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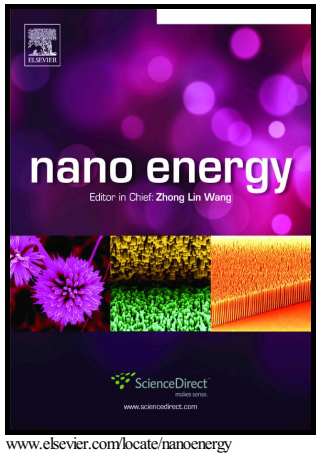

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Piezophototronic effect enhanced luminescence of zinc oxide nanowires

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Abstract:

Experimental findings on electroluminescence or photoluminescence of ZnO nanowires have been drawn much attention due to their promising applications in many areas. One of the current challenges on this technology is a deeper understanding of this phenomenon in order to adopt it into practical device designs. In this work, a theoretical analysis of the stimulated emission of ZnO nanowires taking into consideration of the piezotronics effect has been conducted using the quantum mechanics theory. It is revealed that extra piezoelectric charges induced by applied mechanical forces increase the overall charge density of the nanowire, subsequently enhancing the emission intensity. Electronic bandgap varying with the diameter of the nanowire determines the peak value in the electromagnetic spectrum. Both wavelength and intensity of the stimulated emission can be tuned by controlling the dimension of the nanowires and external applied mechanical forces.

Keywords: ZnO nanowire, quantum mechanics, stimulated emission

Introduction:

The first nanogenerator based on ZnO nanowires was developed to generate electricity from mechanical movements [1]. Due to coupling properties of semiconductor and piezoelectric in wurtzite semiconductors, such as ZnO, GaN, InN and CdS, emerging nanoelectronic applications have been developed based on the basic principle that strain-induced piezoelectric charges can turn/control carriers transport in piezoelectric semiconductors. The new emerging fields of piezotronics and piezophototronics are coined by Zhong lin Wang, which are potentially applied in many engineering areas. Fundamental of the piezotronics effect has been explained in [2] [3] [4]. Transistors made by ZnO nanowires were introduced in [5], and recently high performance transistors based on ZnO nanowires for driving high power light emitting diodes have been fabricated [6]. Resistive switching devices have been realized using ZnO nanowires, both in terms of metal-semiconductor contact [7], and electromechanical relocations of nanowires [8] [9]. ZnO nanowire sensors were developed for high performance gas sensors and pressure sensors [10] [11] [12] [13] [14]. Optical properties such as

photoluminescence and electroluminescence of nanodevices have attracted a great amount of attentions, enduing themselves with potential usage in optical imaging, sensors, and smart systems. Notable developments in this area include an imaging device made of ZnO nanowires array combined with GaN light emitting diodes, whose emitting intensity can be adjusted by the mechanical strains applied on the piezoelectric nanowires [15]. Similar approach has been conducted using ZnO nanowires and GaN light emitting diodes reported in [16], in which the piezotronic effect wasn't mentioned. Electroluminescence of ZnO with UV LEDs has been reporfted in [17]. An intense electroluminescence from ZnO nanowires has been achieved recently using enhanced quality of the nanowires and injections of holes from the p-type ZnO [18]. During the research and development of the electroluminescence or photoluminescence phenomena, there is a lack of in-depth theoretical understanding and explanation from quantum theory point of view.

In this paper, we will theoretically investigate the impact of the nanowire diameters on the spectrum of the stimulated emission (shown schematically in Figure 1), and the enhancement of the emission intensity by the piezotronic effect. This work fills the gap by using quantum mechanics theory and interesting results as to the relations among piezoelectric charges, energy bandgap, emission intensity and peak wavelength are obtained and analyzed in the following sections. The paper is organized as follows: optical transmission of the ZnO thin film is reviewed using dispersive refractive index in the first part of the paper. It is followed by the quantum mechanics simulation of the stimulated emission. The results of the simulation are then presented and discussed.

Optical transmission of ZnO

Transmission of light through a single ZnO thin film can be calculated using classic optical theory taking consideration of wavelength dependent complex refractive index of ZnO, which is expressed as

$$n_r(\lambda) = n(\lambda) - ik(\lambda) \qquad (1)$$

Real part of the refractive index $n(\lambda)$ can be derived from the Sellmeier equation given by $n^2(\lambda) = A + \frac{B\lambda^2}{\lambda^2 - C^2} + D\lambda^2$, where A, B, C, D and E have been extracted to be 2.814, 0.879, 0.304, and 0.00711 respectively [19] [20]. Imaginary part $k(\lambda)$ has been given as $k(\lambda) = E\lambda \exp\left(-F\left(\frac{1}{G} - \frac{1}{\lambda}\right)\right)$, where E, F and G are Cauchy parameters as 0.0178 nm^{-1}, 7327.1 nm, and 337.87 nm respectively taken from the reference [21]. Suppose that the refractive index of air n_0 is 1, the transmitted amplitude is given by [22]

