Modeling of Joule heating based self-alignment method for metal grid line passivation

M. Janka[1], P. Raumonen[2], S. Tuukkanen[1] and D. Lupo [1]

[1] Department of Electronics and Communications Engineering, Tampere University of Technology, P.O.Box 692, FI-33101 Tampere, Finland

[2] Department of Mathematics, Tampere University of Technology,
P.O. Box 553, FI-33101 Tampere, Finland

ABSTRACT

A Joule heating based self-alignment method for solution-processable insulator structures has been modeled for the passivation of metal grid lines, for example for organic light emitting diodes or photovoltaic cells. To minimize overhang of the passivation layer from line edges, we have studied the Joule heating approach using solution-processable, cross-linkable polymer insulator films. Finite element simulations were performed to investigate the heating of the sample using glass and poly(ethylene terephthalate) (PET) substrates. The sample was at room temperature and the current was selected to induce a temperature of 410 K at the conductor. It was found that the selection of substrate material is crucial for the localization of cross-linking. For a PET substrate, the temperature gradient at the edge of the conductor is approximately twice the gradient for glass. As a result, using a glass substrate demands high selectivity from the polymer cross-linking, thus making PET a more suitable substrate material for our application. A flexible PET substrate is, in addition, compatible with roll-to-roll mass-manufacturing processes.

INTRODUCTION

The performance of organic photovoltaic devices (OPV) and light emitting diodes (OLED) is dependent on the device active area. Since known transparent conductors have a relatively high resistivity, the resistance of the transparent anode limits the power conversion efficiency in large devices for OPV applications and brightness homogeneity of OLEDs, due to the large lateral voltage drop inside the electrode. Integration of a metal grid with the transparent conductor improves the performance of OPVs and OLEDs. [1, 2]

Metal grids, however, decrease the device active area and thus they need to have low area coverage and high conductivity; they should be as narrow and thick as possible. This topology makes the anode and cathode prone to shorting. To avoid shorting, an insulating layer is put on top of the grid lines. This layer should cover only the grid lines in order to minimize the non-luminescent and non-illuminated areas; accurate alignment of the passivation layer is thus critical for maximizing the aperture ratio of the device. It is possible to use either photolithography or printing for the definition of the passivation layer. However, printing generally requires large overprinting and photolithography an additional alignment step, which is challenging when aiming at high throughput in roll-to-roll production. A self-alignment method offers better registration than printing without additional alignment steps.

Here we present finite element simulations of Joule heating in an aluminum grid line on PET and glass substrates. The aluminum line is heated by an electric current, causing a localized temperature increase in the vicinity of the conductor. The heat locally cures the insulator on top of the the conductor, while it remains uncured and thus soluble farther away. The uncured dielectric can be rinsed away after crosslinking is completed. The method is described in detail in a previous publication [3]. Localization of the dielectric is dependent on the temperature distribution at the substrate and can be used as an estimate for the length overlap of the dielectric on a grid line. We investigate the effect of an indium tin oxide (ITO) layer on the diffusion of the heat.

The measured geometry of the device consists of domains with large dimensional differences (dimensions of the lines are 2 mm x 70 µm x 500 nm). Using this geometry for modeling would result in a very large mesh size, which would increase the modeling time, and in the worst case the mesh cannot be generated. To alleviate these mesh related problems, we model the problem using an equivalent problem with a “scaled geometry” that has greatly reduced dimensional differences [4].

THEORY

Modeling was carried using a finite element method (Comsol Multiphysics version 4.3 from Comsol, Inc.). The simulation combined a heat transfer model of the Heat Transfer Module and an electrical conductivity model of the AC/DC Module.

In order to investigate the effect of the transparent electrode on thermal diffusion, two geometries were compared; a plain substrate and a substrate coated with 150 nm thick ITO having a sheet resistance of 14 Ω/□. The substrate in the model is either 125 µm thick PET or 1 mm thick glass. A 500 nm thick and 70 µm wide aluminum line is placed either directly on substrate or on ITO. The length of the grid line is 2 mm on PET and 5 mm on glass. The uppermost is a 1 µm thick dielectric layer of poly(methyl methacrylate) (PMMA). Figure 1(a) illustrates the geometry used in the modeling.

