A Numerical Study of the Heat Transfer Phenomena on ZnO Pyroelectric Film Sensor

M. S. Suen, David T. W. Lin, Y. C. Hu, J. C. Hsieh

***Abstract*—This paper proposes a simulated model combined with the finite element method (F.E.M) to obtain the temperature profiles of the ZnO pyroelectric film sensor. A novel design of the top electrode is discussed and it can enhance the rate of temperature variation significantly. This study proves that the temperature variation transform to the corresponding electrical signal by the pyroelectric effect is a very important issue for the response of the pyroelectric film sensor. To go further, we will apply these results to detect the environmental temperature for the artificial skin of robots, and integrate with clothes to perform human health detection. In addition, the knowledge of the thermal-electric conjugated problem can be built through this study gradually.**

***Keywords:* finite element method (F.E.M), pyroelectric film sensor, ZnO**

I. INTRODUCTION

In recent years, the ferroelectric materials have been developed gradually in MEMS. One of them is that pyroelectric film is studied intensively for some applications such as the temperature sensor, the fire alarm, the sensor of pollution monitor, the pyroelectric infrared detector, the thermal image detector and actuator. Consequently, the pyroelectric sensors use the pyroelectric effect to transform the variation of the temperature variation into the electrical signal completely.

The technique of the ZnO thin film is expanded quickly in several years. It is developed many kinds of variety manufactured methods for the ZnO thin film. Those indude the DC or RF sputtering [1], chemical vapor deposition [2], metal organic chemical vapor deposition [3], sol-gel method [4], spray pyrolysis [5] and laser deposition et al.. The sol-gel [4] method is selected for saving the cost device and printing large area of the thin film uniformly. The characteristics of ZnO film which on the aluminum substrate are printable and flexible. In the applications, the flexible film sensors can capture the image from biomedicine, artificial skin, and wearable electronics. In the other part, the pyroelectric film has been applied widely for measring the variation of the temperature. For these reasons, the ZnO pyroelectric film sensors have some advantages, such as low cost, room-temperature operation (300K), and fast and wide spectrum with high sensitivity.

Li et al. [6] use ANSYS to simulate the temperature field of multilayer pyroelectric thin film sensor and show that the porous silica film as a thermal-insulation layer reduce obviously the loss of heat from the pyroelectric film sensor to the Si substrate. Hsiao et al. [7] make the flexible pyroelectric sensor and design four types of the top electrode on ZnO film sensor. Häusler et al. [8] simulate the complex interaction in the physical fields realized by implementing a two-step approach that take advantage of the internal computational routines of finite element programs. Tang et al. [9] present the results of the better pyroelectric response, those can be expected by controlling the temperature below $70\ (°C)$ during the fabrication of the pyroelectric detectors, as selecting the suitable absorption layer with high absorption coefficient, and decreasing the thickness of the ments. Ko et al. [10] verify the theoretical analysis in the micro machined $Pb(Zr_{0.3}Ti_{0.7})O_3$(PZT30/70) thin film pyroelectric detectors with different silicon substrate thickness fabricated and characterized. Vanderpool et al. [11] convert the waste heat into electricity by using pyroelectric materials directly. In addition, they propose a simulation of prototypical pyroelectric converter by F.E.M solved by the momentum, and energy equations. Limbong et al. [12] investigate that the effect of a varying bias field on the pyroelectric properties of sub-micron ferroelectric polymer films. They propose that the magnitude and phase of the pyroelectric signal reflect the hysteresis in the polarisation resulting from the bias field. The simulation and analysis on the design of the top electrode shape are discussed respectively in this paper.

In this paper, a simulation of transient heat conduction in the pyroelectric film sensor is used to design the shape of top electrode. The reason is that the temperature variation rate in the pyroelectric film sensor is an important issue. This investigation proposes a simulation of the temperature variation which is based upon the finite element method. In future, we can combine the optimization method with finite element method to design the shape of the top electrode, and obtain the best benefit for improving the temperature variation rate of pyroelectric film sensor.

It includes four sections in this paper. The first section introduces the characteristics of ZnO pyroelectric film sensor and more investigations are researched for applications and simulations of pyroelectric material. In the second section, it is illustrated the numerical analysis and modeling in this study. The results and discussions of the different design of the top electrode shape on ZnO pyroelectric film sensor are presented in the third section. All contributions and possible applications of this study are concluded in the final section.

