P-20: Shadow Modeling using Z-map Algorithm for Process Simulation of OLED Evaporation

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Abstract

In order to simulate OLED evaporation process, modeling of directional distribution of the vaporized organic materials, film thickness distribution profile and pattern-mask shadow effect are required In accordance with many literatures; all of them except shadow effect modeling are studied and developed.

In this paper, modeling algorithm of evaporation shadow is presented for process simulation of full-color OLED evaporating system. In OLED evaporating process the offset position of the point cell-source against the substrate rotation axis and the usage of the patterned mask are the principal causes for evaporation shadow. For geometric simulation of shadow using z-map, the film thickness profile, which is condensed on a glass substrate, is converted to the z-map data. In practical evaporation process, the glass substrate is rotated. This physical fact is solved and modeled mathematically for z-map simulation. After simulating the evaporation process, the z-map data can present the shadow-effected film thickness profile. Z-map is an efficient method in that the cross-sectional presentations of the film thickness profile and thickness distribution evaluation are easily and rapidly achieved.

1. Introduction

OLED (organic electro-luminescence device) has been studied world-widely because of its simple structure, high resolution, large viewing angle and low driving voltage. Vacuum evaporation allows pure organic material deposition on a substrate without concern of contamination such as water or solvents. [1] It is the most mature and common method already in production for OLED displays.

For optimizing evaporation process, computer simulation is developed. For process simulation of OLED evaporation, modeling of directional distribution of the vaporized organic materials, the thickness uniformity of the organic films and modeling of shadow effect are required. Many investigations have been done to optimize the thickness uniformity on the substrate. [2, 3]

In accordance with many literatures; all of them except shadow effect modeling are developed. The trend of the display size has hauled the enlargement of the mother glass substrate. As the shadow effect becomes more important. Therefore, the shadow modeling can improve the performance the full-color OLED displays

The object of this paper is to simulate the thickness distribution considering the shadow effect over the area of the substrate. Generally, the shadow is larger at the more outside of a substrate. The z-map simulation can show the actual shadow profile over all area of a substrate.

For shadow effect simulation, z-map algorithm is applied. In the simulation, the film thickness profile, which is generated in the evaporating process, is converted to the z-map data. In the OLED evaporating process, the offset position of a point cell-source against the substrate rotating-axis and the usage of the patterned mask are the principal causes for the shadow effect. The shadow effect is strongly influenced by the geometrical position of the evaporation source with the rotating substrate. This physical fact is solved and modeled mathematically for z-map simulation.

2. Simulation of Evaporation Process

2.1 Geometric Modeling

Atoms or molecules evaporating from a cell-source have kinetic energies that are distributed according to their temperature. [4] Many investigations have been done to calculate the thickness distribution in the evaporation process. In the paper, the well-known evaporating model is used to calculate the normalize profile of the film thickness. Figure 1 shows the geometrical arrangement of typical evaporation using a plane rotating substrate. The position of the evaporator is out of center by a section q. The substrates rotate with a radius r in a vertical distance h above the cell-source. (Figure 1)

