Reliable Simulation and Prediction of Water Vapor Transmission Rate in High-Performance Thin-Film Encapsulation

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Abstract

The water vapor barrier capability of the TFE layer is crucial for ensuring the performance and lifetime of OLED devices. WVTR testing typically takes long time, hence using simulation methods to predict the water vapor permeation behavior of OLED devices is a reasonable choice. In this study, we have established a water vapor permeation simulation model based on Fick's law, which can be used to predict the WVTR values of TFE inorganic films and the water vapor concentration at any time or position within the boundary conditions. The simulation model demonstrated high accuracy in predicting the water vapor barrier behavior of TFE films, with simulation results closely matching the experimental results. Finally, we applied the simulation model to assess the water vapor barrier capability of TFE layers corresponding to different isolation column structures in OLED devices, which can be effectively applied to the assessment and prediction of OLED encapsulation materials and structures.

Author Keywords

OLED; WVTR; Simulation; water vapor transmission

1. Introduction

In the realm of display technology, thin-film encapsulation (TFE) has been an indispensable technology in ensuring the reliability of high-performance products, specifically for flexible organic light-emitting diode (OLED) displays. By effectively obstructing the ingress of gases such as H_2O and O_2, which may lead to the device degradation, TFE can prevent film deterioration, thereby guaranteeing the long-term reliability of OLED devices while maintaining their flexibility and performance.

The water vapor transmission rate (WVTR) is a critical parameter for TFE materials, with the objective of achieving a rate below 1×10^{-6} g/m^2/day for practical OLED applications. Conventional approaches to measuring WVTR involve experimental methods, such as coulomb method, tritiated water test, calcium test, infrared imaging method and membrane permeation test with coulometric sensor.[1] Each method has its advantages and limitations, and the selection of method depends on factors such as the material being tested and the required accuracy. Nevertheless, the aforementioned methods are time-intensive, typically spanning several days.

Extensive efforts have been dedicated to simulating the WVTR in TFE. And the barrier effect of organic-inorganic film laminated encapsulations have been systematically studied through finite element simulation. However, the outcomes of this simulation were limited to normalized results and trends, rendering them insufficient for accurately characterizing the actual barrier performance of TFE. The simulation enables the coupling of different physics fields, allowing for the simulation of complex interactions between various physical phenomena. Based on Fick's laws of diffusion and geometric defect penetration, we determine an appropriate finite element simulation model based on the properties of SiN_x and SiO_xN_y inorganic thin films in this paper.

We established a finite element model firstly, guided by the mathematical model and simulation parameters. To enhance accuracy, we integrated experimental results to optimize the model. Subsequently, we reported the simulated WVTR for inorganic thin film encapsulation, demonstrating alignment with experimental results. Additionally, we employed the model to predict the WVTR of TFE with different isolation column structures, to assess the application potential of the model in the OLED display field.

2. Model and Simulation

Firstly, we investigated the diffusion behavior and concentration changes of water vapor in the thin-film encapsulation based on Fick's law. There is a simulation module: transfer of dilute species in porous media, which can be used to solve the equations about Fick's laws. Fick's law has been generally applied to the analysis of water vapor permeation behavior in inorganic layers with uniform and nano-scale defects. The existing inorganic films in TFE deposited by PECVD predominantly consist of nano-defects, which are homogenized and considered to be uniformly dispersed throughout the film. There are mainly intrinsic permeation and defect permeation in the process of water vapor permeation through inorganic TFE films. Thus, it is appropriate to employ Fick's diffusion equation to examine the permeation of water vapor. Based on Fick's second law, the time-dependent diffusion of water vapor within the inorganic TFE film can be described by the following equation:

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial^2 x} + \frac{\partial^2 c}{\partial^2 y} + \frac{\partial^2 c}{\partial^2 z}\right) + f \qquad (1)$$

Where D is the diffusion coefficients, and f is the source term, primarily accounting for defect permeation and chemical reactions in the unsteady diffusion process. The mathematical model captures the influence of the chemical reactions on the water vapor concentration.[2] The initial condition of water vapor concentration is set as follows:

$$c_i(0, x) = 0 \ , \quad 0 < x < h \qquad (2)$$

Where c is the concentration at position x, and h is the thickness of the the inorganic film.