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At last, it also can be combined with the optimal numerical method in the proposed simulation to gain the greatest benefits to the thermal response of the pyroelectric film sensor.

II. NUMERICAL ANALYSIS AND MODELING

The shape design of the top electrode in the pyroelectric film sensor is very important. The dynamic pyroelectric response current of multilayer pyroelectric thin film sensor can be expressed as below: [6]

$$i_p = \eta PA \frac{dT}{dt} \qquad (1)$$

where η is absorption coefficient of radiation

P is the pyroelectric coefficient of pyroelectric thin film
A is the detector area
dT/dt is the temperature variation rate of pyroelectric film

The response current of the multilayer pyroelectric thin film sensor is proportion to the temperature variation rate of the pyroelectric film sensor. A large scale of the temperature variation rate leads to the higher response current. In addition, the top electrode design also affects to the response current and the temperature variation rate of the pyroelectric film sensor. There are four kinds of the top electrode namely the rectangle type, the crisscross type, the target type, and the web type are simulated in this study. The design of top electrode is a critical factor to affect the temperature variation rate in the pyroelectric film which proposed by Hu [7]. This problem is solved by the direct problem commercial solver of package. The governing equation about this model is listed as below:

$$\beta\rho C\frac{\partial^2 T}{\partial t^2}+\rho C\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+Q$$

$$(x_i, y_i)\in V \qquad (2)$$

Here, k ρC and β is the thermal conductivity, heat capacity, and relaxation time respectively. The above governing equations along with the boundary conditions are solved by adopting the well-received multi-physics analysis method.

The present finite element model of the ZnO pyroelectric film sensors is generated with F.E.M including four cases. Fig.1 is real size of the pyroelectric film sensor. Fig.2 shows all type shapes of pyroelectric film sensor. As shown in Fig.3, three layers in the each film sensor are in the present analysis. First, this problem is three-dimensional in thermal conduction. The parameters of various thermal properties of the films given in Table 1 were assigned to corresponding layers. Fig.3 shows that bottom layer made by Al, middle layer made by ZnO, and top layer made by Ag. In order to compare the result of the four models, some parameters of the films are assumed the same properties in the modeling, and changed the designs of the top electrode to get the different the data of the thermal conductibility. Second, the mesh number of the geometry in the modeling is appropriately. In boundary conditions, T_0 is the ambient temperature $(300K)$ and T the top electrode of the surface $(301K)$. At last, the interface between layer and layer is assumed continuity and other outside boundary conditions in the model are assumed insulation.

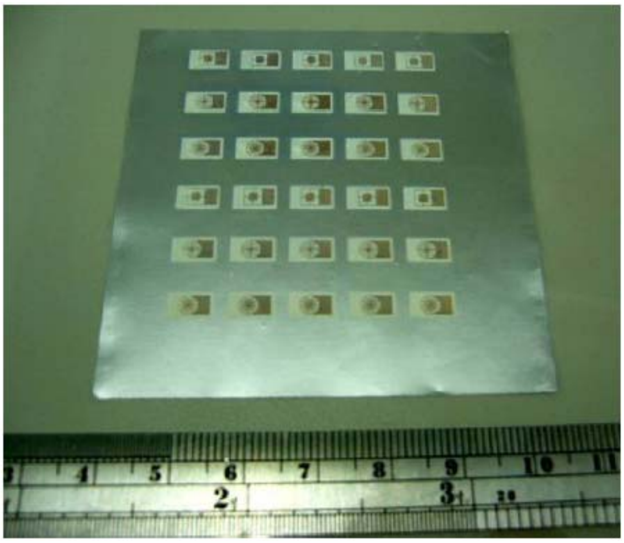
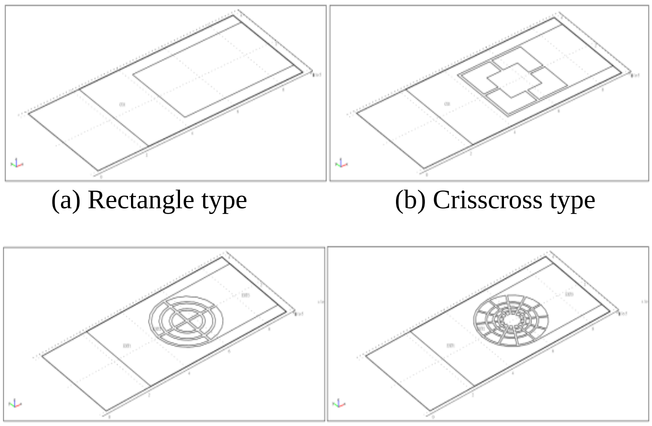


Fig.1 Real size of the pyroelectric film sensor.