$$T_p = \frac{t_1 t_2 \exp(-i\delta)}{1 + r_1 r_2 \exp(-2i\delta)}$$
$$t_1 = \frac{2n_0}{n_0 + n_r(\lambda)}, \quad t_1 = \frac{2n_r(\lambda)}{n_r(\lambda) + n_0}, \quad r_1 = \frac{n_0 - n_r(\lambda)}{n_0 + n_r(\lambda)}, \quad t_1 = \frac{n_r(\lambda) - n_0}{n_r(\lambda) + n_0} \qquad (2)$$
$$\delta = \frac{2\pi}{\lambda} n_r(\lambda) d \cos\varphi$$

where d is the thickness of the film, φ denotes the incident angle of the light. Varying wavelength of the light from 300 nm to 1000 nm, transmission coefficient has been obtained shown in the Figure 2. It is seen that the T-λ curve is analogy to a high pass filter with $1/\sqrt{2}$ pass band from 400 nm. It is also found that the cut-off frequency for transmission curve shifts to longer wavelength as the film thickness increases. Light transmission of ZnO thin films has been experimentally investigated in [23]. Analytical analysis of the light transmission through ZnO films or nanowires provides the background for the further analysis based on quantum mechanics theory. Light-semiconductor interaction theory is utilized to unveil the spectrum of stimulated and spontaneous emissions, two mechanisms that elucidate the electroluminescent or photoluminescence properties of ZnO nanowires in presence of mechanical pressures in their c-axis. The hypothesis behind the experimental observation described in [15] has been made that when the force is exerted on the nanowire, extra charges are generated due to piezotronic effect, subsequently increasing the carrier concentration. The increased carrier concentration leads to enhanced emissions, therefore reflecting increased brightness.

Quantum mechanical analysis:

As an incident photon of energy $\hbar\omega$ ($\hbar$ is the reduced Planck's constant, and ω is the frequency of light) enters to the semiconductor material, in this case a ZnO nanowire, electron absorbs the photon energy transiting from states of valence band to states of conduction band (Figure 1). In the meantime, an electron can migrate back to the energy states in valence band from conduction band, emitting photons. It is thought the interband transition of electrons that governs the process of the luminescent imaging of piezoelectric nanowire LED array. Under incident light energy, transition of electrons from the conduction band (higher energy states) to the valence band (lower energy states) creating a new photon with identical phase, frequency, polarization, and direction of travel as the photons of the incident wave, termed as the stimulated emission. The absorption is ignored in this analysis. There exists a very small amount of spontaneous emission due to electrons transiting from conduction band to valence band in the absence of incident light. As demonstrated in reference [15], images get brighter in the area where a mechanical pressure was applied on the nanowires array, indicating a light amplification, which can be explained by mainly the stimulated emission mechanism. If we measure energy from the top of the valence band, then the energy of an electron in the conduction band with

effective electron mass m^*_e is $E_2 = E_g + \frac{\hbar^2 k^2}{2m_e^*}$ (k is the wave vector, and E_g is the band gap) and the energy of an electron in the valence band with effective electron mass m^*_h is $E_1 = -\frac{\hbar^2 k^2}{2m_h^*}$. Then the energy due to an electronic transition from the conduction band to the valence band is $\hbar\omega = E_2 - E_1 = \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) + E_g$, defining the reduced effective mass m_r, we have $\frac{1}{m_r} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$, so $\hbar\omega = E_2 - E_1 = \frac{\hbar^2 k^2}{2m_r} + E_g$. For an incident electromagnetic wave $A(r,t) = A_0 \cos(q \cdot r - \omega t)$, where the wave vector $q = \frac{\omega n_r}{c}$, n_r is the refractive index of the media, c is the speed of light and ω is the angular frequency of the plane wave. The transition rate from the initial state to a state in the valence band in the presence of electromagnetic radiation is given by Fermi's golden rule. The stimulated emission rate is given by

$$R = \frac{2\pi}{\hbar}\left|\langle \psi_1 | H' | \psi_2 \rangle\right|^2 \delta(E_c - E_v - \hbar\omega) \qquad (3)$$