The Dirichlet boundary conditions are set as follows:

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$$c_1(\mathrm{t},0) = S_1 p_0 \qquad (3)$$

$$c_\mathrm{N}(\mathrm{t},h) = S_N p_h = 0 \qquad (4)$$

Where S_1 is the solubility coefficient of surface in contact with water vapor, while p_0 denotes the initial partial pressure of water vapor at the film surface. S_N is the solubility coefficient of water vapor permeating the surface of inorganic thin films and ph is the partial pressure of the surface outflow from the film surface. [3]

Based on the aforementioned theory, we developed a simulation method for water vapor permeation through the inorganic TFE films; the specific methods are detailed as follows. 1) Determine the physical fields and simulation parameters, and establish the water vapor permeation simulation model based on the mechanism of water vapor permeation (Fick's law). 2) Set environmental conditions and material parameters, and substitute them into the simulation model for solution. 3) Optimize the simulation parameters and simulation model for water vapor permeation based on the experimental results of WVTR. 4) Applied to the assessment of water vapor barrier capabilities of OLED encapsulation films, perform water vapor permeation simulation for the TFE films with specific materials and structural film layers.

To determine the environmental conditions and materials settings in simulations, we investigated the diffusion behaviors of the TFE inorganic films, including SiN_x and SiO_xN_y films deposited by PEVCD. As shown in Figure 1, we observed nano-scale defects of SiN_x film in the SEM images, and the defects exhibited a relatively uniform distribution of 1-10 nm throughout the film. This homogeneity of defects in inorganic films allows for their description using an ideal laminated model during the simulation.

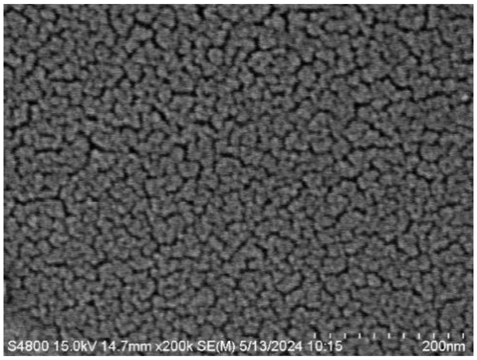

Figure 1. SEM image of the SiN_x TFE film deposited by PEVCD.

The WVTR measurements were conducted using MOCON equipment, and the WVTR value could be obtained at which the water vapor transmission rate stabilized. The steady-state flux (F_{ss}) can be calculated using equation (5):

$$\mathrm{F}_{ss} = \frac{DC_1}{\mathrm{L}} \qquad (5)$$

$$\mathrm{D} = \mathrm{D}_0 \times e^{-\frac{Ed}{RT}} \qquad (6)$$

Where L represents the thickness of thin film and Fss can be considered equivalent to the WVTR value when diffusion time becomes sufficiently large.[4] Based on Arrhenius' law, the activation energy (Ed) of the TFE film can be calculated using equation (6). We also assessed the impact of PECVD process parameters on the WVTR of inorganic films in the process. As depicted in Figure 2, the flow rate of hydrogen (H_2) and plasma power are identified as pivotal factors that significantly influence the WVTR of these films. Predominantly, these parameters affect the density and hydrogen content within the inorganic films, which in turn have a downstream effect on the WVTR. These film properties are reflected in the material parameter settings of the water vapor permeation simulation. Based on these findings, we are able to enhance the accuracy of our simulation model. Moreover, the solubility coefficient (S), the initial pressure (p_0), and other material parameters can be obtained through testing or calculation, which will be applied in the simulation to refine the water vapor permeation simulation model.

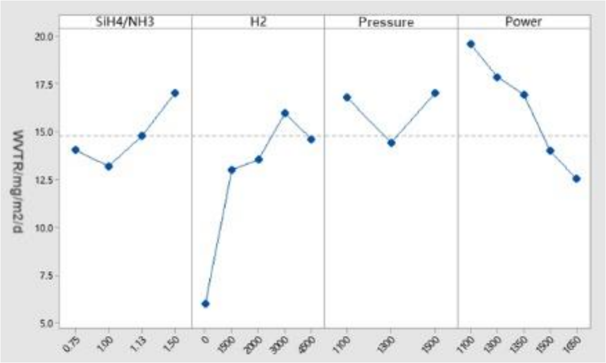

Figure 2. The impact of PECVD process parameters on WVTR of inorganic films.

