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Nanosimulation of electron confinement in cerium doped zinc oxide nanowire structure for light emitting devices

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ABSTRACT

Nanosimulation of Cerium (Ce) doped Zinc Oxide (ZnO) nanowire has been carried out for nanowires structure of Ce doped ZnO/$Mg_xZn_{1-x}O$ using MATLAB. Electron confinement in Ce doped ZnO nanowire has been achieved by deducing wave function intensity from the solutions of Schrodinger equation. Eigen energy has been computed using the Transfer Matrix Method (TMM). It is revealed from our analysis that increasing mole fraction of magnesium (Mg) increases Eigen energy. For 10% magnesium, Eigen energy was found to be 0.07 eV and for 30% magnesium, it has got increased up to 0.09 eV. Effect of Mg mole composition in barrier region on confinement of electron wave function spread has been investigated. Better confinement was obtained for increasing values of Mg mole composition.

1. Introduction

Zinc oxide (ZnO) nanostructures have been a major focus of attention due to their significant performance in electronic and optoelectronic applications. ZnO is the most promising material for the fabrication of optoelectronic devices operating in the blue and ultraviolet region [1]. It is having direct band gap of 3.37 eV with excitonic binding energy of ~60 meV, which is responsible for stimulated emission at room temperature [2,3]. Moreover, ZnO is having nontoxic character, chemical stability, low cost, radiation hardness and better thermal stability. Heterostructure based on ZnO had shown excellent light emission properties proving its potential for light emitting devices [4,5].Ternary compound $Mg_xZn_{1-x}O$ serves as an excellent barrier with ZnO due to its higher band gap to form quantum confined nanostructure [6]. $Mg_xZn_{1-x}O$ tunes band gap without affecting the lattice constant of ZnO. The optical confinement analysis has showed an excellent confinement of optical field intensity within active region for ZnO/$Mg_xZn_{1-x}O$ heterostructure [7].

Various doped ZnO nanostructures with different elements have been realized to improve the electrical, optical and magnetic properties. Recently, rare earth doped ZnO has attracted widespread attention for the high efficiency and ease of large-scale production of light emitting devices. Most of all, the Ce element possessing an exceptional optical characteristic can be a perfect material for visible light-emitting phosphors in displays and light-emitting devices.

Cost and efforts in fabrication of device can be minimized by modeling and simulation prior to its fabrication. Furthermore, the device characteristics can be predicted well in advance with optimized set of parameters using computer simulation. For that reason, Nanosimulation work on Ce doped ZnO nanowire embedded within $Mg_xZn_{1-x}O$ barrier has been proposed for the first time. Electron confinement analysis within Ce doped ZnO quantum nanowire has been carried out by obtaining solutions of Schrödinger equations.

Optical confinement within ZnO/$Mg_xZn_{1-x}O$ heterostructure has been already studied [5,8]. Despite of this, the electrical confinement within active region of quantum wire is required for stimulated emission. The work invoves Eigen energy evoluation using TMM. The electrical confinement has been investigated by obtaining solutions of Schrödinger equation. Proposed modeling and simulation work deals with analysis of quantum confinement in Ce doped ZnO/$Mg_xZn_{1-x}O$ nanowire structure. Here, effect of Mg mole fraction in barrier region on quantum confinement has been explored. Furthermore, the FWHM has been observed to study the spread of the wave function along with probability density. This work has been carried out for the nanowire considering wire region of Ce doped ZnO and barrier of $Mg_xZn_{1-x}O$ as depicted in Fig. 1. Blue shaded region is of the barrier, i.e. made up of $Mg_xZn_{1-x}O$, and white region defines the wire region of Ce doped ZnO.

Paper is organized as follows: follwing section intricates idea about the mathematical modeling, which is followed by results and discussion in Section 3. Finally, conclusions are highlighted.

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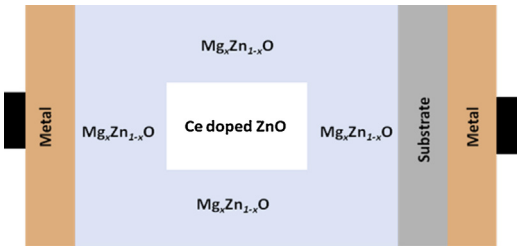

Fig. 1. Nanowire structure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

Table 1
Materials parameters considered for nanosimulation.

	Barrier region	Wire region
Material	$Mg_xZn_{1-x}O$	Ce doped ZnO
Layer length	20 nm	7–10 nm
Mg mole fraction	0.1–0.3	
Electron mass	$m_0 = 9.1 \times 10^{-31}$	
Electron effective mass	$(0.23 + 0.05x)m_0$	$0.28m_0$
Band gap energy	$3.373 + 1.046x + 0.87x^2$	3.29 eV [12]

2. Mathematical modeling

The band gap discontinuity in Ce doped ZnO/$Mg_xZn_{1-x}O$ quantum nano-wire structure provides a great opportunity for the electron confinement. For this reason, mole composition of Mg in the barrier region of $Mg_xZn_{1-x}O$ plays a crucial role in modulating band gap of barrier region and controlling band gap discontinuity. Analysis of quantum confinement has been carried out by solving Schrödinger equation in 2-D using MATLAB. Eigen energy has been deduced using Transfer Matrix Method as it is simple and accurate method [9].

