HEFAT2010
7th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics
19-21 July 2010
Antalya, Turkey

CHARACTERISTICS OF THERMAL-STRUCTURAL INTERACTION ON ORGANIC THIN FILM TRANSISTORS

Lee D.-K., Lee N.-E. and Kim Y.-J.*
*Author for correspondence
School of Mechanical Engineering,
University of Sunkyunkwan,
300 Cheoncheon-dong, Suwon 440-746,
South Korea,
E-mail: yjkim@skku.edu

ABSTRACT

Organic thin film transistors (OTFTs) on a flexible substrate offer many advantages in the fabrication of low-cost sensors, e-paper, smart cards, and flexible displays. The performance of OTFTs in upper and lower contact structured devices is affected by parameters such as the temperature and field effects. Regarding the key device parameter that affects the performance, the heat transfer and thermal stress of layers are matters of grave concern for maintaining the stability. In this study, we simulated the physical characteristics through coupled thermal, electrical, and structural analysis of OTFTs under various drain-voltage conditions. The electrical characteristics such as current vs. voltage were estimated by the measurement of various temperatures ranging 293 to 393K at a fixed drain voltage (V_{SD}), viz, either -1 V or -20V. The result shows that because the top layer in an OTFT features poor chemical union and differential thermal expansion coefficients between the Au electrodes and the Pentacene layer, hole mobility increases when the temperature raised from 370K. The analytical model estimated that how much current and increase in temperature displace the layers, because the thermally induced stress loads the material and deforms the OTFTs. As a result, the crystals of the pentacene layer are affected by the specific stress of the relative layers, which causes thermal resistance. Also, the heat-transfer characteristics lead to displacement of layers through the thermal expansion of the OTFTs.

INTRODUCTION

Various semiconducting organic materials have been used up to now for the fabrication of thin film transistors due to the attractive characteristics such as cheap, flexible, large-area organic-based solar cells. Pentacene is one of the most investigated organic materials to maintain the high performance of flexibility [1, 2]. However, the performance of all-organic TFTs has been limited by the low conductivity of the organic conductors as well as by the low adhesion between the pentacene and the Au source/drain electrodes in top contact structure because there no chemical interaction [3, 4]. Of the parameters affecting device performance, temperature is the key parameter of interest, which can cause damages to crystals of Pentacene and poor adhesion between organic layers and metal electrodes. The very fine turning of the structural characteristics of the semiconducting layer in the early 1990s allowed an understanding of the key relationship between carrier mobility and surroundings temperatures [5, 6]. As reported previously [7], the Lucent Bell Labs group has been able to propose clear evidence of the morphological origin of the very high field-effect mobility in pentacene-based thin film transistors. As for the correlation between the morphology of the interface at source and drain electrode and the effective field-effect mobility in OTFTs, a study performed by Bratina et al. [8] showed a strong correlation between contact regions. Furthermore, Varahramyan et al. [9] studied the temperature dependence of the hole mobility in pentacene with different temperature ranges and that hole mobility peaked between 300K and 450K. More recently, Chang et al. [10] investigated the thermoviscoelastic stress in thin films/substrate system. As a result, it is necessary to understand the characteristics of thermal-structural interactions in the context of surroundings temperatures. There are few published numerical analyses for thermal stress of thin film transistors by means of numerical study and the operational suitability such as the hole mobility in various temperature conditions. In addition, it is quite interesting to analysis the how much thermal stress is effect on electric field including Au electrode and pentacene layer in condition of steady state.

In the present study, the operational stability of OTFTs, in the hole mobility and I-V characteristics has been evaluated for various temperatures. Moreover, COMSOL Multiphysics (3.5a) was used as the commercial CFD code to analyze the thermal-structural interactions such as the effects of the thermal stress effects on all the layers.

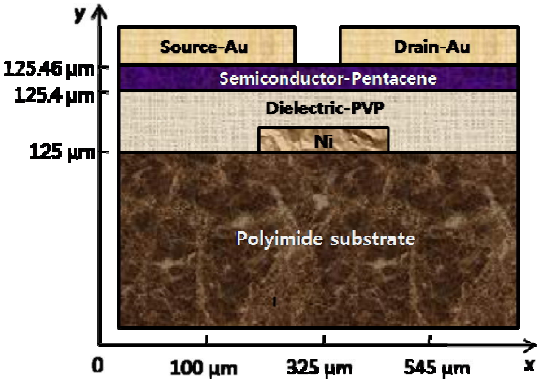

Figure 1 Schematic of the fabricated OTFT.

