Numerical Procedure for Modeling of Light Emitting Diode with Mesh-Like Electrode

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Abstract. A computational procedure is presented for numerical modeling of the light emitting diode (LED) with top p-electrode designed as a mesh with the strips of rectangular cross section. Isotropic light emission in the LED’s active region and light reflection from the bottom electrode are considered. Three-dimensional Laplace equation for electric potential is solved by finite element method. The numerical model incorporates mapped infinite element to account for potential decay far away from the LED structure and finite element model developed for boundary condition at semiconductor-air interface in the mesh opening. Simulation results demonstrate the effect of the mesh’s geometrical parameters on the total output power.

1. Structure and physical model of the LED
Patterning of the top metal electrode of light-emitting diodes (LEDs) was proposed to enhance their output optical performance. To assess the effect of mesh-like electrode one needs to invoke numerical modeling. In the present study, we consider an LED with vertical structure schematically shown in Fig. 1. It consists of the narrow-gap active layer sandwiched between bottom n- and top p-doped wide-gap layers with thicknesses \( d_1 \) and \( d_2 \), respectively. Metal electrode attached to the bottom n-layer is solid while that one attached to the top of p-layer is designed as a mesh with pitch \( a \). Mesh strips have rectangular cross section of width \( w \) and height \( h \). The periodicity of the mesh allows to consider a portion of the LED structure beneath a single mesh cell which will be referred as a unit cell. Directions of coordinate axis are shown in Fig. 1. The planes of the bottom electrode and active region have coordinates \( z = 0 \) and \( z = z_{\text{act}} \), respectively.

To find distribution of electric potential along active region one needs to solve three-dimensional Laplace equation. The boundary conditions at the bottom surface and the mesh strips are set to be constant, i.e. \( \varphi(x,y,0) = 0 \) for bottom surface and \( \varphi(x,y,z)|_{\text{node}} = \text{const.} \) for mesh strips, respectively. Also, the potential should decay far away from the top surface, i.e. \( \varphi(x,y,\infty) = 0 \) and continuity of normal component of electric flux at the semiconductor-air interface in the mesh opening is taken into account:

\[
\frac{\partial \varphi}{\partial z}|_{\text{int}_+} = \varepsilon \frac{\partial \varphi}{\partial z}|_{\text{int}_-},
\]

where \( \varepsilon \) is the dielectric constant of semiconductor, \( \text{int}_\pm \) indicate top (air) and bottom (semiconductor) sides of the interface. Due to the periodicity of the mesh the electric field
normal to the side walls of unit cell is equal to zero, or in differential form: $\frac{\partial \varphi}{\partial x}|_{y=0,a} = \frac{\partial \varphi}{\partial y}|_{x=0,a} = 0$.

Current injected into each elementary volume $\Delta V$ is determined by the electric potential $\varphi(x, y, z_{act})$ at its location and can be expressed as [1]

$$J(x, y, z_{act}) = J_0 \exp \left( \frac{q}{a_f kT} \varphi(x, y, z_{act}) \right),$$  \hspace{1cm} (2)$$

where $k$ and $T$ are the Boltzmann constant and the temperature in Kelvin, respectively, $q$ is electron charge. For simplicity we set an ideality factor $a_f = 1$. Saturation current density $J_0$ can be evaluated from the total current injected into the LED and measured as the current flowing in the external circuit [2]. Each elementary volume is treated as a point source with isotropic light emission. Power of light generated in a volume with coordinates $\{x, y, z_{act}\}$ can be expressed as [1]

$$dP(x, y, z_{act}) = \frac{h\nu}{q} J(x, y, z_{act}) dx dy, \hspace{1cm} (3)$$

where $h$ and $\nu$ are the Planck’s constant and the frequency of light photons, $\eta$ is the internal quantum efficiency. Due to total internal reflection, only light coming within the escape or acceptance cone determined by the critical angle $\theta_c$ can be extracted via semiconductor-air interface. We assume that at any point of the mesh opening $\{x, y, z_{opn}\}$, the extracted light consists of a primary and secondary contributions collected from the encircled portions of the active region and bottom reflecting plane subtended by acceptance (or escape) cone (Fig. 1). The radii of these acceptance circles are $r_{c1} = d_1 \tan \theta_c$ and $r_{c2} = (d_1 + d_2) \tan \theta_c$, respectively. Output optical power density for primary contribution can be expressed as [1]

$$P_{prm}(x, y, z_{opn}) = \int_{\text{circ1}} \cos(\theta_i) T(\theta_i) \ dP(x_{circ1}, y_{circ1}, z_{act}), \hspace{1cm} (4)$$

