Optimization of single - mode electrically - pumped ZnO nanowire laser design structure with distributed Bragg reflector

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Optimization of design structure of single-mode electrically-pumped ZnO nanowire laser (NWL) with including of distributed Bragg reflector (DBR), acting as a rear mirror, has been achieved. Numerical simulation results show that the design structure of ZnO NWL with DBR has better performance compared to the same design structure but without DBR. Lower threshold current, higher output power, and higher quality factor (Q-factor) is observed of ZnO NWL with DBR.

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1. Introduction

Currently, ZnO is considered as one of the most important materials for ultraviolet (UV) optoelectronic devices, such as detectors, sensors, LEDs and lasers, due to its wide bandgap of 3.37 eV, large exciton binding energy around 60 meV, as well as ZnO is not toxic.

Random ZnO-based NWLs have been demonstrated with both optical and electrical pumping, but these random LDs suffer from reduced output powers, unstable emission spectra and beam divergence [1-4]. S. Chu1 et al. demonstrated good directional electrically pumped Fabry-Perot (F-P) ZnO NWL that consists of Sb-doped p-type ZnO NWs and n-type ZnO thin films [4]. An electrically pumped nitrogen doped p-type ZnO NWs/undoped n-type ZnO thin film homojunction random laser with a 10-period SiO₂/SiNx DBR is demonstrated by J. Huang et al. [5]. This random laser behaved with a low threshold of around 3 mA and output power was measured to be 220 nW at a drive current of 16 mA [5]. An electrically pumped UV random laser diode (LD) based on an Au-ZnO NW Schottky junction on top of a SiO₂/SiNx DBR has been fabricated by Sunayna B. Bashar et al. [6]. However, there is still a lack of high directionally and efficiency NWLbased on ZnO.

Electrically pumped ZnO NWL is critical for practical applications. In current issues, the output powers of the electrically pumped NWLs are relatively low and need to be increased. To achieve this goal, one way is to reduce the loss at the light reflection or scattering by adding DBR which is acting as a rear mirror. Both theoretical calculations and experiment results show that DBR gives desirable optical quality and the reflectivity at the wavelengths ranged between 380–390 nm up to be 95% [5] or more than this value depending on the number of DBR pairs. As a result, DBR structures which are formed from multiple layers of alternating materials with different

refractive indexes can significantly reduce the threshold pumping current and enhance LD output power and performance [6-8]. On the other hand, including DBR in NWL design structure may affect the other characterises of the LD. Therefore, the balance between characterises and requirements should be considered.

The aim of this study is designing a single-mode electrically-pumped ZnO NWL with uniform NWs to get low threshold current, high output power and good directionality of LD with DBR assisted.

2. ZnO nanowire laser design structure

In general, the under study design structure of ZnO NWL with DBR is similar, in some sides, to S. Chu et al.'s design structure [4] and J. Heo et al.'s design structure [5]. The top p-type contact of ZnO is designed and engineered to offer both good optical transparency for LD output and low electrical resistivity as it has been reported in the real structure fabricated in the LAB. [4]. The cavity length, *L*, between the top and the bottom ends of the ZnO NW is assumed to be 4.5 μ m. The area of design structure, *A*, is taken to be around (21× 21) μ m². Fig. 1 shows the design of single ZnO NW with its two contacts and substrate; while the schematic diagram of ZnO NWL design structure with DBR is shown in Fig. 2.



Fig. 1. The single ZnO NW with its contacts and substrate (color online)



Fig. 2. The schematic diagram of ZnO NWL design structure with DBR (color online)

As it is shown in Fig. 1, ZnO NW consists of two parts, n-type ZnO NW and p-type ZnO NW, this acting as Fabry-Perot (F-P) cavity by contrasting a high refractive index of ZnO NW against the surrounding medium which is air. In the other hand, DBR acts as a high rear mirror reflector as it is shown in Fig. 2. However, there are several differences between fabricated NWLs reported in refs [4,5] and the ZnO NWL design structure under study, which can be listed below:

I. NWs in real devices have different lengths in the same device; while in ZnO NWL design structure under study, NWs lengths are assumed to be the same.

II. The diameters of NWs in real structure are not the same in the same device; while in ZnO NWL design structure under study, diameters are assumed to be the same. III. Space between each two adjusted NWs is uniform and is taken to be 240 nm; while in real structure the spaces between each two adjusted NWs are non-uniform.