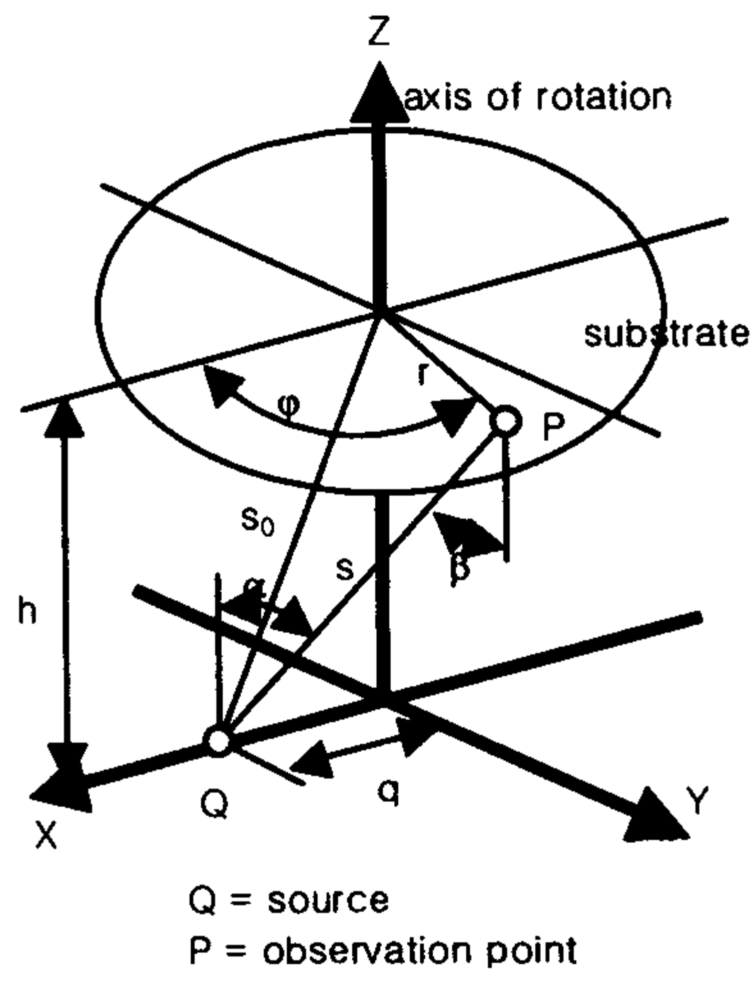


Figure 1 Geometry of evaporation process

Generally, the mass m of material emitted from an evaporation source at a solid angle w is

$$dm = m(w)\,dw = m(w)\cos^n \alpha\, dw \quad (1)$$

The evaporated material transported in the solid angle dw condenses on the substrate element dA. The relation existing between mass m, density ρ and thickness is

$$dm = \rho\, d\, dA \quad (2)$$

By substituting Eq. (2) into Eq. (1), the thickness on the substrate element of the distance s is

$$d = \frac{m(n)}{\rho}\frac{\cos^n \alpha \cos\beta}{s^2} \quad (3)$$

In the Eq. (2), α denoted the angle between the direction of the emitted molecule and the symmetry axis of the evaporation source. The substrate has a point, the center of rotation, whose relative position to the evaporation source remains unchanged during the rotational motion. This center of rotation is the best suited position as a normalization point for the thickness d_0.
In normalized representation is obtained

$$\frac{d}{d_0} = \left(\frac{s_0}{s}\right)^2\left(\frac{\cos^n \alpha \cos\beta}{\cos^n \alpha_0 \cos\beta_0}\right) \quad (4)$$

Substituting the parameters with the q, h, and r, Eq. (4) yields

$$\frac{d}{d_0} = \frac{\left[1+\left(\frac{q}{h}\right)^2\right]^{\frac{n+3}{2}}}{\left[\left(\frac{r}{h}\right)^2 - 2\left(\frac{r}{h}\right)\left(\frac{q}{h}\right)\cos\varphi + \left(\frac{q}{h}\right)^2 + 1\right]^{\frac{n+3}{2}}} \quad (5)$$

Eq. (5) describes the relation of the thickness of an arbitrary point to the thickness of the point on the axis of rotation under stationary conditions. In practice, the glass substrate is rotated.

2.2 Least Square Fit

According to Eq. (5), the shape of the thickness profile is strongly influenced by the effusion shape and the geometrical position of the evaporation source. The geometrical position of the cell-source is easy established, but the effusion profile must be determined experimentally. The experimental determination of the exponent is done by measuring the thickness profile on substrates and fitting the measured profile with those calculated. (Figure 2) The least square method (sometimes called regression model) applied for obtaining the best fit between experiments and calculations.
Least square method is a statistical approach to estimate an expected value n with the highest probability from the observations with random errors. The highest probability is replaced by minimizing the sum of square of residuals in the least square method.

In case measurements (α_i,t_i) - emission angle and film thickness - are given, the relationship between α and t (thickness at a point) is estimated by the function Eq. (1). Residual is defined as the difference between the observation and an estimated value of a function. (Eq. 6)

$$E = \sum_{i=1}^{n}(n \ln\cos\alpha_i - \ln t_i)^2 \quad (6)$$

By minimizing the square sum of residuals, the unknown parameters n will be determined as shown in Figure 2.

