Modeling and Simulation of Organic MEM Relay for Estimating the Coefficient of Thermal Expansion of PEDOT:PSS

Nabeela Zabin Khan

Rutgers – The State University of New Jersey, New Brunswick, NJ, USA, nzk7@rutgers.edu

ABSTRACT

Thermomechanical properties such as Coefficient of Thermal Expansion of the popular transparent electrode material PEDOT:PSS have not been reported which would be of interest to researchers in the fields of material science and solid state electronics. In a recent paper, our group presented the development of two polymer based (purely and partially polymeric) electrostatically actuated relays, which use PEDOT:PSS as a conductive layer in the three polymer layer movable gate. This paper presents the modeling and simulation of these prototype micro electro mechanical relays on finite element analysis (FEA) software CoventorWare. A number of simulations were run on compound field solver CoSolveEM, using different values of Coefficient of Thermal Expansion of PEDOT:PSS aiming at each of ten available data points on V_{NPI} at different temperatures. From the simulated results an upper estimate of thermal expansion coefficient of PEDOT:PSS was extrapolated.

Keywords: PEDOT:PSS, conducting polymer, MEMS simulation, CoventorWare, relay

1 MEM RELAY BASICS

A MEM relay is a mechanical switch that mimics the behavior of Field Effect Transistors. There are two parallel plate electrodes: a static bottom plate and a movable top plate, usually suspended from beams. When a voltage is applied between the two electrodes, the resultant electrostatic force pulls the top electrode downward. As the two electrodes come into contact, a current flows through the relay; hence the device is in its " On" state. To turn off the relay, the applied voltage has to be reduced below a certain amount known as the release voltage. In the off state there is no current flow as there is an air gap between the conductors. Since they are physically separated there is no off state leakage whereas transistors leak current in their idle state. The minimum required voltage to turn the relay on is called Pull In Voltage. The two features protruding from the top electrode are called dimples and the gap between the dimples and the bottom plate is called dimple gap, g_d. The gap between the two parallel plates is called actuation gap, g. Depending on the relative sizes of dimple gap and actuation gap a relay will operate in either pull in mode or non-pull in mode. If g_d is small (less than one third of g) the relay operates in non-pull in mode; if it is larger than one third of g, then it operates in pull in mode [1]. For pull in mode V_{PI} is given by the following equations:

$$V_{PI} = \sqrt{\frac{8K_{eff}\,g^3}{27\varepsilon_o A_{OV}}} \tag{1}$$

For the non-pull in mode V_{NPI} is given by:

$$V_{NPI} = \sqrt{\frac{2K_{eff}\,g_d(g-g_d)^2}{\varepsilon_o A_{ov}}} \tag{2}$$

$$K_{eff} = \frac{4t_m^3 W E_{eq}}{L^3}\,, \quad E_{eq} = \text{equivalent elastic modulus}$$

A_{ov} is the effective area of overlap between the two electrodes and ε_o is the permittivity of free space. K_{eff} is the effective spring constant of the structure.

2 ORGANIC MEM RELAY

In an earlier published work by the Rutgers Devices group, two prototype MEM relays: fully and partially polymeric relays were fabricated and the influence of temperature on their switching characteristics was investigated [2].

2.1 Modeling on CoventorWare

Six terminals: a movable gate, a body and two pairs of source/drain make up the relay structure [3]. The movable structure, suspended by serpentine springs, has three polymer layers: structural polymer (SU-8 shown in Cyan), conductive polymer (PEDOT: PSS shown in Red) and dielectric polymer (Cytop shown in Green). The pair of channels, dimples, sources and drains are made of PEDOT: PSS in the purely polymeric structure whereas ITO replaces PEDOT:PSS in the partially polymeric relay [2]. Both these relays were modeled on CoventorWare using the same materials, layout and process flow (as described in the previous paper) as the ITO electrode layers are insignificant in thickness compared to the rest of the structure.