V. NWs in design structure under study are perpendicular to the substrate; while in real devices some of them are title.

Experimentally, high quality, such as high smooth, end facets are no longer requisite in NWL structures, since multiple reflections can occur at non-normal incidence with respect to the side faces, leading to a variety of possible resonator geometries [9]. Consequently, such phenomena, enable this type of NWLs of producing high gain in order of 10^4 cm⁻¹ which allows for the observation of lasing in ZnO NWL, which can be enhanced with including DBR.

3. Result and discussion

3.1. Parameters assignment and calculation

ZnO NWL design structure is based on many fundamental laser diode parameters and nano concepts. The initial parameters for this design structure have been adopted from related experimental works [4-6,10-12]; while the others have been assigned and calculated using suitable LD concepts and equations as will be shown.

Owing to the large difference in refractive index between ZnO NW, $n_z \approx 2.5$, and the embedding medium which is air, $n_a \approx 1$, NW acts in the same time as the optical gain medium and the optical cavity, as a result it is allowing of lasing despite the limited volume of ZnO gain material.

The cross-section of ZnO NW, which is actually hexagonal prismatic, can be treated as being approximately cylindrical [9]. Cylindrical semiconductor nanoscale lasers offer a means for improving, at the same time, both optical confinement and modal gain in such lasers [9]. Wide bandgap of ZnO semiconductor nanostructures, such as nanowires, with near-cylindrical geometry and large dielectric constants exhibit twodimensional UV waveguide [9] with an emission wavelength around 385 nm.

It is noticeable that the waveguide modes of the wires, and nanowire, can be treated with the aid of classical optical waveguide theory [9]. The fractional mode power within the core of the waveguide, NW is this case of this study, of radius r can be roughly estimated as [11]:

$$\eta_{mo} = 1 - \left[2.405 \exp\left(-\frac{1}{V}\right)\right]^2 V^{-3},$$
 (1)

where $V = kr(n_z^2 - 1)^{1/2}$, $k = 2\pi/\lambda$, and λ is the wavelength which is 385 nm. For ZnO NW with r > 100 nm, > 90% of the field intensity is retained in the nanowire for the lowest-order guided mode [9] as shown in Fig. 3. Fig. 3 also shows that the fractional mode power of ZnO NW with diameter of 120 nm is equals to 0.96 which equivalents the optical confinement factor, Γ , of the active region.



Fig. 3. Fractional mode power of ZnO NW as a function of its radius (color online)

As NW waveguide radius is increased, additional transvers modes being exist. However, there are critical values of the NW waveguide radiuses for operating in single-mode. In general, NW will function as a single-mode optical waveguide when the following condition is satisfied [12]:

$$1 \approx (\pi D/\lambda) \ (n^2 - n_a^2)^{0.5} < 2.4, \tag{2}$$

where 1 is a practical lower limit, D is the NW diameter. In the case of ZnO NW, the minimum and maximum diameters needed to support a single-mode are in the order of 50 and 128 nm, respectively. As a result, it is expected that the fundamental waveguiding mode at around 385 nm is strongly guided in 120 nm diameter of ZnO NW.

However, it is difficult to determine a value of the gain coefficient for an LD, and ZnO NWL, because the conventional methods, for this purpose, requires the length of a sample to be varied with constant cross-section [13]. A good design should have an appropriate gain length region where electrons and holes coexist, mainly near p-n junction where large amount of electron-hole pairs exist.

NW length is considered to be 4.5 µm, but in NWLs it isn't necessary to be the same of the gain length (L_{ac}). It can be noticed that the gain length in NWL is determined by the minority carrier diffusion lengths in the p-type NW ($L_n \approx 2$ mm) and n-type ZnO film ($L_p \approx 200$ nm), as well as the width of the space charge region (<100 nm) [4, 14,15]. Hence, the total gain length of ZnO NWL is calculated as:

$$L_{ac} = L_n + L_p + L_S \approx 2.3 \,\,\mu\text{m} \tag{3}$$

As a result, the threshold gain, G_{th} , of F-P ZnO NWL design structure is determined as:

$$G_{th} = \frac{1}{2\Gamma L_{ac}} ln(\frac{1}{R_1 R_2}) \tag{4}$$

In NWL, normally G_{th} is calculated by considering mirror losses (α_m) only because the mirror losses >>