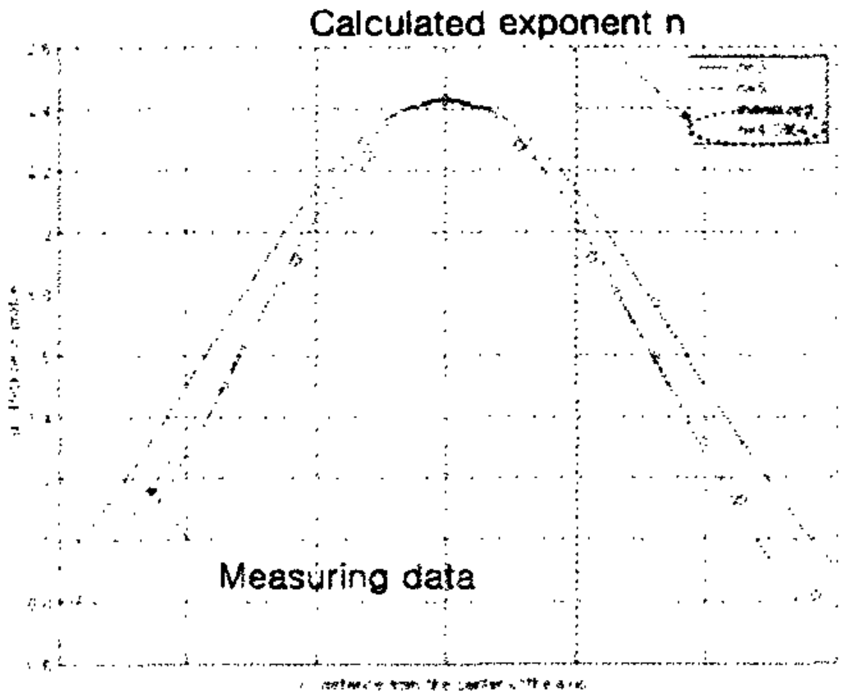


Figure 2 Least-square fitting to determine the exponent n

2.3 Deposition Profile

With the calculation exponent n, the deposition profile can be predicted at an arbitrary position with the Eq. 5. (Figure 3 and 4)