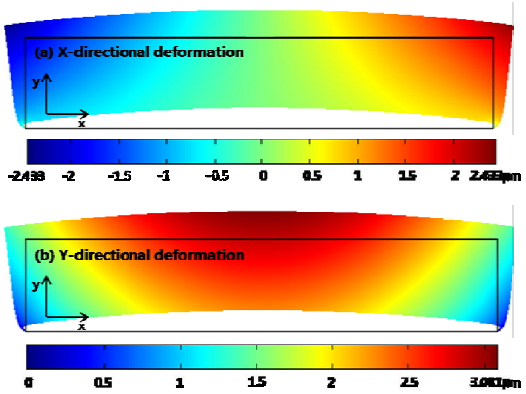

Figure 2 Numerical results of the deformation at a temperature of 373K: (a) x-direction and (b) y-direction.

EXPERIMENTS

A schematic of the fabricated OTFT is shown in **Figure 1**. OTFTs with a pentacene layer (30nm), gold S/D electrodes (70nm), cross-linked PVP (400nm-poly-4-vinylphenol), and gate dielectric layer (150nm) were fabricated on 125-μm-thick PI film (Du Pont : Kapton®) [3, 11].

The fabricated devices were tested with Semiconductor Parameter Analyzer (HP-4145B) at dark atmospheric ambient and N_2 blowing condition. The characteristics of I-V and transfer of OTFTs have been measured, while heating the stationary temperature conditions from 293K to 373K.

For higher values of V_d, after pinch-off of the channel, the saturation regime is described by

$$I_{d,sat} = \left(\frac{W}{2L}\right)\mu C_i\left(V_g - V_T\right)^2 \quad (1)$$

$$V_T = (qdp_0)/C_i \quad (2)$$

Equation (1) shows that the value of the carrier mobility is critical parameter defining semiconductors, for it directly controls the level of current output of OTFT. Where μ is the field-effect carrier mobility, V_T is the threshold voltage, given by Eq. (2), where q is the absolute electron charge and p_0 is the hole density at zero voltage and d is the semiconducting film thickness.

NUMERICAL METHOD

The problem-specific numerical model was validated numerically through the commercially available computational package, COMSOL. The main geometrical parameters are shown in Table 1. In order to analyze the thermal loads and expansion in the x- and y-directions including all the layers, the OTFT is designed for simplicity in a 2-D structure, which assumes that the z-component of the strain is zero.

Table 1 Dimensions of the modeled layers of the OTFT.

Pentacene layer	Ni Gate electrode	Au S/D Electrode
60 nm	150 nm	70 nm
Thick PI Film	Cross-linked PVP	Channel Length
125 μm	400 nm	40 μm

For subsequent analysis of the thermal-structural interaction, the 2-D plane strain application mode and general heat transfer mode are used. The lower-left and lower-right corners of the substrate are fixed for assuming rigid-body movements but the other layers, excepting the substrate, are not fixed so that a free body can be assumed. The thermal-structural characteristics of the OTFT are estimated by the measurement of the temperature that ranges from 290K to 373K. The model of the simulated OTFT contains only thermal loads, which are introduced into the constitutive equations according to the following equations:

$$\sigma = D\varepsilon_{el} + \sigma_0 = D(\varepsilon - \varepsilon_{th} - \varepsilon_0) + \sigma_0 \quad (3)$$

$$\varepsilon_{th} = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{xz} \end{bmatrix}_{th} = \alpha_{vec}\left(T - T_{ref}\right) \quad (4)$$

where σ is the stress vector, D is the elasticity matrix, ε_x, ε_y, ε_z, γ_{xy}, γ_{yz}, γ_{xz} are the strain components, α_{vec} is the thermal expansion coefficients, T is the actual temperature, and T_{ref} is the reference temperature. For analyzing the pentacene layer as an excessively narrow region with a thickness of 70 nm in the y-direction, in the grid system the numerical meshes, a number of elements are concentrated in the pentacene channel, which causes most of the electrical characteristics. As a result, the grid systems and degrees of freedom for all the layers have a total of 7,570 and 61286 elements, respectively.

Table 2 Material parameters used in numerical study.