internal losses (α_i). α_m accounts for the losses at the end facets (the mirror losses). For ZnO NWs, the cavity length is much smaller and the reflection coefficient is small, as a result the dominant loss mechanism is considered to be the mirror loss, $\alpha_m \gg \alpha_i$, so the waveguide loss (internal loss, α_i) can be neglected [16,17]. Therefore, G_{th} for ZnO NWL, and other types of NWLs, can be written as in Eq.(4). G_{th} of F-P ZnO NWL design structure without DBR is calculated to be 1.27×10^4 cm⁻¹, this is high value, which requires a high threshold bias current. As it seen, L_{ac} is considered to determine G_{th} ; while NW length, L, determines the average spacing between adjusted modes ($\Delta\lambda$) according to the following formula:

$$\Delta \lambda = \frac{\lambda^2}{\left[2L(n-\lambda\left(\frac{dn}{d\lambda}\right)\right]}\tag{5}$$

Where $dn/d\lambda$ denotes the dispersion relation for the refractive index, which is = - 0.015 nm⁻¹ [4]. For a 4.5 µm cavity length between the top end of the ZnO NWL designed structure and the bottom ZnO film/silicon interface, $\Delta\lambda$ is calculated to be around 2 nm.

First, it has been designed quarter-wavelength DBR with SiO_2 and SiN_x acting as two dielectric layers using the following equation [6]:

$$n_H l_H = n_L l_L = \lambda/4 \tag{6}$$

The designed DBR structure of many-period alternating 65.07 nm SiO_2 and 47.5-nm SiN_x layers provides high reflectivity at the bottom of the ZnO NW, acting as a rear mirror, thus causing more light to be scattered among the NWs [6].

The reflection response, R_r , from the DBR at operating wavelength ranged between 380-390 nm can be simply expressed as [5,6]:

$$R_{r} = \frac{1 - \left(\frac{n_{H}}{n_{L}}\right)^{2N} \frac{n_{H}^{2}}{n_{a}n_{b}}}{1 + \left(\frac{n_{H}}{n_{L}}\right)^{2N} \frac{n_{H}^{2}}{n_{a}n_{b}}},$$
(7)

where n_a is the refractive index of air, n_b is Si substrate refractive index, and N is the number of bilayer in the DBR, which is assumed to be varied from 2 to 16 in this study.

Without DBR, the facet end reflectivities of ZnO NW are extremely low, the reflectivity of the front facet is 0.04 and the reflectivity of rear facet is 0.09 [4]. Since DBR is assumed to be in the bottom of the ZnO NW design structure under study, it is acting as a rear mirror, so the reflectivity of the rear mirror is altered according to the number of the DBR pairs, as indicated in Figure 4, which represents the DBR pairs as a function of the average reflectivity ($\mathbf{R} = \sqrt{R_1 R_2}$) of the NW end mirrors.



Fig. 4. The average mirror reflectivities as a function of DBR pairs (color online)

Photon lifetime (T_p) for ZnO NWL without DBR is expressed as:

$$\frac{1}{\tau_p} = \frac{c}{n} \left(\alpha_i + \alpha_m \right)$$
$$\frac{1}{\tau_p} = \frac{c}{n} \left(\alpha_i + \frac{1}{2L} ln \frac{1}{R_1 R_2} \right), \tag{8}$$

since $a_m >> a_i$, a_i can be neglected, as it is shown above, hence, τ_p is mainly determined by a_m . For ZnO NWL without DBR, τ_p is calculated to be 6.8 fs, it is noticeable that τ_p is extremely low, this due to low facet reflectivities of ZnO NWs. As a result, including DBR on ZnO NWL design structure can increase the value of photon lifetime, Fig. 5 shows the photon lifetime as a function of DBR pairs.



Fig. 5. Photon lifetime as a function of DBR pairs (color online)

Quality factor (Q-factor) is another important parameter to be determined, it depends on the NW length and two facet mirror reflectivities, which can be calculated from the following formula:

$$Q = \frac{2\pi n_z L}{\lambda (1 - \sqrt{R_1 R_2})},\tag{9}$$

for ZnO NWL design structure without DBR, Q-factor is calculated to be 200. The low value of Q-factor is attributed to the low two facet mirror reflectivities and as indicated in Eqs. (8) and (9). Since Q-factor depends on the R_1 and R_2 , it is altered by including DBR in ZnO NWL design structure depending on the number of DBR pairs as indicated in Fig. 6.