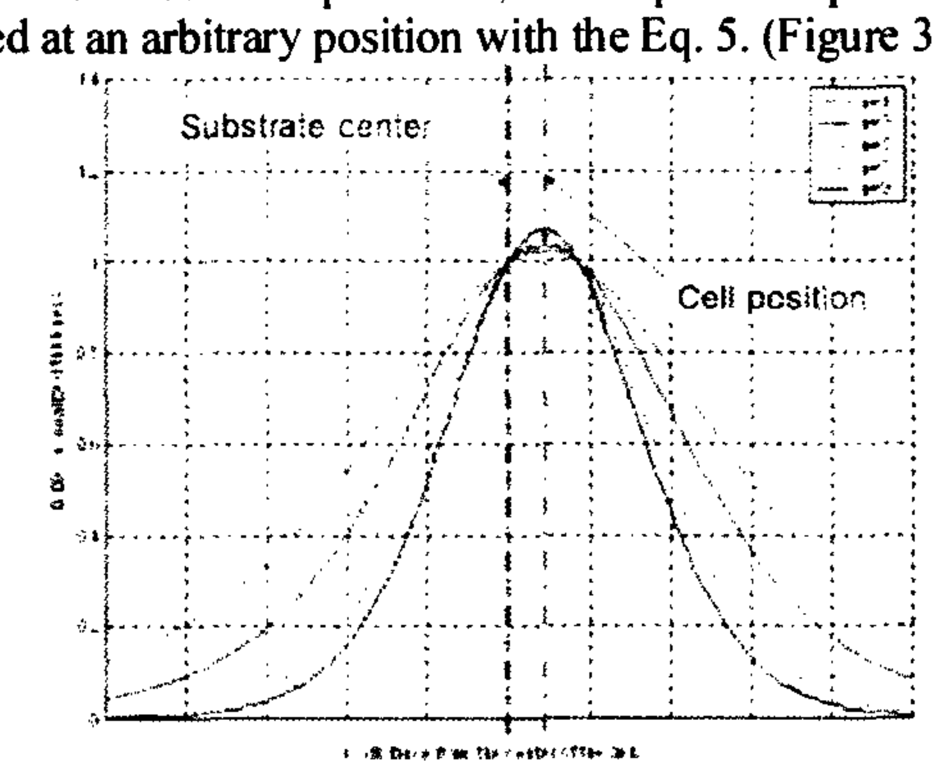


Figure 3 Film thickness profiles under stationary condition

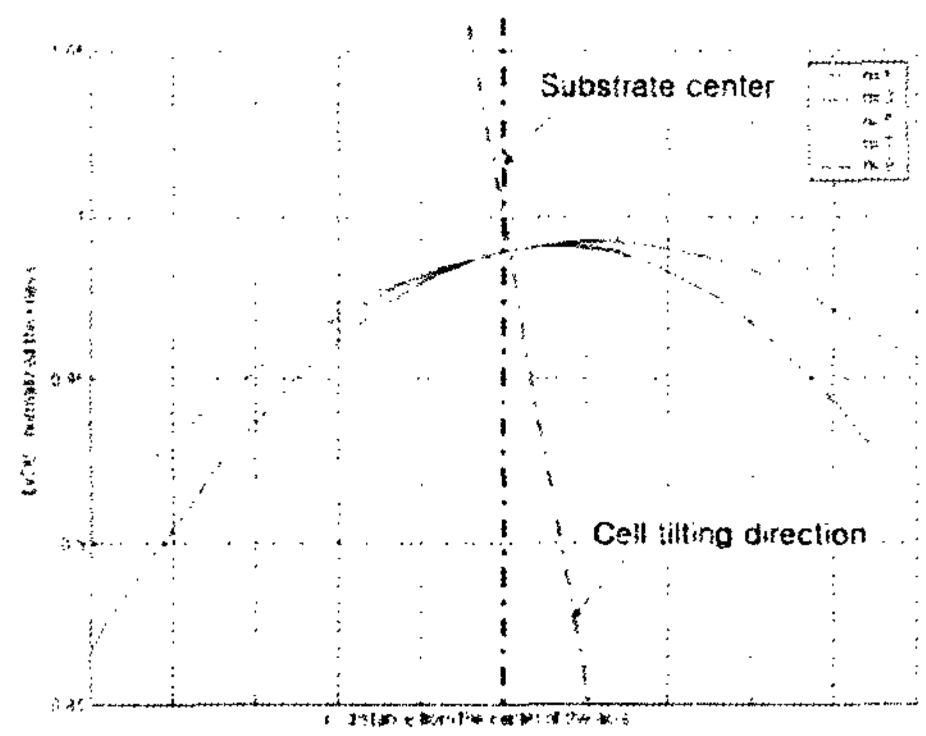


Figure 4 Film thickness profiles with an inclined cell

For the verification of the thickness profile calculation algorithm, the experiments had been performed. Results from the experiments on film thickness comparison are shown in Table 1. Table 1 shows the thickness calculation error. The maximum error is 4.66 %.

Table 1 Thickness comparison

No.	Predicted Thickness (A)	Experimented Thickness (A)	Difference (%)
1	2132.7	2061	-3.48%
2	3214.4	3299	2.56%
3	4601.8	4827	4.66%
4	6085.3	6120	0.57%
5	7228.8	7108	-1.70%
6	7573.0	7573	0.00%
7	7228.8	7230	0.02%
8	6085.3	6284	3.16%
9	4601.8	4817	4.47%
10	3214.4	3217	0.08%
11	2132.7	2068	-3.13%

Figure 3 and 4 describe the thickness profiles to the thickness of the point on the symmetry center of the substrate under stationary condition. In practice, however, the substrate holder is rotated. This physical fact is solved mathematically by forming the integral of Eq (5) with the integration variable. The resulting thickness distribution on a rotating substrate holder is Eq. (7)

$$\frac{D}{D_0}=\frac{1}{\pi}\int_0^{\pi}\frac{d}{d_0}d\varphi \qquad (7)$$

Solving Eq. 7, the solution of the integral does exist for all possible n values by using a numerical calculation method. If we approximate the Eq. 7 by a piecewise linear function (polygon of chords of the curve of the equation), we obtain the trapezoidal rule The numerical integration method is obtained by approximating the integrand by polynomials as shown Eq. 8.

$$J=\int_a^b f(x)dx \approx \frac{(b-a)}{n}\left[\frac{1}{2}f(a)+f(x_1)+f(x_2)+\cdots+f(x_{n-1})+\frac{1}{2}f(b)\right] \qquad (8)$$