In the simulation process, the physical field of transfer of dilute species in porous media based on Fick's second law is initially selected. Subsequently, the initial conditions, boundary conditions, and respective boundary parameters are incorporated into the physical field. Consequently, water vapor concentration and flux (corresponding to WVTR) at any position within the thin film geometry and at any given time can be calculated through simulation. To validate the accuracy of the aforementioned water vapor permeation simulation, SiN_x TFE films of varying thickness were deposited by PECVD, and their WVTR were simultaneously tested and simulated. It was observed that the peak values of the water vapor permeation simulation curves for different samples closely approximated the measured values and were within the same order of magnitude, with the simulation deviation value below 3.92E-04 $g/m^2/d$ (Figure 3). The simulated and tested WVTR values were of the same order of magnitude, and the accuracy of the simulated WVTR curve could be further enhanced through more appropriate parameter settings within the simulation model, among other factors. Furthermore, the WVTR results obtained through the simulation model demonstrated high reliability.

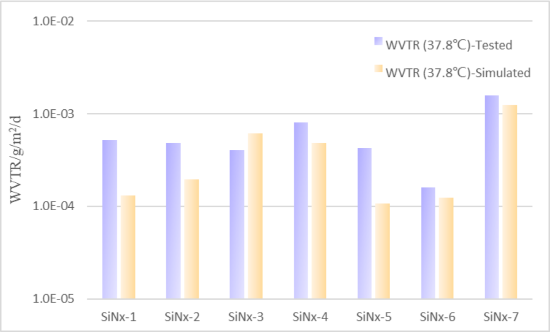

Figure 3. Test and simulate WVTR of different samples

3. Cases and Results

Subsequently, the water vapor permeation simulation model was applied to predict and evaluate the moisture barrier capability of the TFE layers in OLED devices. OLED isolation columns are a critical component of OLED devices, playing a crucial role in ensuring the proper functioning and longevity of the display by providing electrical isolation between pixels (Figure 4). A well-designed isolation structure can enhance the durability and lifespan of OLED devices by protecting them from external factors such as moisture and stress.

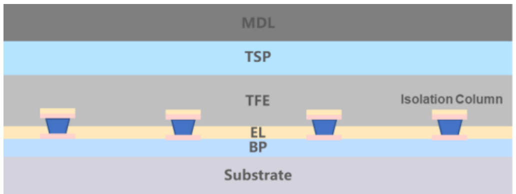

Figure 4. Stacked structure of OLED devices.

Therefore, the water vapor permeation simulation is of substantial practical significance in forecasting the moisture barrier efficacy of TFE layers above the isolation columns and subsequently refining the structure of these columns, which is beneficial for improving the lifetime of OLED devices and mitigating performance degradation caused by GDS (Growing Dark Spot).

As illustrated in Figure 5, there are three distinct types of isolation columns, with varying undercut structures and pixel isolation capabilities. The cross-sectional view above the isolation column represents the corresponding encapsulation layer (CVD layer), which was utilized to establish the simulation model for water vapor permeation. Additionally, the environmental conditions for the simulation were set at 85℃/85% RH, and the length of TFE layers was consistently modeled at 14.7um.

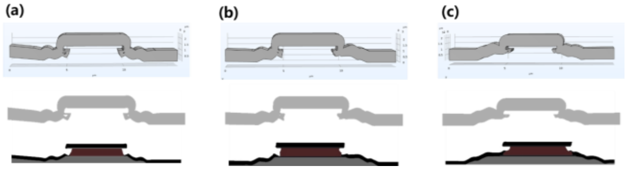

Figure 5. Structures of different types OLED isolation column, their encapsulation layers and the corresponding simulation model of TFE layer.

The water vapor permeation simulations were conducted based on the aforementioned simulation models, with the water vapor direction proceeding from the upper surface of the encapsulation film layer towards its lower surface. The permeation simulation was executed for 2000 hours, at which point the water vapor permeation process of different models had attained an equilibrium state. As illustrated in Figure 6, the efflux surface of three permeation models reached water vapor permeation equilibrium between 800H and 1000H, at which point the encapsulation layers were rendered completely ineffective. Furthermore, the simulation results indicated that the order of encapsulation layer failure, when water vapor permeation occurred from top to bottom, was b (803H) < a (888H) < c (917H). Consequently, the order of their water vapor blocking capacity was b < a < c, which aligned with the results of our experimental evaluation in the trend of sample failure sequence. This phenomenon may be attributed to the variations in height and width of the undercut structures. For instance, the encapsulation film layer of structure b exhibits relatively thinner weak spots compared to the other two structures (Fig 7), rendering it more susceptible to failure during the water vapor permeation process. Thus, the simulation can be utilized for evaluating the lifetime of the OLED device.