(a) Rectangle type (b) Crisscross type

(c) Target type (d) Web type

Fig.2 Shape of the top electrode in the pyroelectric film sensor.

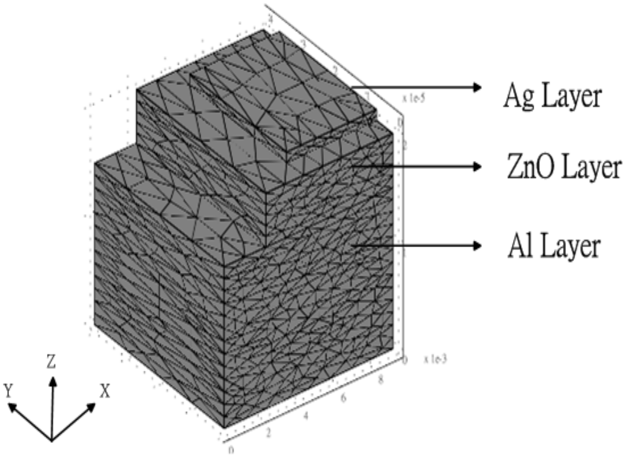


Fig.3 Layers of the pyroelectric film sensor.

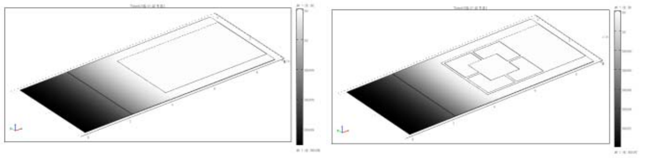
Table.1 Parameters of the model for Simulation

Material	Thermal conductivity $(W/m-K)$	Density (kg/m^3)	Heat capacity at constant pressure $(J/kg-k)$	Length (m)	Width (m)	Height (m)
Al	237	27000	940	9×10^{-3}	4×10^{-3}	1.5×10^{-5}
ZnO	6	5676	385	6.775×10^{-3}	4×10^{-3}	5×10^{-6}
Ag	429	10500	235	-	-	-

III. RESULTS AND DISCUSSIONS

The simulated results are assumed to expose $0\,(s)$ to $1\,(s)$ under the room-temperature. This paper uses the transient process to solve the temperature profile of the pyroelectric film sensor. In the finite element method package, it is hard to mesh the model that is why the length and height of the model have the different proportion obviously.

Fig.4(a)-4(d) show the temperature profiles of the different kinds of shape on the top electrode in the pyroelectric film sensor clearly and compare the influence of the temperature profile, respectively. Throughout these figures, it is obvious that the film sensor with the rectangle type electrode is better than the one with the web type electrode.


(a) Rectangle type
(b) Crisscross type

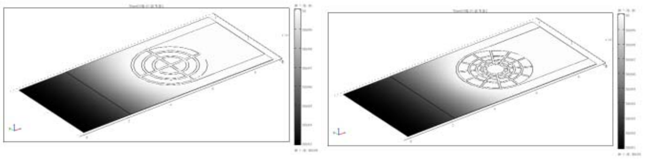

(c) Target type
(d) Web type

Fig.4 The temperature profiles of the top electrode in the pyroelectric film sensor.

In the Fig.5, it shows that the respone time of the temperature field from $0\,(s)$ to $1\,(s)$ and we can discover the temperature to increase during $0.1\,(s)$ to $0.4\,(s)$ rapidly. As can be seen in Fig. 5, the temperature response of the pyroelectric film sensor is affected by the electrode shape exactly. When the simulated time arrives at $0.1\,(s)$, the temperature of the film sensor with rectangle type electrode approaches to 300.8(K), and the one with the web type electrode approaches to 300.6(K). Through the comparison between two shape of the different top electrode on ZnO film sensor, Fig.5 shows that the heat transfer rate of the film sensor with the rectangle type electrode is higher 20% than the one with the web type electrode at $0.1\,(s)$. The other kinds of the top electrode have the similar trends as the temperature variation of the film sensor with the web type electrode.

