Optical simulation of surface textured TCO using FDTD method

I L Elviyanti, H Purwanto and Kusumandari
Department of Physics, Faculty of Mathematics and Natural Sciences, Sebelas Maret University, Jl. Ir. Sutami 36A Kentingan Surakarta 57126, Indonesia

*E-mail: isna_elviyanti@yahoo.co.id

Abstract. The purpose of this research is simulating the transmittance of surface textured transparent conducting oxide (TCO) for Dye-Sensitized Solar Cell (DSSC) application. The simulation based on finite difference time domain (FDTD) was performed using the MatLab software for flat and pyramid surface textured TCO. Fluorine-doped tin oxide (FTO) and indium tin oxide (ITO) were used as TCO material. The transmittance simulation of flat TCO was compared to UV-Vis spectrophotometer measurement of real TCO to ensure the accuracy of the simulation. Then, the transmittance simulation of pyramid surface textures of TCO is higher than a flat one. It suggested that surface texturing enhance the path of light through dispersion and reflectance light by the pattern of the surface. This result indicates that surface textured increasing the transmittance of TCO through a complex light trapping mechanism which might be used to increase the light harvesting for DSSC application.

1. Introduction
Dye-Sensitized Solar Cell (DSSC) is one of type solar cell which based on photoelectrochemical process. The DSSC has a sandwich structure with transparent conductive oxide (TCO) as a glass substrate, TiO$_2$ as working electrode, dye as an absorbent of light, electrolytes as a medium of exchange electron and Pt or carbon as counter electrode [1].

Recently, the DSSC has an efficiency of 11-12.3%. It smaller than conventional Si solar cell which has an efficiency of 25% [2]. Many methods for increasing the efficiency of DSSC such as modification of TiO$_2$ and variation of dye have been done. Surface texturing is another method to increase the efficiency by scattering or diffraction the incident light so that the optical path length and light absorption within the active layer of the solar cell is increased. Recently, conventional solar cell prepared on periodic surface textures have shown conversion efficiency exceeding of 10% [3]. However, the experimental of surface texturing on DSSC is still rare and need more investigation.

Optical simulation is often used to analyze wave propagation and transmittance within solar cell structure to derive optimal textures [4,5]. In this study, simulation uses finite difference time domain (FDTD) two dimension (2D) method computing by Matlab software. The purpose of this study is comparing transmittance and reflectance of flat and pyramid surface textured of TCO.

2. Method
FDTD is a method to solve Maxwell’s equations problem [6]. In this study, FDTD simulation uses Transverse Magnetic (TM) type. TM has component vector of $\vec{E}_x$, $H_x$ and $H_y$. With $\vec{E}_x$, $H_x$ and $H_y$ is
electric field in x direction, magnetic field in x and y direction, respectively. Two dimension Maxwell’s equation at $z = 0$ depend on media that used as perfect matched layer (PML) [7,8]:

Where $S$ is PML equation, $m$ is vector constant, and $L$ is the length of PML.

\[
\begin{align*}
\nabla x \vec{E}(\omega) &= -j\omega \mu_0 [\mu_r] [S] \vec{H}(\omega) \\
\nabla x \vec{H}(\omega) &= \sigma \vec{E}(\omega) + j\omega [\varepsilon_r] \vec{D}(\omega) \\
\vec{D}(\omega) &= \varepsilon_0 [\varepsilon_r] \vec{E}(\omega)
\end{align*}
\]

The simulation is dividing into four steps. First, we define parameters of object, such as object constant which used in this simulation as shown in Table 1, velocity of light ($c_0$), maximum refractive index $n_{\text{max}}$, frequency, wave length ($\lambda$), resolution grid and size of object. The source frequency are $375 – 857 \text{ THz}$. The object have size of width and length of 6000 nm and 2000 nm, respectively.

**Table 1. Object constant of FDTD 2D simulation**

| Object | N | $\mu_r$ | $\varepsilon_r$ |
|--------|---|---------|-----------------|
| Glass  | 1.46 | 0.57 | 3.75 |
| FTO    | 1.47 | 1.01 | 2.14 |
| ITO    | 1.86 | 0.99 | 3.45 |
| Air    | 1   | 1     | 1               |

Second, calculation of modeling of object, source of Gaussian pulse, PML, and field of the coefficient. Third, we start the simulation for 26182 steps of electric and magnetic field using Maxwell [7,8]. And, the last step is analyzing of an electric field to obtain the reflectance and the transmittance. Figure 1 shows optical layout of a TCO structure and incident of the light source. In this study, we use Indium doped Tin Oxide (ITO), and Fluorine doped Tin Oxide (FTO) as TCO.