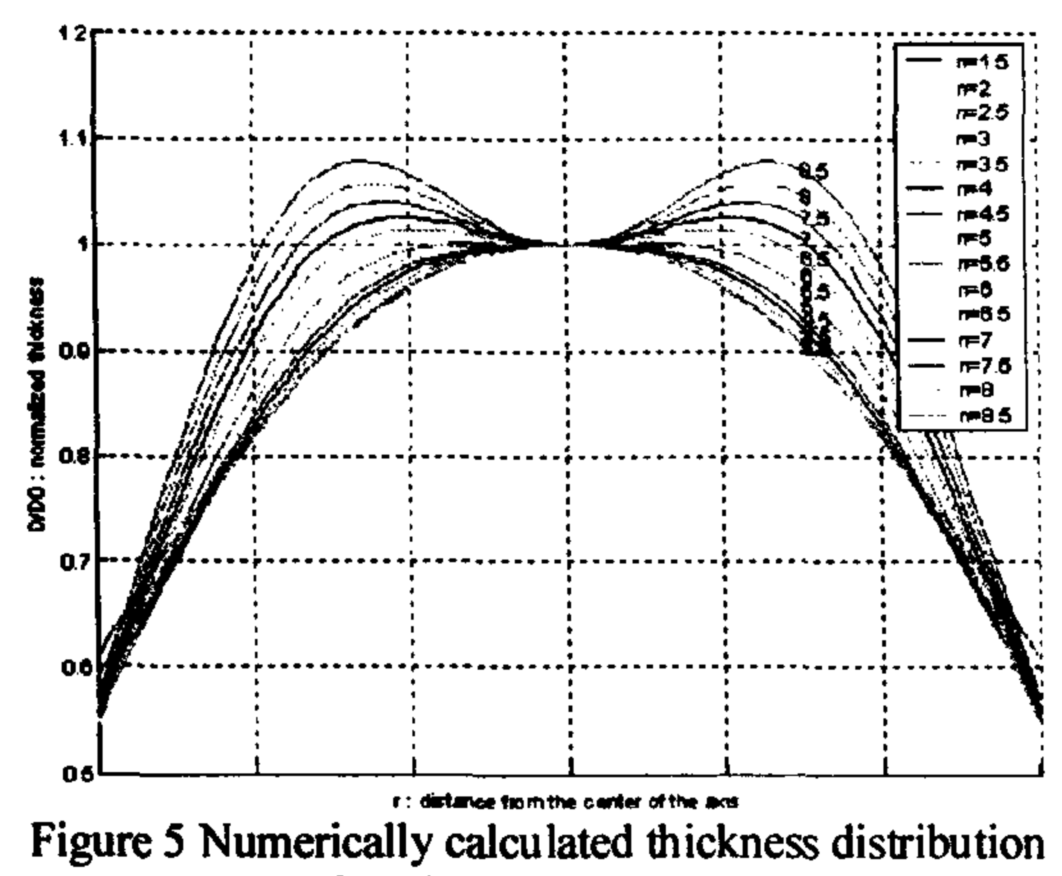


Figure 5 Numerically calculated thickness distribution as function of real number n

The shape of resulting thickness profile in the direction of the radius is shown in Figure 5. A cell-source position outside the rotation axis produces not only a monotonic decreasing thickness distribution but also, depending on the characteristic of the source, to some extent peaks. This behavior can be seen in Figure 5.

3. Mask Shadow Simulation

3.1 Concept of z-map

For solid geometric simulation, z-map method is widely used. The z-map concept is very similar to the z-buffer method of displaying shaded images in computer graphics. In order to display a graphic image on a raster device, a frame buffer is used. A frame buffer is organized as an X-Y matrix of memory locations, and each memory location corresponding to a pixel of the display screen, contains a color data to be displayed. Instead of color data, z-map data contains a corresponding thickness z value of the organic film at each frame buffer location. (Figure 6)