where ψ_1 and ψ_1 are the final and initial wave function of the electron respectively, H' is the perturbation Hamiltonian $H' = \frac{e}{2m} A_0 e^{iq\cdot r} \cdot q$. Generally speaking the transition rate depends on the strength of the coupling between initial and final states, and the number of ways the transition can occur, i.e. the density of states. It is assumed that a number of transitions happening per unit volume of material per second. The total transition rate is given by

$$E_{St} = \frac{2}{V}(\sum_k R) f_e f_h \qquad (4)$$

where $f_e = f_1$ and $f_h = 1\text{-}f_2$, and f_1 and f_2 are Fermi-Dirac distribution functions of electron states in the conduction band and valence band respectively ($\frac{1}{e^{(E-\mu)/k_B T} + 1}$). After several derivation procedures such as the separation of fast varying and slow varying exponents in the integrand and breaking up the integral over the entire crystal into integrals over all the primitive cells. Finally one can arrive at the following equation

$$\frac{2}{V}\sum_k R = \frac{2\pi}{\hbar}\left(\frac{qA_0}{2m}\right)^2 \left\langle \left|\hat{\bar{p}}_{cv} \cdot \hat{n}\right|^2 \right\rangle 2 \times \int \frac{d^3k}{(2\pi)^3} \delta(E_c - E_v - \hbar\omega) \qquad (5)$$

The squared momentum matrix element $\left|\hat{\bar{p}}_{cv}\cdot\hat{n}\right|^2$ depends on the electron wavevector k and also the polarization direction of the electromagnetic wave. In most of III-V and II-IV semiconductors, the average value of the momentum matrix element can be treated as constant [24], expressed in terms of the *Kane* energy E_p, as $\left\langle\left|\hat{\bar{p}}_{cv}\cdot\hat{n}\right|^2\right\rangle=\frac{mE_p}{6}$. The value of E_p for most of II-IV and III-V semiconductors can be found from the preferences [25] [26]. $\int\frac{d^3k}{(2\pi)^3}\delta(E_c-E_v-\hbar\omega)$ is the density of states $g(E)$ in three-dimensions. Density of states (DOS) is defined as the number of states in a conductor per unit energy. The DOS for bulk materials with no confinement is expressed as

$$\int\frac{d^3k}{(2\pi)^3}\delta(E_c-E_v-\hbar\omega)=\frac{1}{4\pi^2}\left(\frac{2m_r}{\hbar^2}\right)^{3/2}(\hbar\omega-E_g)^{1/2} \tag{6}$$

Combining equations (4), (5), and (6), the stimulated emission is expressed as

$$E_{St}=\frac{2\pi}{\hbar}\left(\frac{qA_0}{2m}\right)^2\left\langle\left|\hat{\bar{p}}_{cv}\cdot\hat{n}\right|^2\right\rangle\frac{1}{2\pi^2}\left(\frac{2m_r}{\hbar^2}\right)^{3/2}(\hbar\omega-E_g)^{1/2}f_ef_h \tag{7}$$

For nanostructures, electrons are likely confined in three dimensions, akin to quantum dots. The DOS for electrons confined in 3D is

$$g(E)=\frac{2}{\pi}\frac{\hbar/2\tau}{(\hbar\omega-E_g)^2+(\hbar/2\tau)^2} \tag{8}$$

Equation (8) is known as a Lorentzian equation. The width of the Lorentzian at half its peak value (full width at half maximum, or FWHM) is $\hbar/\tau$. The coupling between the photon and the electron within the nanowire can be described by the coupling energy $\Gamma=\hbar/\tau$. In this work, the Γ is taken to be 20 meV. Stimulated emission using 3-D confined density of states, $E_{st\text{-}c}$ is given by

$$E_{St-c}=\frac{2\pi}{\hbar}\left(\frac{qA_0}{2m}\right)^2\left\langle\left|\hat{\bar{p}}_{cv}\cdot\hat{n}\right|^2\right\rangle\frac{2}{\pi}\frac{\Gamma/2}{(\hbar\omega-E_g)^2+(\Gamma/2)^2}f_ef_h \tag{9}$$

In addition to the stimulated emission process, an electron in the conduction band can spontaneously emit a photon and migrate to the valence band, named as spontaneous emission. The rate of spontaneous emission is comparably much smaller than the stimulated emission for this particular material. For the application of LED+ZnO nanowires, only the $E_{st\text{-}c}$ will be considered. Re-arrange equations (7) and (9), let $M=\left\langle\left|\hat{\bar{p}}_{cv}\cdot\hat{n}\right|^2\right\rangle$, and substitute q by $(\omega n_r)/c$, we get

$$E_{St} = \frac{\sqrt{2}\pi A_0^2 m_r^{3/2} M}{m^2 \hbar^6 c^2} (\hbar\omega)^2 n_r{}^2 (\hbar\omega - E_g)^{1/2} f_e f_h$$
$$E_{St-c} = \frac{4 A_0^2 M}{m^2 \hbar^3 c^2} (\hbar\omega)^2 n_r{}^2 \frac{\Gamma/2}{(\hbar\omega - E_g)^2 + (\Gamma/2)^2} f_e f_h \qquad (10)$$