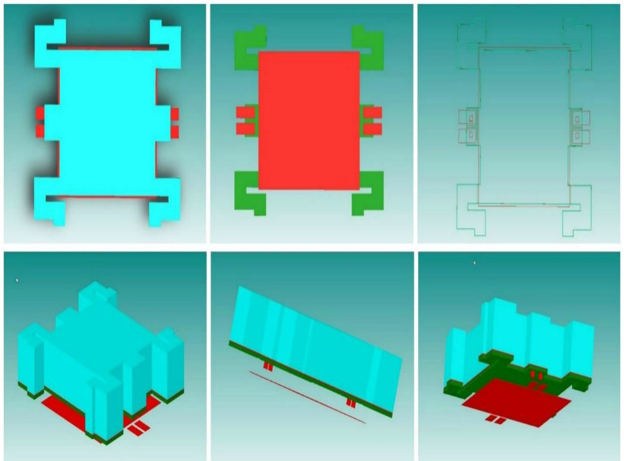


Figure 1: Top, Bottom and wireframe rendered 2D and 3D views of the prototype MEM Relay on PreProcessor.

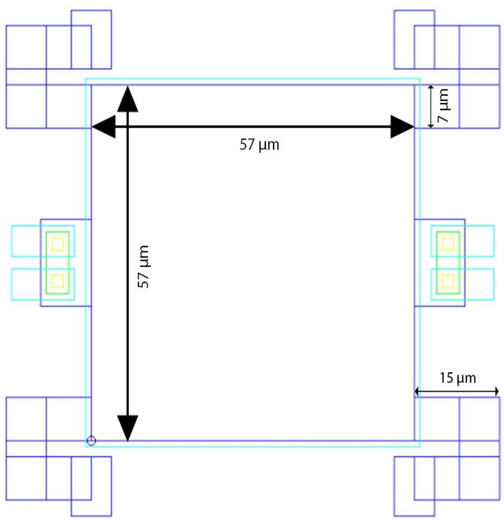


Figure 2: Organic MEM Relay layout

In the MEM relay layout Blue denotes top plate, green denotes channel, yellow denotes dimples and cyan denotes bottom plate. A new material database was created and characteristics of PEDOT:PSS, SU-8, Cytop were defined inside it. Two existing materials – SILICA and SILICON_100 were added from the built in database. Since the geometry of the MEM rely is orthogonal, Manhattan Bricks was chosen as mesh type. CoSolveEM was chosen as field solver for the simulations.

2.2 Temperature Dependence of V_{PI}

Due to a low degree of crystallinity, changes in temperature influence the mechanical properties of polymers much more than that of metals. Young's modulus of SU-8 is reduced by > 5 times when temperature increases to 150˚ C [4, 5]. The temperature dependence of young's modulus of PEDOT: PSS and Cytop are not known. Nonetheless, its common knowledge that young's modulus of polymers usually decrease with increasing temperature [6]. From the expressions (1) & (2), its seen that V_{PI} and V_{NPI} are directly proportional to the equivalent elastic modulus, √Eeq of the materials composing the top plate. Hence, both V_{PI} and V_{NPI} decrease with increasing temperature. The decrease in switching voltages can also be attributed to deformation of the movable structure in response to thermally created strain gradient. The composite polymer structure has three layers made of three different materials, each with different coefficient of thermal expansion. The top layer: Cytop has CTE value of 74 ppm/˚C [7] while bottom layer: SU-8 has a CTE value of 52 ppm/˚C [8]. The conductive layer in the middle is made of PEDOT:PSS; reporting a Thermal Expansion Coefficient value of PEDOT:PSS is the objective of this paper. With a uniform temperature rise of ΔT, the three layers elongate unequally: Cytop expands more than SU-8. Since the three layered materials are tightly joined together at the interfaces the top plate must bend downward forming a concave shape at the center. As a result, the actual actuation gap becomes narrower than the as-fabricated gap g_o and from the eqns. (1) & (2) the switching voltages V_{PI}, V_{NPI} being proportional to g, decrease with temperature.

