispersed structure. The left pictures are optical images under crossed polarizers and right pictures are cross-sectional image as observed by scanning electron microscopy(SEM).

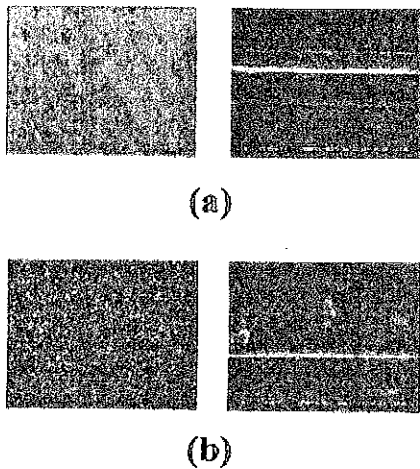


Fig. 2 Optical texture and cross sectional image of (a) well separated case and (b) polymer dispersed case.

In numerical simulation, we studied for values of  $R = 25$  and  $L=0.1$ , for given unit cell gap 1. According to  $R$ , the morphologies are changed from film-like separation to polymer dispersed structure. And then we change cell gap, which results change of  $R$  and  $L$  simultaneously. Figure 3 shows the numerical simulation results.

The results seems not to be consistent with Q. Wang et. Al's experimental result[6]. However the boundary morphology of LC and polymer is not involved in this 1-dimensional simulation. This means morphologically, lower cell gap serves more uniform LC/polymer boundary. And even lower cell gap generate polymer dispersed morphology again. Our numerical results implies the for given bulk parameters, there is optimized cell gap range. From the above definition of  $R$  and  $L$ , this may be written as  $1/b < d < (D/kI)^{(1/2)}$ .

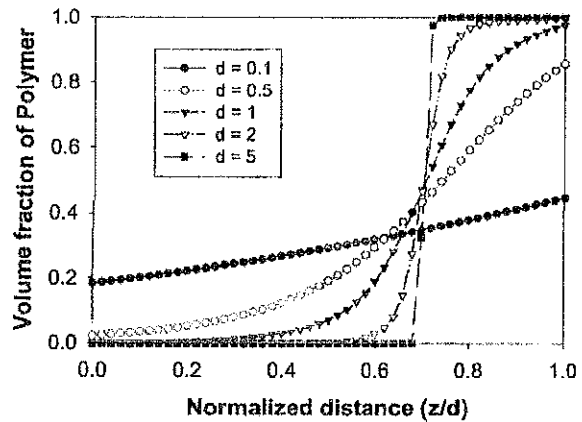


Fig. 3 Numerical simulation of 1-dimensional phase separation as cell gap varying.

### 4. Conclusions

We studied the cell gap dependence on phase separation morphology through numerical simulation. Although lower cell gap can serve more uniform LC/polymer boundary, but it can generate polymer dispersed structure. In a viewpoint of application, one should choose proper cell gap range for constructing suitable film-like structure.

### 5. References

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Program : October 21, 2005 (Fri.)

Chairman : Seiji Kurihara

10:20-10:40 : Invited Paper

"Development and Industrialization of Liquid Crystal Materials"

Haruyoshi Takatsu

DAIIPPON INK & CHEMICALS INC.

10:40-10:50 : Coffee Break

10:50-11:20 : Invited Paper

"Synthesis and Electroluminescent Properties of Fully Substituted Ethylene Moieties"

Jong Wook Park

Department of Chemistry/Display Research Center, The Catholic University of Korea  
Catholic University

Chairman : Keun-Byoung Yoon

11:20-11:40 : Invited Paper

"Numerical simulation study of cell gap dependence on anisotropic phase separation"

Min-Young Jin

Department of Electronics and Computer Engineering, Hanyang University

11:40-12:00 : Invited Paper

"Fabrication of Twisted Nematic Structure in Phase Separated Composite Film"

Hak-Rin Kim

Department of Electronics and Computer Engineering, Hanyang University

12:00-13:30 : Lunch