Material	Young's modulus (GPa)	Poisson's ration	Thermal expansion coefficient (10^{-6}/K)
Au	70	0.44	14.2
Ni	219	0.31	13.4
PVP	200	0.33	100
Pentacene	2.7	0.33	150
Polyimide	3.1	0.33	55

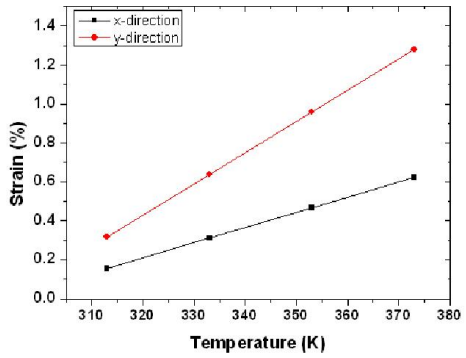

Figure 3 The normalized maximum values of strain at the coordinates (x=200μm, y=125.4μm; refer Figure 1) between the Au electrodes and Pentacene layer by means of cross section analysis when different temperatures are forced.

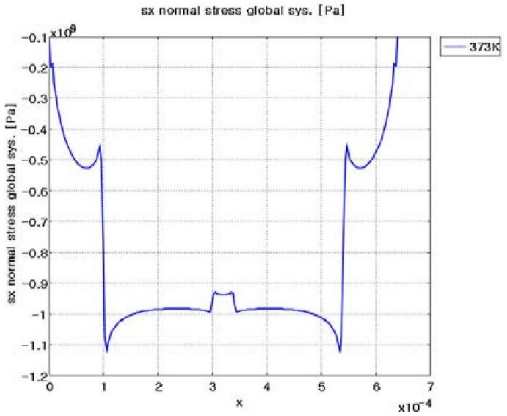

Figure 4 The normal stress distribution in x-direction from numerical COMSOL results at temperature of 373K.

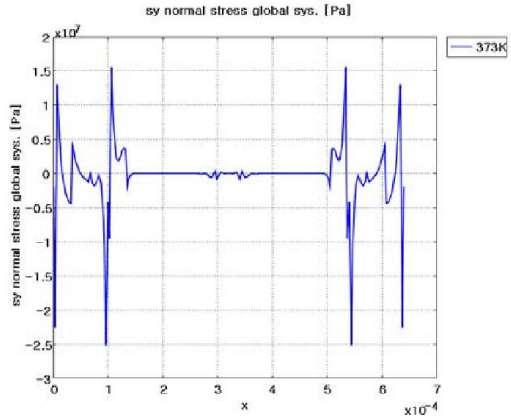

Figure 5 The normal stress distribution in y-direction from numerical COMSOL results at temperature of 373K.

RESULTS AND DISCUSSION

In this paper, the effects of the thermal stress of OTFT layers, σ_{xy}, electrical characteristics such as hole mobility with temperature variations were studied by numerical and experimental methods respectively. In the numerical analysis, the thermal-structural interaction was taken to obtain the stress, strain and deformation at the conditions of temperature dependence. The material properties of the OTFT are listed in Table 2. In real applied boundary conditions, the uncertainty in given input parameter may be considered and independently estimated from several different sources. However, the effect of uncertainty in the input parameters for relative thin layers such as 30nm-semiconductor layer than 125μm-polyimide layer could assume to have specific values of Young's modulus (E), Poisson's ratio (ν), and thermal expansion coefficient (α).

Figure 2 shows a representative transition of the total deformation at a specific temperature at 373K. The temperature causes thermal stress to the OTFT layers in the stationary condition, and causes deformation in xy-direction since each different thermal expansion coefficients of layers. This figure noted that there is curled shape in x-direction of 2.433μm and y-direction about 3.081μm. In **Figure 3**, the maximum values of xy-strain values at the region of contact between the pentacene layer and PVP layer as a channel region are plotted as a function of the temperature. The main strain inclination can be derived from the difference in deformational transition at this contact region because of, this region of contact point is shows that the y-strain value of 1.28% are better deformed than x-directional its 0.623% when maximum temperature (373K) applied. It is worth mentioning that most deformation occurred in y-direction and gave form to a curve when thermal energy loads to OTFT. From that curled form, it is also noticed that distances between crystals in lower the pentacene region can be narrowed.