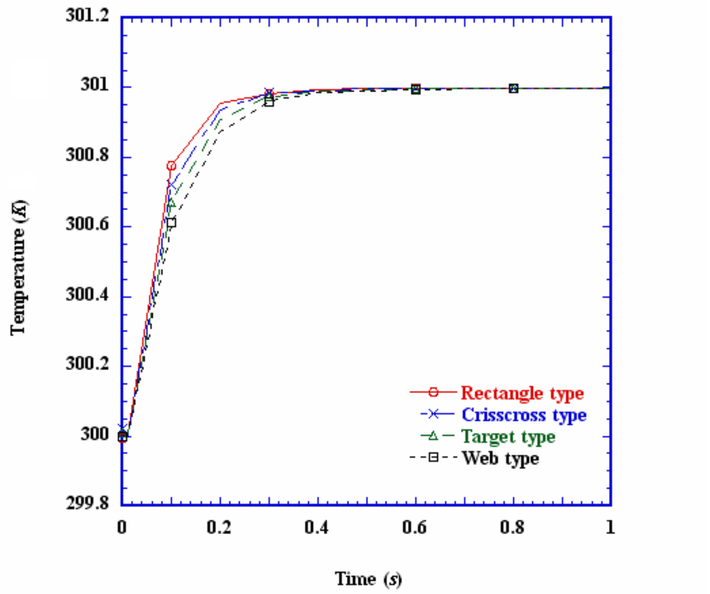


Fig.5 The temperature profiles of the pyroelectric film sensor with different shape type of the top electrode.

Fig.6 presents the temperature variation rate (dT/dt) with different types of the top electrode in the pyroelectric film sensor. The value of the temperature variation rate on ZnO film sensor decreases from $0\,(s)$ to $0.4\,(s)$. After the time is equal to $0.4\,(s)$, the temperature variation rate converges to 0. From these results, it is concluded that the effect of the electrode area is important. Fig.6 shows that initial temperature variation rate of the rectangle type is higher than others. It is obviously that the temperature response of the film sensor with the rectangle type electrode is faster than the ones with other type electrode. But, the temperature variation rate of the other type of the film sensor will be larger than the rectangle type of the film sensor gradually as the time after $0.1\,(s)$. This means that the response of the film affected by the different type of the film sensor is important within $0\sim0.1\,(s)$. This is the reason that the hyperbolic heat transfer phenomena happen in this model. More clear phenomena can be see from Fig. 7.

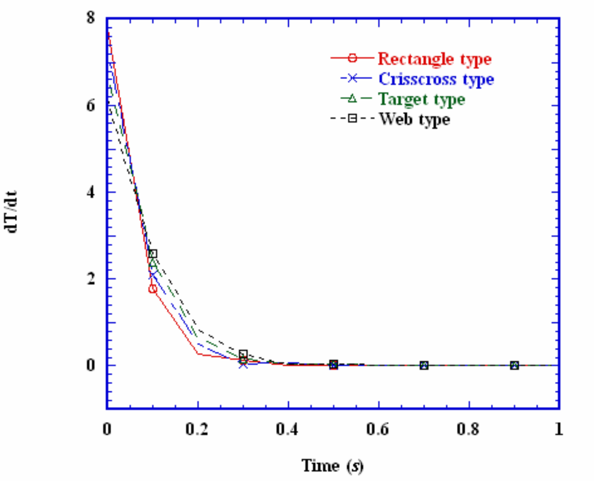


Fig.6 The temperature variation rates of the pyroelectric film sensor with different shape type of the top electrode.

From Fig.7, the second order derivative temperature (d^2T/dt^2) is proposed in the different type electrode of the pyroelectric film sensor. As can be seen from Fig.6 and Fig.7, the temperature variation rate (dT/dt) of the film sensor with the rectangle type electrode not only increases highest than the others, but also the second order temperature derivative decreases highest. As deduced from here, we know that each of the different shape type of the top electrode trends the same response after $0.1\,(s)$. In the other words, the temperature variation rate before $0.1\,(s)$ is an important issue on the speed of the temperature response.

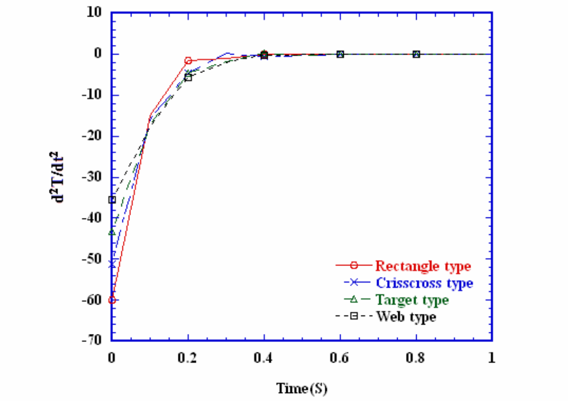


Fig.7 The Second order derivative of the temperature with different shape type of the top electrode.