3 SIMULATION RESULTS

There are varied reports on thermal and mechanical properties of common polymers in literature, which is anticipated taking into account disparity in testing conditions, concentration etc. Nevertheless, material properties which were roughly consistent across the references have been reviewed. From the litearture review, following the trend in which CTE changes with Poisson's ratio in polymers such as PMMA [9], PolyCarbonate, PVC, PDMS [10], a first degree approximation was made that CTE of PEDOT:PSS may lie between 40 ppm/˚C – 60 ppm/˚C.

The table below shows measured V_{NPI} of fully and partially polymeric relays as a function of temperature. These ten data points were collected from experiments for our previous paper [2]. There might be minor inaccuracies in the temperature measurements. As expected we see in the experimental data when the relays are heated V_{NPI} decreases with increasing temperature.

Fully polymeric		Partially polymeric	
Temperature	Measured V_{NPI}	Temperature	Measured V_{NPI}
˚C	V	˚C	V
21.5	11	21.5	10.4
41	10.4	41	9.95
60	9.93	60	9.54
85	9.41	85	8.86
103.5	8.83	103.5	8.24

Table 1: Measured V_{NPI} at different temperatures.

A number of simulations were run using different CTE values of PEDOT:PSS between 40 ppm/˚C and 60 ppm/˚C for a temperature of 21.5 ˚C. By trial and error, a simulated V_{NPI} was found that came very close to the experimental V_{NPI} of 11 V.

Simulated V_{NPI} at 21.5 ˚C (Experimental V_{NPI} = 11 V)	
CTE (ppm/˚C)	V_{NPI} (V)
60	10.842-10.843
55	10.93457-10.9355
45	11.0625-11.25
44	11.0625-11.25
46	11- 11.0625
47	11.05664-11.05762
49.2	11.01562-11.02344

Table 2: Simulated V_{NPI} of the fully polymeric relay

Above are the simulated V_{NPI} from several attempts. A CTE value of 49.2 ppm/˚C was picked out from these as it produced a V_{NPI} of 11.02 V which approximately matches the measured V_{NPI} at the corresponding temperature. The same process was repeated for the other nine data points. Ten CTE values were obtained from a large number of simulations performed. The average of these values came out to be around 49.92 ppm/˚C.