Figures 4 and **5** respectively show the normalized stress distributions in the x- and y-directions as a function of the x-directional length at temperature of 373K. By comparing these two figures, it is inferred that the values of x-directional stress shows negative values but its y-directional stress shows positive at the same channel region.

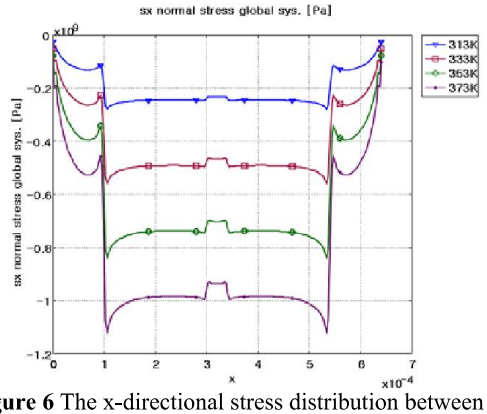

Figure 6 The x-directional stress distribution between the pentacene layer and PVP layer from numerical results for temperatures ranging from 313 to 373K.

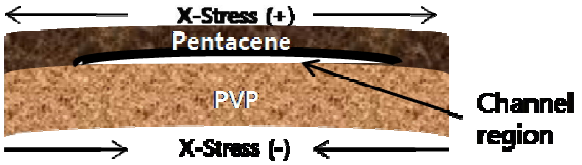

Figure 7 Schematic of the curl of pentacene / PVP dielectric due to thermal stress.

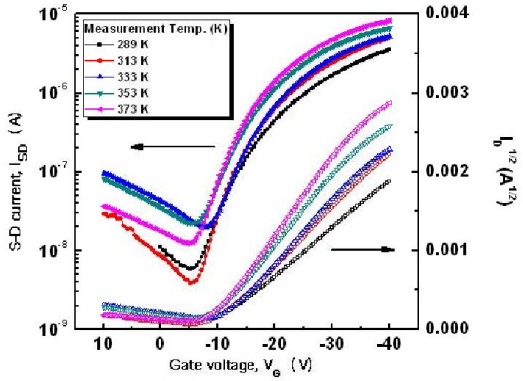

Figure 8 Transfer characteristics measured at temperature ranging from 289 to 373K. V_{GS} was swept from 10 to -40V at V_{DS} = -20V.

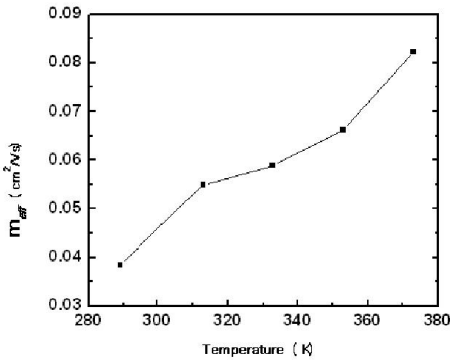

Figure 9 Temperature dependent hole mobility at V_{DS}=-20V and V_{GS}=-40V.

Besides, it can be found that the situation is symmetric around 320μm in x-axis. This phenomenon is because of the symmetric geometry around the channel region and the uniformly loaded thermal stress. As expected, the region of contact region such as channel, 100μm and 540μm, in the x-direction layer has negative value of stress in x and y directions of -600MPa and 150MPa respectively, since there is shrink phenomena. To obtain a more useful result, the normalized x-directional stress is analysed in **Figure 4**. By comparing **Figures 4** and **6**, they display similar pattern of stress distribution in x-direction. In **Figure 6,** four different cases of x-directional stress values with temperature increase are analyzed for thermal stress between the Au electrode layer and pentacene layer. The patterns of x-stress distribution of other cases, like the preceding analysis of **Figure 4**, appeared similar pattern since assumed elastic structure.

According to the analysis of these figures, the x-directional stress as an effective parameter for thermal expansion occurred almost at whole layers when the thermal energy loads to OTFT. Furthermore, it is observed that in each curve there exist negative values of x-directional stress in the region of channel and symmetric diagram around the channel region. In addition, as shown in **Figure 7,** in order to understand what type of deformation generated on interface between the pentacene layer and PVP layer, schematic geometry is described.

The experimental results of the hole mobility as a function of temperature are shown in **Figures 8** and **9**. It is found that over the temperature range of 287-373K, the mobility increases to a peak value. Hole mobility reflects the number of carriers that contribute to the condition at a channel [12]. Furthermore, the temperature dependence of hole mobility characteristics can be affected by the device structure, especially by the contact resistance between the pentacene layer and Au electrodes and channel length. As shown in Figure 7, we can observe a decrease of channel length; this effects can induce a increase of electrical performance such as hole mobility.