where $r_1$ is the distance between a point $\{x_{circ1}, y_{circ1}, z_{act}\}$ within an acceptance circle in the active region plane and a point $\{x, y, z_{opn}\}$ in the mesh opening, i.e., $r_1 = [(x - x_{circ1})^2 + (y - y_{circ1})^2 + (z_{act} - z_{opn})^2]^{1/2}$, $\theta_i$ is the angle of incidence, $\cos(\theta_i)$ is a geometric factor which scales properly the inclined photon flux, $T(\theta_i)$ is polarization dependent transmission coefficient for the semiconductor-air interface. To evaluate secondary contribution $P_{scn}$ we use Eq. (4) with proper substitution of coordinates at the bottom plane and $r_2 = [(x - x_{circ2})^2 + (y - y_{circ2})^2 + (z_{opn})^2]^{1/2}$ instead of $r_1$. 

![Figure 1. Schematic structure of the LED with top p-electrode patterned as a mesh.](image)

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To evaluate total output optical power $P_{tot}$, we integrate power densities of both primary and secondary contributions obtained using Eq. (4) over the mesh opening and multiply by the number of mesh cells $N_{opn}$

$$P_{tot} = N_{opn} \int_{opn} (P_{prm} + P_{scn}) \, dx \, dy. \quad (5)$$

where $N_{opn} = S_{LED}/a^2$, $S_{LED}$ is total surface area of the LED.

2. Numerical results

The developed procedure is applied to evaluate the performance of the LED. In the computations the following parameters are used: bias voltage $V = 2$ V, internal quantum efficiency $\eta = 1$, $T = 300$ K, refractive index $n = 2.5$, dielectric constant of semiconductor layers $\varepsilon = 8.9$, and layer thicknesses and boundary conditions are indicated in Fig. 2. Total area of the LED was set $S_{LED} = 1296$ $\mu$m$^2$.

![Figure 2. Computation domain of the LED’s unit cell with geometric parameters and boundary conditions.](image)

Fig. 3 shows distributions of the potential along the active region plane and the normalized output power density at mesh opening plane for mesh pitch $a = 900$ at different width of the strips: $w = 100$, 200, and 300 nm. One can see in Fig. 3 that an increase in strip width at a fixed mesh pitch boosts the potential and causes modification in the shape of distribution. It also boosts the average value of power density but smaller peak values are observed with decreasing area of mesh opening.

Fig. 4 shows total normalized output optical power $P_{tnor}$ versus mesh pitch at different strip widths. Solid curves with filled symbols correspond to the situation when light emitted towards the top surface as well as reflected from the bottom plane was taken into account (primary plus secondary contributions) and only primary contribution was taken into account in the case of dashed curves with open symbols. It should be pointed out that at all strip widths $w$ total output power drops with increasing mesh pitch $a$ and approaches some saturation value when only regions in the vicinity of the strip edges contribute to the optical output, as expected. It should be noted also that at $w = 300$ nm the total output power with contribution of the reflected light reveals saturation in the range of the mesh pitches $a = 300 - 600$ nm. It can be attributed to modification of potential distribution while effect of the reduced size of mesh opening is less pronounced. However, at strip width $w = 300$ nm reduction in the size of mesh opening becomes crucial at mesh pitch $a = 600$ nm. Thus, the interplay between modification of potential distribution and reduction in size of the mesh opening at a fixed mesh pitch and increasing strip width should be addressed properly when we choose the geometrical parameters of the mesh-like electrode.
Figure 3. Potential distributions along the active region plane (top panel) and normalized output optical power density along the mesh opening (bottom panel) at mesh pitch $a = 900$. The distributions are shown for width of strips $w = 100, 200, \text{ and } 300 \text{ nm}$.

Figure 4. Normalized total output optical power versus mesh pitches at different width of the strips. Solid curves with filled symbols correspond to the situation when light emitted towards the top surface as well as reflected from the bottom plane was taken into account (primary plus secondary contributions); dashed curves with open symbols - only primary contribution was taken into account.

3. Conclusion
Numerical model and procedure are developed and used to study the output optical performance of the light-emitting diode with top metal electrode designed as a mesh with the strips of rectangular cross-section as in realistic LEDs. The developed model also accounts for the contribution of light reflection from the bottom electrode. Three-dimensional Laplace equation is solved by finite element method. The mapped infinite element is introduced into numerical model to account for potential decay far away from the LED structure and finite element model developed for boundary condition at semiconductor-air interface in the mesh opening. Simulation results demonstrate the effect of the mesh pitch and width of the strips on the distribution of electric potential and total output optical power. The saturation of the total output optical power is demonstrated at significant increase in mesh pitch at all strip widths. It is also shown that the interplay between increase in potential values and reduction in size of the mesh opening should be taken into consideration during design of the mesh-like patterned electrodes.

References
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