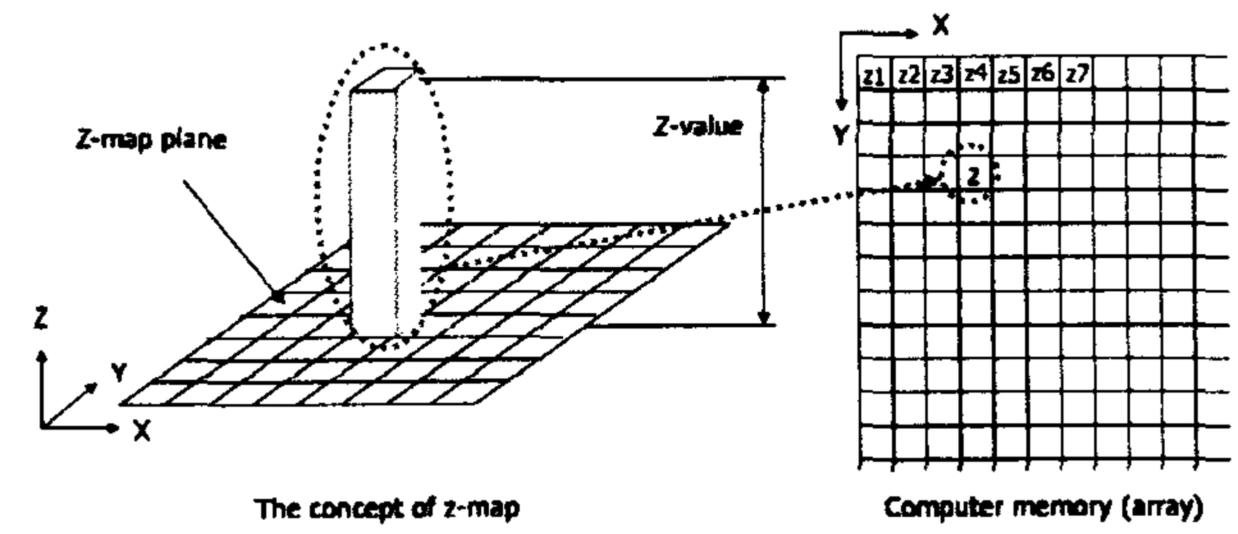


Figure 6 The concept of z-map

A z-map is an array of data elements that represent the thickness values of points on a substrate. (Figure 6) The z-map algorithm, from which this algorithm derives its name, is an n_x x n_y arrary for which the (n_i, n_j)th element corresponds to the (n_i, n_j)th point of the substrate. This array holds the z value of the film thickness at the point. For simulating an evaporating process, z-map plane is perpendicular to the rotation axis direction.

3.2 Shadow Effect

In the evaporation process, the molecules leave the vaporizing surface with direction defined by the cosine law. At very low pressures, the mean free path of the vapor organic molecules exceeds the usual distance between evaporation source and the substrate. [5] The molecules travel to the substrate without any collision in the residual gas. Thus, the substrate receives a flux of organic material vapor which travels in straight lines with the spatial distribution of the condensate obeys purely geometrical laws.