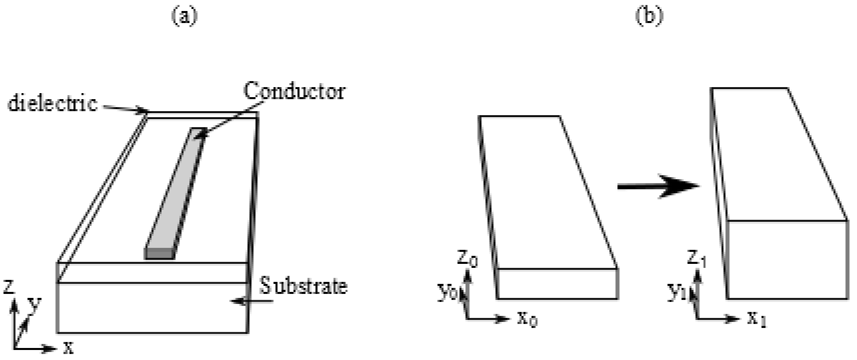

Figure 1. (a) Geometry of the model (dimensions not in scale) and (b) the scaling of the geometries

Since the dimensions of the different material blocks have large differences, the ratio between the dimensions is on the order of 10^3. The larger the dimensional differences are, the longer the calculation time is, and in the worst case a mesh cannot be generated. To overcome the problems caused by the dimensions, thicknesses of the materials are scaled so that there are no large differences between the dimensions. The scaled thicknesses are 50 µm for ITO, 100 µm for PMMA and 50 µm for Al. The scaling is illustrated in Figure 1 (b).

To transform the original problem to a new geometry so that the problems are equivalent, we need a mapping F between domains:

$$\mathbf{x}_1 = F(\mathbf{x}_0) \quad (1)$$

The mapping F must be piecewise smooth and one-to-one, giving the correspondence between points and material blocks in the original geometry and the scaled geometry. Then, to make the problem with scaled geometry equivalent to the problem with original geometry, we need to modify the material parameters. This is done with the Jacobian matrix J of the mapping F. Material parameter matrices δ in the domains are related as follows [4]:

$$\delta_1 = \frac{1}{\det(J)} J \delta_0 J^T \quad (2)$$

where J^T and $\det(J)$ are the transpose and determinant of the Jacobian matrix. Each material was scaled separately in the model. Notice that material parameters in the scaled geometry are anisotropic.

Heat transfer in bulk material was modeled with the Fourier law of heat conduction [5], and the surface of the dielectric was described with a heat flux condition [6]. The bottom face of the substrate was set to room temperature corresponding to a situation where a heat sink is placed under the substrate, and the current was selected to induce a temperature of 410 K at the conductor. The modeling was done using stationary equations. This assumption is valid since the modeling indicated that the temperature stabilizes in less than a second and the heating time is a few minutes.

DISCUSSION

Even though the modeled grid line is only a few millimeters long the results are valid for longer lines as well. Heat conduction decreases the temperature at the ends of the conductor, thus temperature is not uniform along the conductor. The modeled conductor should be long enough that the ends do not have an effect on the temperature. For the glass substrate conductor length should be at least 5 mm and for PET 1 mm is enough. This result was used as a guideline for the geometry selection.

Scaling the thicknesses of the layer does not have a significant effect on the results. For example, increasing the scaled PMMA thickness 500 % decreased the calculated temperature at the conductor only 3 %. The mesh density, however, has an effect on the temperature gradient, which is the key parameter in investigating the selectivity of heating. In this sense the closer the scaled dimension are to each other, the better the gradient estimation is. Nevertheless, the scaling comes with a cost: The mesh is still generated as if there is no scaling in the geometry, which results in mesh elements that correspond to very elongated ones in the original geometry. This makes the condition number of the system matrix worse and can also affect the interpolation [7]. To improve this, the elements should be anisotropic, i.e. they should be elongated in the scaled geometry, in which case they correspond to “nice” elements in the original geometry. However, this option was not available in the version of the software used.

Figure 2 shows the temperature distribution along the x-axis for PET and glass substrates without and with ITO coating. Due to its higher thermal conductivity the glass substrate was shown to be a more challenging material choice for Joule heating than PET. The temperature gradient near the conductor for plain glass is approximately 1 K/µm, while for plain PET substrates it is approximately 2 K/µm. This means lower localization of the cured dielectric. However, a glass substrate enables the use of higher temperatures, which decrease the time needed for the curing of the dielectric film. By a careful selection of the curing parameters it should be possible to create a well-aligned dielectric layer on glass.