These simulations prove that the design the shapes of the top electrode influences the thermal response of the pyroelectric film sensor is an important and interest problem. The results of these simulations can combine the finite element method and the optimal method to design the top electrode of the optimal shape and it would gain greatest benefits for improving the temperature variation rate of the pyroelectric film sensor.

IV. CONCLUSION

The temperature variation rate of pyroelectric film sensor is simulated by the finite element method in this paper. The simulated results prove that the shape of top electrode of pyroelectric film sensor affects the temperature variation rate is an important issue. And, it also shows that the response variation value of dT/dt and d^2T/dt^2 obviously varies from $0\,(s)$ to $0.1\,(s)$. In general, the temperature variation rate is an important problem on the ZnO pyroelectric film sensor. In order to obtain the different response, it presents the simulation for the different kinds of shapes design of the top electrode in this study. It can improve that the thermal response of the ZnO pyroelectric film sensor can be affected by the different kinds of the electrode. In future, we can combine optimal numerical method to gain the greatest benefits in the shape design of top electrode on the pyroelectric film sensor.

REFERENCES

[1] U. Ozgur, A. Teke, Liu, S. J. Cho and H. Morkoc, “Stimulated emission and time-resolved photoluminescence in rf-sputtered ZnO thin films,” *Applies Physics Letters*, Vol.84, pp.3223-3225.

[2] B. S. Li, Y. C. Liu, Z. S. Chu, D. Z.Shen, Y. M. Lu, J. Y. Zhang, and X.W. Fan, “High quality ZnO thin films grown by plasma enhanced chemical vapor deposition,” *Journal of Applied Physics*, Vol.91, pp.501-505, 2002.

[3] S. T. Tan, B. J. Chen, X. W. Sun and W. J. Fan, “Blueshift of optical band gap in ZnO thin films grown by metal-organic chemical-vapor deposition,” *Journal of Applied Physics*, Vol.98, pp. 013505-013505-5, 2005.

[4] B. Pal and M. Sharon, “Enhanced photocatalytic activity of highly porous ZnO thin films prepared by sol–gel process,” *Materials Chemistry and Physics*, Vol.76, pp.82-87, 2002.

[5] R. Ayouchi, D. Leinen, F. Martin, M. Gabas, E. Dalchiele and J. R. Ramos-Barrado, “Preparation and characterization of transparent ZnO thin films obtained by spray pyrolysis,” *Thin Solid Films*, Vol.426, pp.68-77, 2003.

[6] L. Li, L. Zhang, X. Yao, and B. Li, “Computer simulation of temperature field of multilayer pyroelectric thin film IR detector,” *Ceramics International*, Vol.30, pp.1847-1850, 2004.

[7] C. C. Hsiao, K. Y. Huang and Y. C. Hu,”Fabrication of a ZnO pyroelectric sensor,” *IEEE SensorJoutrnal*, Vol.8, pp. 185-192, 2008.

[8] C. Häusler, G. Milde, H. Balke, H. A. Bahr and G. Gerlach, “3-D modeling of pyroelectric sensor arrays part I: multiphysics Finite-Element simulation,” *IEEE Sensor Journal*, Vol.8, No. 12, December 2008.

[9] Y. Tang and H. Luo “High-performance pyroelectric single crystals for uncooled infrared detection applications,” *Infrared Physics & Technology*, Vol.52, pp. 180–182, 2009.

[10] J. S. Ko, W. Liu, W. Zhu snd B. M. Kwak, “Influence of the silicon substrate thickness on the response of thin film pyroelectric detectors,” *Solid-State Electronics*, Vol.46, pp.1155–1161, 2002.

[11] D. Vanderpool, J. H. Yoon and L. Pilon, “Simulations of a prototypical device using pyroelectric materials for harvesting waste heat,” *International Journal of Heat and Mass Transfer*, Vol.51, pp. 5052–5062, 2008.

[12] A. Limbong, and I.L. Guy, “Pyroelectric hysteresis in ferroelectric polymers,” *Thin Solid Films*, Vol.325, p.p 187–191, 1998.