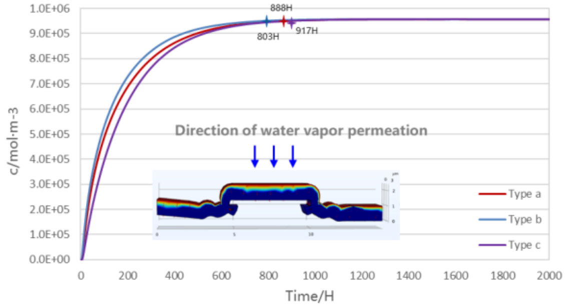

Figure 6. Results of water vapor permeation simulations in vertical direction.

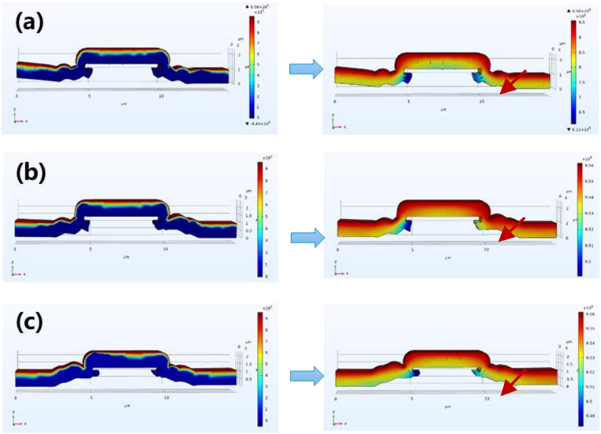

Figure 7. Results of water vapor concentration distribution at 0h (left) and 1000h (right), respectively.

Following the permeation simulations in the vertical direction, water vapor permeation simulations in the lateral direction were performed to compare permeation in different directions. The simulation results, depicted in Fig 8, demonstrate a different order of encapsulation ability among the three types of isolation columns (c < b < a), and this could be attributed to the differences in effective encapsulation distance. Additionally, the simulated water vapor permeation process did not reach an equilibrium state within 8000 hours, which contradicts the results of the experimental evaluation. Therefore, it is postulated that the primary direction of water vapor permeation in the aforementioned models is from top to bottom, while lateral water vapor permeation existed but did not cause encapsulation failure within 8000 hours. In the absence of interface peeling and bubbling, the predominant cause of encapsulation failure is vapor permeation from top to bottom. Consequently, the water vapor permeation simulations accurately portray the trend of water vapor permeation in different TFE structures.

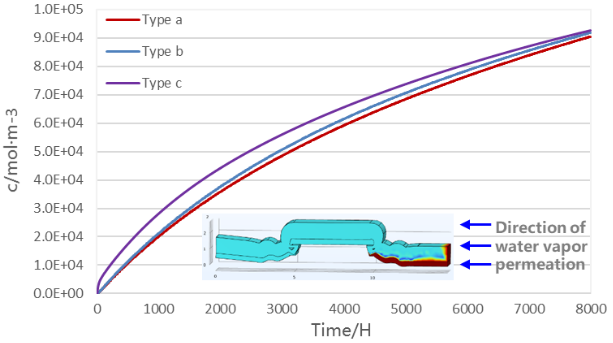

Figure 8. Results of water vapor permeation simulations in lateral direction.

4. Conclusion

Based on Fick's law, we established a water vapor permeation simulation model, which can be apllied in the simulation to evaluate and predict the water vapor permeation behavior of inorganic TFE films. Under appropriate simulation conditions, the simulation model successfully predicts WVTR values for fifferent SiN_x and SiO_xN_y film thicknesses, and the simulated WVTR closely aligns with the experimental results with the simulation deviation value below 3.92E-04 $g/m^2/d$. Moreover, the simulation model enables the prediction of failure time and barrier performance of different TFE films, corresponding to different isolation column structures of OLED device. To conclude, the simulation model is of great significance in assessing and predicting the encapsulation capability of OLED devices.

5. References

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