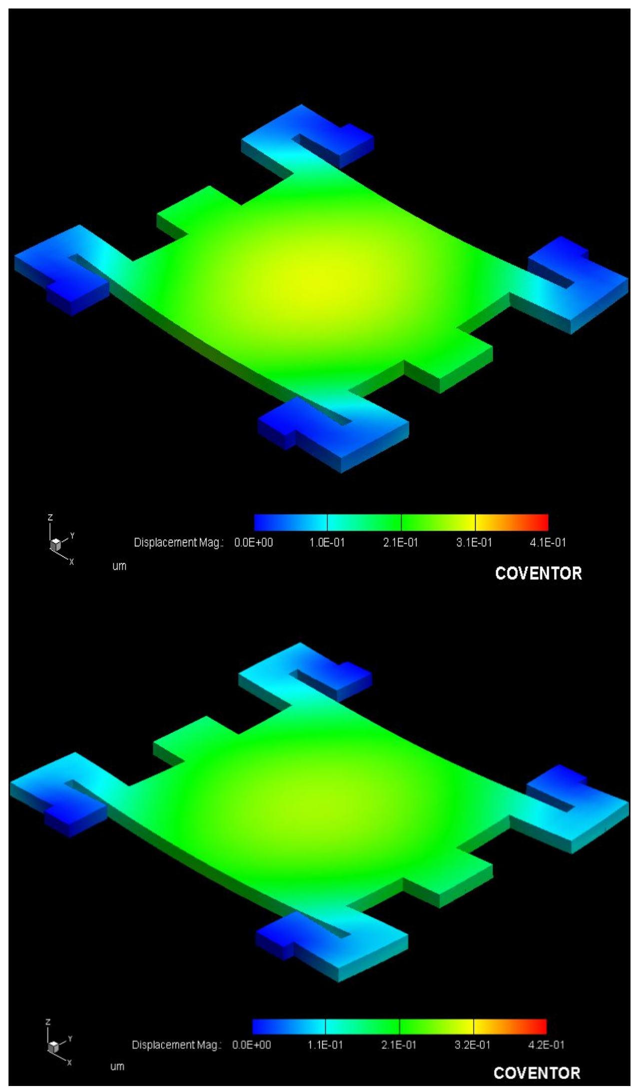
4 DISCUSSION

To get a sense of the accuracy another batch of simulations were run for the fully polymeric relay V_{NPI} using the discovered PEDOT:PSS CTE. From Table 3, we see that the difference between the simulated and measured V_{NPI} increases with temperature. CoventorWare did not model temperature dependent behavior of young's modulus instead a constant value was used for all temperatures. During the trial and error simulation stage, in the absence of this effect (decrease in young's modulus) the CTE values had to compensate with extra deformation to account for the reduction in V_{NPI}. If the decline in young's modulus was accounted for, the corresponding CTE values would have come out progressively smaller and smaller than what was found. As a result the average CTE would have been smaller as well. Thus, here we report an upper estimate of 49.92 ppm/˚C for CTE of PEDOT:PSS.

Temperature	Simulated V_{NPI}	Measured V_{NPI}	Error
˚C	V	V	V
21.5	11.02	11	- 0.02
41	10.28	10.4	+ 0.12
60	9.56	9.93	+0.37
85	8.59	9.41	+0.82
103.5	7.84	8.83	+0.99

Table 3: Experimental and simulated (at CTE of 49.92 ppm/˚C) V_{NPI} of fully polymeric relay

Table 3 data discrepancies can be explained as following. The real CTE is smaller which if used would have produced bigger simulated V_{NPI} (closer to experimental V_{NPI}). Using the upper estimate of 49.92 ppm/˚C is making the V_{NPI} smaller in the simulations. Employing constant Young's modulus (2 GPa) in the material property database, whereas in reality it drops with increasing temperature, has an opposing effect. Its making the simulated V_{NPI} progressively larger. At 21.5˚ C, the effect of constant Young's modulus is more dominant since barely any thermal expansion occurs below room temperature. As a result simulated V_{NPI} (11.02 V) turns out larger than experimental V_{NPI} (11 V). At 41˚C and onwards significant thermal expansion takes place and both opposing effects play a role. Nonetheless the effect of *a larger coefficient of thermal expansion* is superseding the effect of *a constant young modulus*. As the temperature increases the error becomes more pronounced as thermal strain multiplies with temperature and produces larger deformations in the movable structure. Following simulation results on the visualizer corroborates this theory.