Fig. 6. Quality factor as a function of DBR pairs (color online)

Parameters that have been adopted and calculated to be used in this numerical simulation are listed in Table 1.

Table 1. Parameters of ZnO NWL design structure

Parameter	Symbol	Value	Unit
Laser wavelength	λ	385	nm
NWL cavity length	L	4.5	μm
(Nanowire length)			
Nanowire diameter	D	120	nm
Active region length	L_{ac}	2.3	μm
Aria of NWL	Α	451.6	μm ²
Active region volume	V_a	9×10 ⁻¹¹	cm ³
ZnO refractive index	n_z	2.5	
Carrier lifetime	$ au_n$	0.2	ns
Carrier number at transparency	No	$\approx 7 \times 10^7$	
Photon lifetime (without DBR)	$ au_p$	6.8	fs
Optical confinement factor	Г	0.96	
Front facet reflectivity	R_{I}	0.09	
Rear facet reflectivity (without	R_2	0.04	
DBR)			
Internal efficiency	η_i	0.5	
Si refractive index	n_b	3.5	
Air refractive index	n _a	≈ 1	
Dispersion relation for the	$dn/d\lambda$	-0.015	nm ⁻¹
refractive index			
Threshold gain (without DBR)	G_{th}	1.27×10^{4}	cm ⁻¹
Q-factor (without DBR)	0	200	

3.2. Applying rate equations

Many valuable information of ZnO NWL design structure under study can be obtained by applying the well-known rate equations. A simple single-mode rate equations feature of the photon number, S, and electron number, N, under continuous wave, CW, operation and electrical pumping are used [18]:

$$\frac{dN}{dt} = \frac{I(t)}{q} - \frac{N}{\tau_n} - \Gamma gS \tag{10}$$

$$\frac{dS}{dt} = \beta \frac{N}{\tau_n} - \Gamma g S - \frac{S}{\tau_p}$$
(11)

The material gain can be simplified then expressed as:

$$g = \alpha(N - N_o), \tag{12}$$

where I(t)/q is the electrically driven rate, τ_n and τ_p are the carrier lifetime and photon lifetime, respectively, Γ is optical confinement factor and α is slope gain constant.

Appling a steady-state condition on Eq. 11, carrier number at threshold is obtained as:

$$N_{th} = N_o + (g_{th}/\Gamma\alpha) \tag{13}$$

Appling the steady-state condition again on Eq. 10, photon number as a function of the electrical driven current is obtained as:

$$s = \frac{(l/q)(n_{th}/\tau_n)}{\Gamma g}, \qquad (14)$$

where n_{th} is the carrier number at threshold. The power emitted by LD above threshold is:

$$P_{out} = \eta d(hv/q)(I-I_{th}) \tag{15}$$

Volume of nanowire (V_n) = Length of active area $(L_{ac}) \times$ cross sectional area (A):

$$V_n = L_{ac} \times A$$
 (16)
= 2.60×10⁻¹⁴ cm³

The total equivalent volume (V_T) = volume of one nanowire × number of nanowire per unite area:

=

$$V_T = 2.60 \times 10^{-14} \times 3484 = 9.059 \times 10^{-11} \text{ cm}^3$$



Fig. 7. Output power of NWL as function of current with and without 16 DBR pairs (color online)

Since the one attractive way for increasing the output powers and decreasing the threshold currents of NWLs is by including DBR in the LD structures, the output power of ZnO NWL is enhanced with the assistance of DBR as indicated in Fig. 7, threshold current is also reduced with including DBR as indicated in Fig. 7.

For the purpose of the comparison with related experimental works, the results presented in this work agree with experimental works, the results of increasing of output power and Q-factor, as well as reducing threshold current with increasing the number of DBR pairs are in line with experimental works reported in refs [4-6].

4. Conclusion

ZnO NWL with DBR has better performance than that without DBR, enhancing output power and reducing threshold current with DBR ZnO NWLs is critical for LD applications especially in optical communication systems. Since, ZnO NWL properties are altered with including DBR, the applications of such LDs are also enhanced and altered.

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