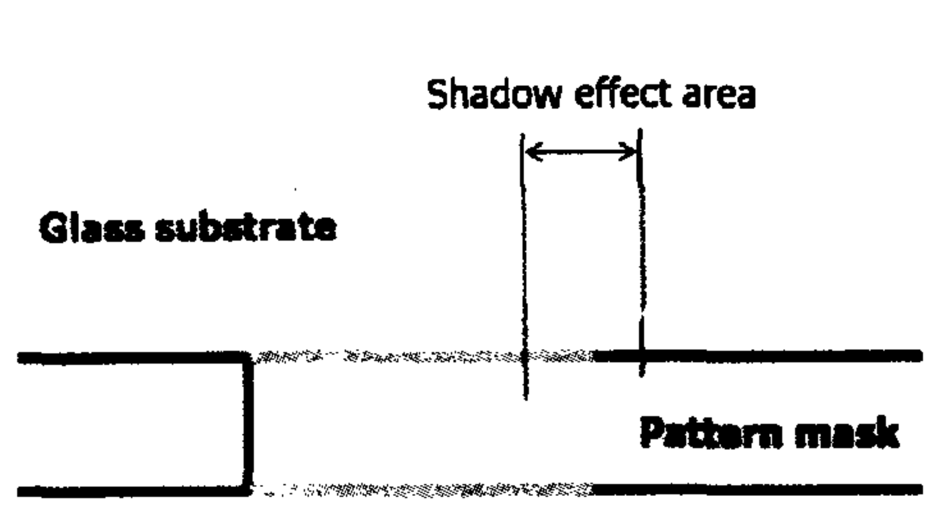
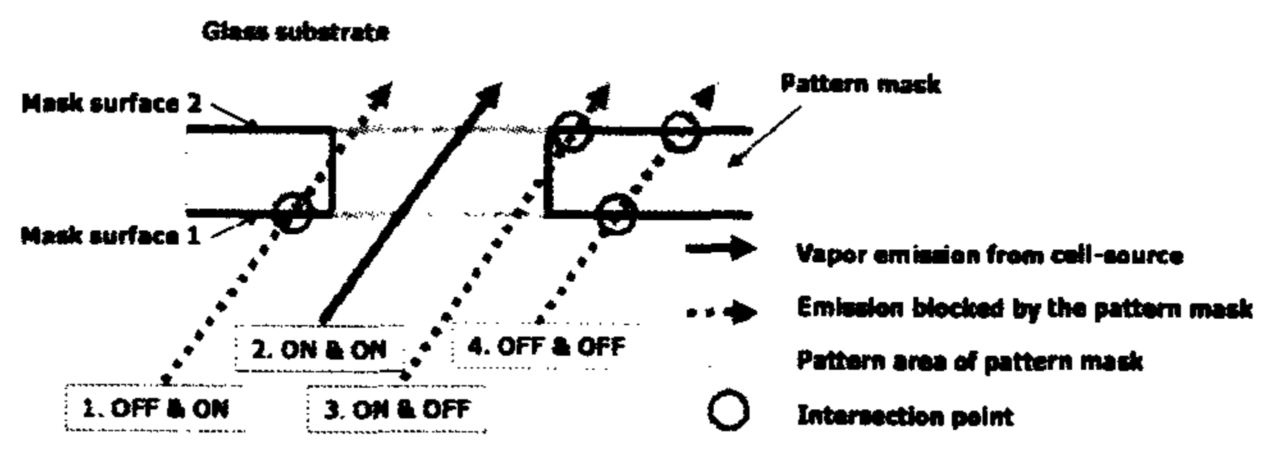


Figure 7 The shape of the mask shadow

The cause of the shadow effect is the usage of a pattern mask for fabricating the full color OLED. As an obstruction, the pattern mask may cut off the molecule travel to the substrate during evaporation process. The main defect of the shadow effect is the different thickness distribution according to the position in a pixel. (Figure 7)

With the physical fact, the organic material vapor is assumed to go from a cell-source to a substrate without collision. In the case of the rotation process, there are only collisions between a molecule and a pattern-mask. In this paper, the collision between an organic molecule and a pattern-mask is simulated with an only geometric calculation. (Figure 8)



No	1	2	3	4
Mask surface 1	OFF	ON	ON	OFF
Mask surface 2	ON	ON	OFF	OFF
Deposited or not ?	X	O	X	X

Figure 8 Deposition interference by a pattern mask.

3.3 Shadow Modeling

For shadow modeling, the z-map plane is defined with respect to the world coordinate whose z-axis is along the rotation axis direction and the origin is the rotation center of the substrate. The z-map segments are generated by subdividing a square region on the z-map plane into equally sized squares in a pattern-mask pixel. (Figure 9)