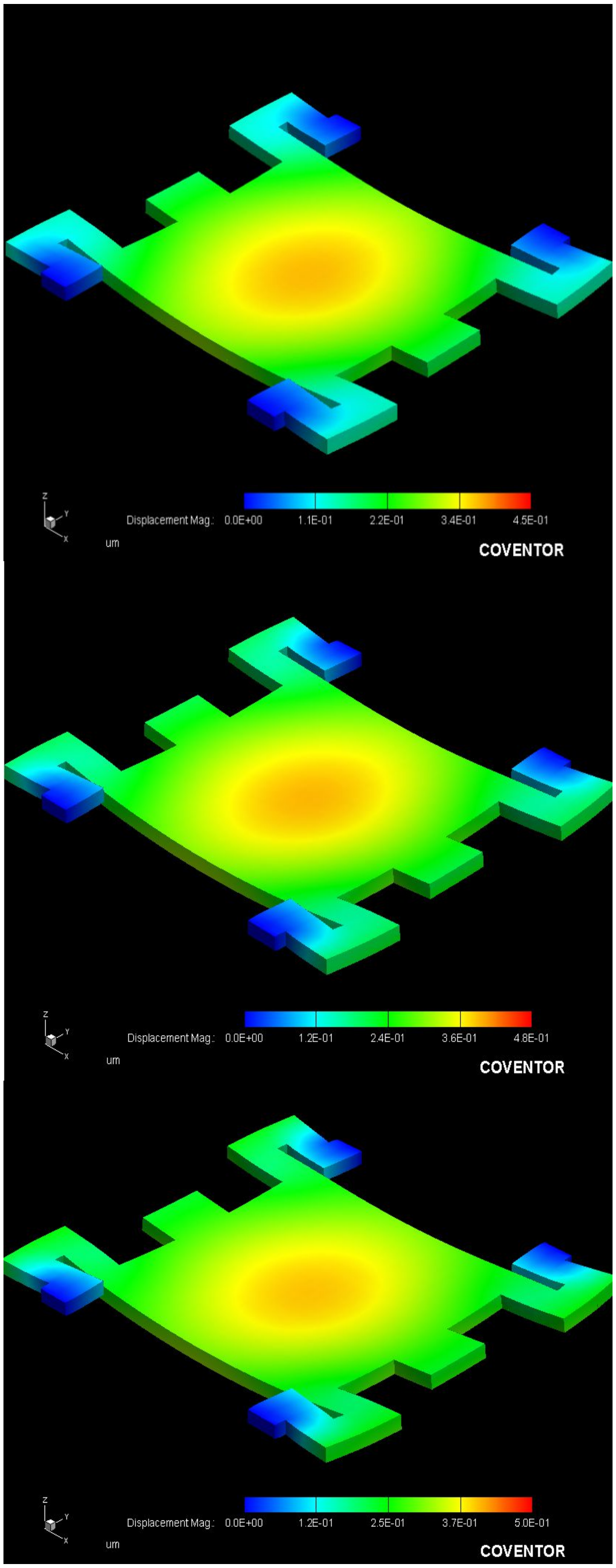


Figure 3: Deformation of the MEM relay top electrode consecutively at 21.5 °C, 41°C, 60 °C, 85 °C & 103.5°C

5 CONCLUSION

V_{NPI} of organic MEM relays decreases with increasing temperature, due to the thermal strain gradient produced in the composite polymer structure and the temperature dependence of young’s modulus, E of polymers. Thermo mechanical analysis was applied on FEA tool to find a set of V_{NPI} values at different temperatures which best fit the experimental (measured) data. The simulation results led to an upper estimate of PEDOT:PSS CTE which came out to be 49.92 ppm/˚C.

6 ACKNOWLEDGEMENT

Author would like to acknowledge Yanbiao Pan’s experimental data used in the simulations. John Scafidi and Nahid Khan contributed in the styling of the illustrations.

REFERENCES

[1] J. Yaung, L. Hutin, J. Jeon and T. Liu, J. Microelectromech. Syst., vol. 23, no. 1, pp. 198-203, 2014

[2] Y. Pan, N. Khan, M. Lu and J. Jeon, IEEE Trans. Electron Devices vol. 63, no. 2, pp. 832-840, 2016.

[3] Y. Pan, F. Yu and J. Jeon, Proc. 28th IEEE Int Conf. Microelectromech. Syst., 2015, pp. 940-943.

[4] J. Hammacher, A. Fuelle, J. Flaemig, J. Saupe, B. Loechel, and J.Grimm, MicrosystemTech., vol. 14, nos.9–11, pp.1515–1523, 2008.

[5] S. Chung and S. Park, J. Mech. Sci. Technol., vol. 27, no.9, pp. 2701–2707, 2013.

[6] N. Lagakos, J. Jarzynski, J. H. Cole, and J. A. Bucaro, J.Appl. Phys., vol. 59, no. 12, pp. 4017–4031, 1986.

[7] MicroChem Corp., SU-82000DataSheet, Newton, MA, USA, 2009.

[8] Asahi Glass Corp., CYTOP Data Sheet, Tokyo, Japan, 2009.

[9] http://www.mit.edu/~6.777/matprops/pmma.htm

[10] http://www.mit.edu/~6.777/matprops/pdms.htm