![Figure 1](image-url)

**Figure 1.** Optical layout structure and incident of light source in (a) flat and (b) pyramid surface textured of TCO

3. **Result and Discussion**

The transmittance of the flat surface of TCO was measured using UV-Vis spectrophotometer. The frequency of incident of light is $375 – 857 \text{ THz}$. Then, FDTD 2D simulation uses Gaussian pulse as a source, which is consists of an electric and magnetic field for 26182 steps of propagation.
The source of Gaussian pulse appears from glass since we consider that glass is not absorbing the incident of light. Gaussian pulse propagates from glass toward to TCO as shown in Figure 1(a) for flat and 1(b) for pyramid surface textured. Pyramid surface textured, showed in Figure 1, have ten pyramids with 200 nm and 292 nm of width and length, respectively. Figure 2(a) and 2(b) show comparison the transmittance of a flat surface as a result of UV-Vis spectrophotometer measurement and simulation of FDTD 2D.

![Figure 2](image)

**Figure 2.** Measurement and simulation transmittance of (a) ITO and (b) FTO

As shown in Figure 2(a) and 2(b), the simulation transmittance not exactly agree with measurement one. In the simulation, we assume that the surface of TCO as the perfectly flat surface. However, in the real TCO, it suggests there is soft roughness caused by a fabrication process which will affect the transmittance.

Then, we compared flat and pyramid surface textured of ITO and FTO. Figure 3(a) and 3(b) show the propagation of light and corresponding transmittance of flat and surface textured ITO, respectively, at 26182 of simulation steps. As a result, the transmittance of pyramid surface textured is higher than flat surface as shown in Figure 4.

![Figure 3](image)

**Figure 3.** Light propagation in (a) flat and (b) pyramid surface textured of ITO.
Figure 4. Transmittance and reflectance of flat and pyramid surface textured of ITO

Then, Figure 5(a) and 5(b) show the propagation of light and corresponding transmittance of flat and surface textured FTO, respectively, at 26724 of simulation steps. Similar with ITO, the transmittance of pyramid surface textured of FTO is higher than flat surface as shown in Figure 6. This result indicates that surface texturing on TCO will increase the transmittance which might be caused by scattering in the edge of the texture. The increasing of transmittance is a benefit to enhance the efficiency of DSSC.

Figure 5. Light propagation of (a) flat and (b) pyramid surface textured of FTO.

Figure 6. Transmittance and reflectance of flat and pyramid surface textured of FTO
4. Conclusion
This research investigated the transmittance of flat and pyramid surface textured of TCO using finite difference time domain (FDTD) 2 Dimension (2D) method computing by Matlab software. Our result revealed that pyramid surface textured on TCO exhibit higher transmittance than a flat one. Based on the result, pyramid surface textured might be used as a method to increase the efficiency of DSSC.

References
[1] Mona B, Siamak N, Kenneth K S L, Daeyeon L and Masoud S 2013 Theoretical and Experimental Study of a Dye-Sensitized Solar Cell American Chemical Society
[2] Green M A, Emery K, Hishikawa Y and Warta W 2011 Solar cell efficiency tables (version 37) Prog. Photovolt: Res. Appl. 19 84–92
[3] Battaglia C, Hsu C M, Soderstrom K, Escarre J, Haug F J, Charriere M, Boccard M, Despeisse M, Alexander D T L, Cantoni M, Cui Y, and Ballif C 2012 Light Trapping Solar Cell: can periodic beat random? ACS Nano 6 (3) 2790-2797
[4] Jäger K, Isabella O, Zhao L and Zeman M 2010 Light scattering properties of surface textured substrates Phys. Status Solidi C 7 945–948
[5] Kusumandari K and Risa S 2014 Transmittance Simulation of Surface Textured Fluorine Doped Tin Oxide (FTO) for Dye-Sensitized Solar Cell (DSSC) Application Advances in Physics Research, 7th International Conference on Physics and Its Applications 2014 (ICOPIA 2014) 86-89
[6] Mohapatra N B and Mohapatra K R 2013 FDTD Optical Simulation To Enhance Light Trapping. International Journal A Scientific & Engineering Research 6 2890-2897
[7] Rathi V, Shrivastava K P and Pokhariya H S 2012 1-D implementation of maxwell’s equations in Matlab to study the effect of absorption using pml. International Journal of Electronics Signals and Systems (IJESS) 1 2231-5969
[8] Sullivan M D 2000 Electromagnetic simulation using the finite difference time domain method. IEEE Press Inc. New York