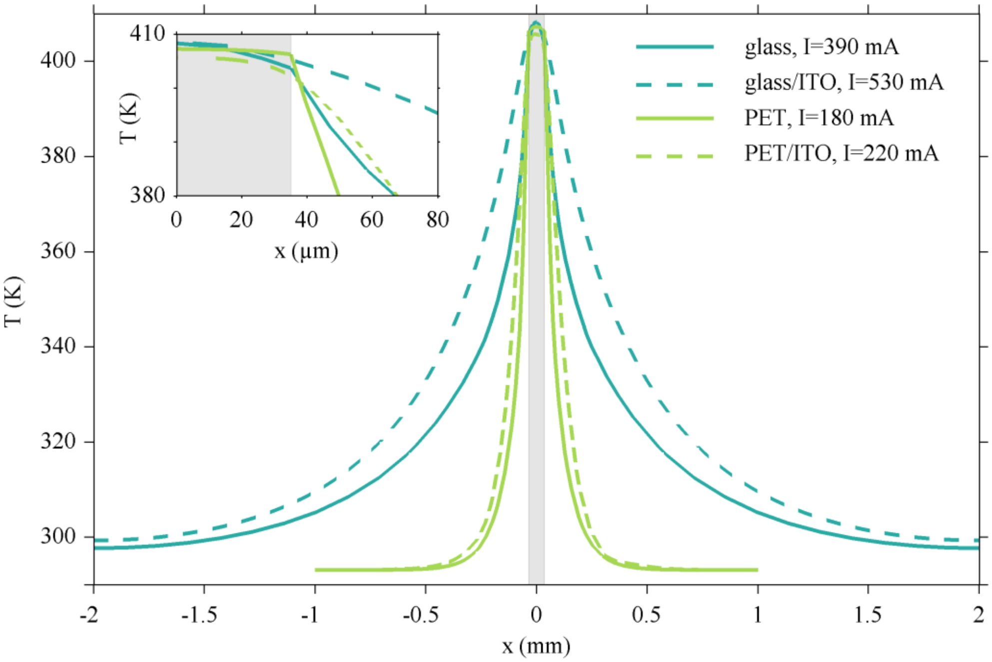

Figure 2. Temperature profile along x-axis (perpendicular to the conductor). The conductor is indicated with the gray bar at graph. Inset: magnification near the edge of the conductor.

The inset of figure 2 shows the magnification of the temperature profile near the conductor edge. Whereas the temperature gradient with the plain substrates is highest at the edge of the conductor, ITO shifts the maximum gradient further away from the edge. At the edge of the conductor temperature gradient for the PET/ITO substrate is 0.6 K/µm and for glass/ITO 0.2 K/µm. This indicates a need for careful optimization of the curing parameters in order to achieve high locality of the dielectric.

An ITO layer on PET does not have a significant effect on the distance from the conductor where the heat is stabilized to room temperature. For the glass substrates, the temperature is stabilized at the distance of 2 mm from the conductor, whereas for PET substrate the corresponding distance is only 0.5 mm. Based on this it can be estimated that for multiple conductors heated simultaneously, the heating selectivity does not degrade when the conductors are separated at least by the distance needed for the temperature to reach room temperature. For PET this distance is 1 mm and for glass it is 4 mm. This, however, should be verified by modeling multiple gridlines.

Higher current is needed to create sufficient temperature on a glass substrate than on a PET substrate. This is because a large area of glass is heated during Joule heating. To reach a temperature of approximately 410 K, the Joule heating current for glass substrate is 390 mA whereas the corresponding current for PET is 180 mA. The ITO layer increases the required current. For PET substrate, the ITO layer increases the required current to 220 mA, (approximately 20 % increase) and for glass/ITO substrate 530mA (35 % increase). The increase results from current flowing in the ITO, as well as the increased heat spreading into the substrate. The actual current that passes through the conductor is 204 mA for the ITO/PET substrate and 452 mA for the ITO/glass substrate as the rest of the current flows through ITO. Even though a small current flows in the ITO, resistive heating in ITO is negligible.

The degree of heat localization is affected by the thermal conductivity of the materials under the conductor. The differences between the substrate materials are explained by the 10 times higher thermal conductivity of compared to PET. [8, 9] Thermal conductivity of ITO is, however, 100 times higher than thermal conductivity of PET.[10] Based on these values it is surprising how small an effect the ITO layer on PET has on the heat spreading. This predicts that heat tends to move to air rather than spread along the thin layer of ITO. By decreasing the ITO thickness it might be possible to increase the temperature gradient at the edge of the conductor. However, decreasing the ITO thickness decreases its sheet resistance and thus affects negatively the device performance. Other transparent conductors might offer better heat localization during Joule heating. For example thermal conductivity of PEDOT:PSS (poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate)) is 0.17 $Wm^{-1}K^{-1}$ [11]. As a comparison, the corresponding value for PET is 0.15 [9], predicting that with a PEDOT:PSS transparent anode layer, the localization of the passivation should not differ from that of plain PET. The effect of the ITO thickness as well as PEDOT:PSS should be studied further.

CONCLUSIONS

Self-aligned passivation of anode grid lines for OPV and OLED applications using Joule heating was studied by a finite-element method. Suitability of glass and PET substrate for the Joule heating method was compared. Due to large dimensional differences in the material layers, the mesh can be too large or impossible to generate. Therefore the geometry of the model used for computations was scaled to reduce the dimensional differences.

Joule heating on glass consumes more energy than on PET, since higher current is required to create sufficient temperature due to the higher thermal conductivity. More heat is conducted into a glass substrate than into PET, where less energy is consumed to heat the substrate. When heating multiple conductors simultaneously, the heating area increases, and more heat will be transferred in to the substrate. With the substrate having higher tendency to store heat this may have a negative effect on the localization. We conclude that PET is a more suitable material for Joule heating method than glass. An ITO layer on PET decreases the temperature gradient at vicinity of the conductor edge, demanding more careful optimization of curing parameters.

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