2.1. Band gap engineering

The basic idea behind the quantum confinement is the band gap discontinuity between two materials. Increasing degree of confinement enhances the efficiency of the device. Nanowire structure provides considerable improvement over quantum well structures [10]. Moreover, the nanowire structure can be formed in more controlled manner [11].

Mole composition of Mg in Ce doped ZnO/$Mg_xZn_{1-x}O$ nanostructure plays an important role in band gap engineering as increase in the Mg mole fraction in ZnO changes its band gap energy from 3.37 to 7.7 eV. In this work, the impact of Mg composition in barrier has been studied for quantum confinement in active region of Ce doped ZnO nanowire structure. The band discontinuity between barrier and wire region has been successfully enhanced as a result of Ce doping in ZnO which reduces band gap of original ZnO. It leads to better quantum confinement and decreases the tunneling possibility of electron from active region to barrier. Materials parameters considered for modeling and simulation has been summarized in following Table 1.

2.2. Solutions of Schrodinger equation

The transportation of electron from one state to other can be described by the Schrödinger equation that leads to probability density arise due to the probability current and imaginary part of the potential. The Schrödinger equation in the X and Y direction has been solved for the arbitrary constants. Following two dimensional Schrödinger equations has been considered for Ce doped ZnO/$Mg_xZn_{1-x}O$ nanowire structure.

$$\left[\frac{\partial^2(x,y)}{\partial x^2} + \frac{\partial^2(x,y)}{\partial y^2}\right] - \frac{2m^*}{\hbar^2}V(x,y)\psi(x,y) = E_{x,y}\psi(x,y) \quad (1)$$

As the weak approximation does not involve the possibility of propagation of electron outside the structure, application of appropriate boundary conditions to forecast the behavior of electron in the nanostructure is must. The interface conditions are applied to the Schrödinger equation and general solutions for each layer have been obtained as follows:

$$\psi(x,y) = Ae^{(qz)} + Be^{(-qz)} \quad \text{for } z_x \le 0 \text{ and } z_y \le 0 \quad (2)$$

$$\psi(x,y) = C\sin(kz) + D\cos(kz) \quad \text{for } z_x \le a \text{ and } z_y \le a \quad (3)$$

$$\psi(x,y) = Fe^{(qz)} + Ge^{(-qz)} \quad \text{for } z_x \ge a \text{ and } z_y \ge a \quad (4)$$

t this juncture, terms A, B, C, D, F, G representing the arbitrary constants, q and k representing the wave vectors in barrier and wire region respectively.

$$\text{Here, } q = \frac{\sqrt{2m_w^* E}}{\hbar} \text{ and } k = \frac{\sqrt{2m_b^*(V-E)}}{\hbar}$$

The Schrödinger equation in 2-D form with above boundary conditions has been solved by using the separation of variable method [9].

2.3. Transfer matrix formulation

The Eigen energy has been deduced using the transfer matrix method and matrices obtained for nanowire structure are

$$\begin{bmatrix} 1 & 1 \\ q & -q \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ k & 0 \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix} \quad (5)$$

$$\begin{bmatrix} \sin(ka) & \cos(ka) \\ k\cos(ka) & -k\sin(ka) \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} e^{(qa)} & e^{(-qa)} \\ qe^{(qa)} & qe^{(-qa)} \end{bmatrix}\begin{bmatrix} F \\ G \end{bmatrix} \quad (6)$$

Eqs. (5) and (6) are written as

$$M_1\begin{bmatrix} A \\ B \end{bmatrix} = M_2\begin{bmatrix} C \\ D \end{bmatrix} \text{ and } M_3\begin{bmatrix} C \\ D \end{bmatrix} = M_4\begin{bmatrix} F \\ G \end{bmatrix}.$$

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_1^{-1}M_2M_3^{-1}M_4\begin{bmatrix} F \\ G \end{bmatrix}$$

$$A = M_{11}F + M_{12}G \quad (7)$$

$$B = M_{21}F + M_{22}G \quad (8)$$

The wave function has been interpreted so that it tends to zero into outer barrier region. It means coefficient of growing exponentials must be zero, i.e. $B = F = 0$. Hence, energy is sought which satisfies $M_{22}(E) = 0$. The Eigen energy computed has been used to determine the arbitrary constants and the wave function intensity.

3. Results and discussion

Eigen energy for different Mg mole composition in the $Mg_xZn_{1-x}O$ barrier and nanowire widths has been evaluated using Transfer Matrix Method. This Eigen energy has been used to deduce wave function and wave function intensity in the Ce doped ZnO/$Mg_xZn_{1-x}O$ quantum nanowire structure.

Fig. 2 depicts the Eigen energy as a function of nanowire dimensions for various values of Mg mole composition. It is apparent from our analysis that an increase in Mg composition increases the Eigen energy. It has been attributed to increase in band offset with