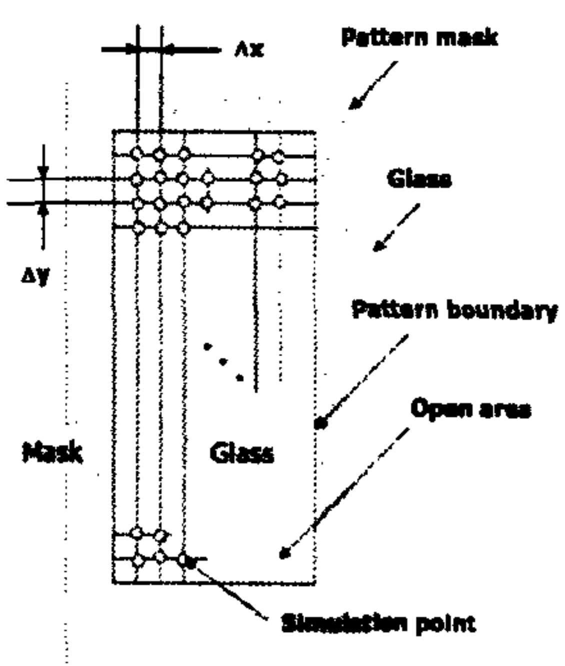
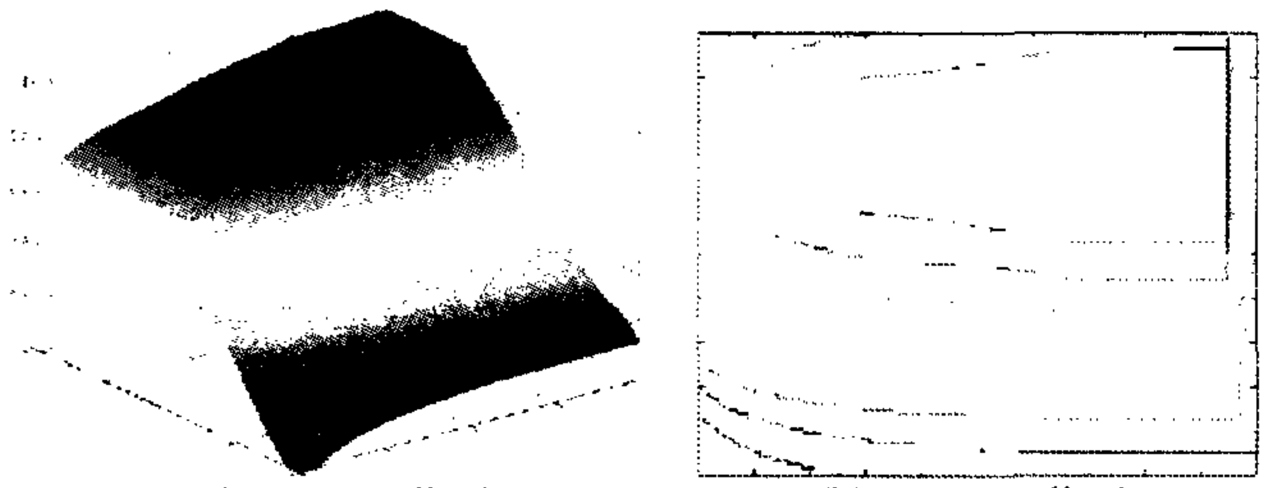


Figure 9 Z-map for shadow modeling

For geometric shadow simulation using z-map method, the film thickness profile data is converted to z-map data. According to the substrate rotation, the organic film is condensed and the new thickness value is converted into the z-map data. The z-value of the film thickness is determined by calculating with the developed method in the simulation. The results of the simulation are shown in Figure 10.

The resolution of the geometric shadow simulation with z-map representation is dependent on both the z-map size and the mask-pattern size to be processed in the z-map. In Figure 10, a 500 x 500 size z-map plane for computing 250μm x 250μm size region is allocated, and then the approximated resolution of the geometric simulation is 0.5μm. Higher resolution is achievable, but it costs more computing time and larger virtual memory. To achieve the higher resolution, the processing time and cost should be increased.



(a) 3-dimension display (b) contour display

Figure 10 The film shape with simulated shadow effect on a pixel

4. Conclusion

In this paper, the geometric simulation algorithm of evaporation shadow is developed by using z-map algorithm. The geometric model simulates the film thickness profile affected by the evaporation shadow.

For geometric simulation of shadow using z-map, the film thickness profile, which is condensed in the evaporating process, is converted to the z-map data. In practical evaporation, the glass substrate is rotated. This physical fact is solved and modeled mathematically for z-map simulation. After simulating the evaporation process, the z-map data can present the shadow-effected film thickness profile.

The geometric simulation makes an OLED evaporator designer be able to check the amount of the mask shadow. Thus, the performance of OLED displays can be improved by precisely coming to the allowable specification of the evaporation shadow.

Z-map is an efficient method in that the cross-sectional presentation of the film thickness profile, and point evaluation are easily and rapidly achieved.

The developed method was verified by the evaporation experiments and the measurements. With the presented method, OLED displays can be manufactured with the high performance.

5. Acknowledgements

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6. References

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