CONCLUSIONS

This paper has proposed thermal-electrical and thermal-structural interaction for the layers of sampled OTFT in order to take into account the thermal stress, and used it to estimate the deformational effects of hole mobility between the Au electrodes and the pentacene layer with temperatures ranging from 273 to 373K. The findings are as follows.

The experimental results of thermal-electrical analysis indicate that at a higher temperature value of 373K, hole mobility have displayed hole mobility of 0.082cm^2/Vs, threshold voltage of -10V; furthermore, this mobility is found to a peak value between 287-373K. According to the numerical results of thermal-structural analysis, the deformed shape of curl the region of channel had a negative value of x-directional stresses of -600MPa when hole mobility approach to peak value at temperature of 373K. Finally, it was found that, the influences of induced thermal stress to OTFT can cause shrink of the channel length which causing decrease of crystal distances in lower the pentacene layer and also an effect on hole mobility increase.

ACKNOWLEDGMENTS

Financial aid from the Korea Ministry of Education through the Brain Korea 21 Project is gratefully acknowledged. The authors are also grateful for financial support provided by the Korea Research Foundation (Grant R01-2008-000-20533-0).

REFERENCES

[1] Cherie R., Kagan, Paul A., Thin-film transistorss, *Proceedings of the 2nd International Conference on Integrated Power Systems (CIPS),* 2002, pp. 25-34.

[2] Klauk H., Gundlach D.J., Nichols J.A., Jackson T.N., Pentacene organic thin film transistors for circuit and display applications., *IEEE Trans Electron* Dev., Vol. 46., 1999, pp. 1258-1263.

[3] Seol, Y.G., Lee, N.-E., Park, S.H., Bae, J.Y., Improvement of mechanical and electrical stabilities of flexible organic thin film transistor by using adhesive organic interlayer, *Organic Electronics 9*, 2008, pp. 413-417.

[4] Noh H.Y., Seol Y.G., Kim S.I., Lee N.E., Improvement of Electrical and Mechanical Characteristics of Organic Thin Film Transistor with Organic/Inorganic Lamicated Gate Dielectric, *J. Kor. Inst. Sur. Eng*., Vol. 41, 2008, pp.1-5.

[5] Garnier F., Yassar A., Hajlaoui R., Horowitz G., Deloffre F., Servet B., Ries S., Alnot P., Molecular engineering of organic semiconductors. Design of self-assembly properties in conjugated thiophene oligomers. *J Am Chem Soc.* 115 pp. 8716-8721.

[6] Servet B., Horowitz G., Ries S., Lagorse O., Alnot P., Yassar A., Deloffre F., Srivastava P., Hajlaoui R., Lang P., Garnier F., Polymorphism and charge transport in vacuum-evaporated sexithiophene films. *Chem Master 6*, 1994, pp. 1809-1816.

[7] Laguindanum J.G., Katz H.E., Lovinger A.J., Dodabalapur A., Morphological origin of hogh mobility in pentacene thin-film transistors., *Chem Master 8*, 1998, pp. 2542-254.

[8] Petrovic A., Pavlica E., Bratina G., Carpentero A., Tormen M., Contact resistance in organic thin film transistors, *Syntheric Metals*, Vol. 159, Issue 12, 2009, pp. 1210-1214.

[9] Zhu M., Liang G., Cui T., Varahramyan K., Temperature and field dependent mobility in pentacene-based thin film transistors, *Solid-State Electronics*, Vol. 49, Issue 6, 2005, pp. 884-888.

[10] Chang W.J., Fang T.H, Weng C.I., Thermoviscoelastic stress in thin film/substrate system, *Thin Solid Films*, Vol 515, 2007, pp. 3693-3697.

[11] Seol Y.G., Lee J.G., Lee N.-E., Effects of different electroplated gate electrodes on electrical performances of flexible organic thin film transistor and flexibility improvement, *Organic Electronics*, Vol. 8, 2007, pp. 513-521.

[12] Takamatsu Y., Sekitani T., Someya T., Temperature dependence of Hall effects in organic thin-film transistors on plastic films, *Applied Physics Letters*, Vol. 90, 2007, pp. 133516-133518.