Hence scaled stimulated emissions for both scenarios ($E'_{St} = \frac{E_{St} m^2 \hbar^6 c^2}{\sqrt{2}\pi A_0^2 m_r^{3/2} M}$, $E'_{St-c} = \frac{E_{St-c} m^2 \hbar^3 c^2}{4 A_0^2 M}$) is given by

$$E'_{St} = (\hbar\omega)^2 n_r{}^2 (\omega)(\hbar\omega - E_g)^{1/2} f_e f_h$$
$$E'_{St-c} = (\hbar\omega)^2 n_r{}^2 (\omega) \frac{\Gamma/2}{(\hbar\omega - E_g)^2 + (\Gamma/2)^2} f_e f_h \qquad (11)$$

where $\hbar\omega$ is the photon energy E_p. It is seen that the stimulated emission is proportional to the photon energy, refractive index, DOS and distributions of electrons and holes. Numerical solution to this equation is followed in the next section. Please be noted that emitted photon energy is at the same frequency as the incoming photon energy. The spontaneous emission E_{spon} is related to the stimulated emission based on the *Einstein* relation, express as

$$E_{spon} = \frac{\hbar\omega^3}{\pi^2 c^3} E_{St} \qquad (12)$$

Results and analysis

According to equation (11), stimulated emissions have been calculated numerically. Dispersion in the refractive index ($dn_r/d\lambda = 0$) is considered in the quantum mechanics simulation. The chemical potential for a number of electrons and holes per unit volume at certain temperatures is required to calculate the f_e and f_h. To calculate the chemical potential for electrons or holes, the following process is used. First of all, an initial value of the chemical potential needs to be estimated. The maximum possible value of the chemical potential is given by the Fermi energy $\mu_{\max} = E_F = \frac{\hbar^2 k_F^2}{2m}$ $k_F = (3\pi^2 n_c)^{1/3}$, n_c is the carrier density. The minimum possible value of the chemical potential is given by the high-temperature limit ($T \to \infty$). In this limit the Fermi-Dirac distribution becomes Boltzmann distribution

$$f(E)|_{T\to\infty} = \frac{1}{e^{(E-\mu)/k_B T} + 1}\Big|_{T\to\infty} = e^{(E-\mu)/k_B T} \qquad (13)$$

A three dimensional electron gas in this high temperature limit has chemical potential

$$\mu_{\min} = k_B T \ln\left(\frac{n}{2}\left(\frac{2\pi\hbar^2}{mk_B T}\right)^{3/2}\right) \qquad (14)$$

Carrier density n can be calculated using an integral over energy

$$n = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_{E_{\min}=0}^{E_{\max}=\infty} E^{1/2} \frac{1}{e^{(E-\mu)/k_B T}+1} dE \qquad (15)$$

A computer iteration process is used to calculate the chemical potential for both electrons and holes respectively (μ_e, μ_h). In the process, an initial chemical potential value taking the average of the maximum and minimum chemical potential is used to calculate a carrier density *n'* for a given temperature by calculating the integral described by the equation (15). If the *n'* is less than the actual value n_c, the new best estimate for $\mu_{\min} = \mu'$. The new estimated μ is given, and the process iterate until the value reaches to a desired level of accuracy. The calculated chemical potentials for electrons and holes are then used in equation (11) to calculate the stimulated emission rate. The bandgap of ZnO nanowire varies with its size and force induced strains [27]. For the strain-free condition, E_p is taken as 3.28 eV. In this simulation, E_p = 3.2 eV is used, as the applied force reduces the value of E_p value to 3.17 with 7.3 % strain for 100 nm diameter nanowire according to reference [27]. Other parameters and constants used in the simulation are listed in the Table 1.

Table 1: constants and parameters used in the simulation

Physical parameter	Value
Electron charge	1.60 x 10^{-19} C
Reduced Planck's constant	1.05 x 10^{-34} Js
Speed of light	2.99 x 10^{8} m/s
Boltzmann constant	8.62 x 10^{-5} eV/K
Permittivity of free space	8.85 x 10^{-12} F/m
Electron mass, m_0	9.11x10^{-31} Kg
Effective electron mass [28]	0.2 x m_0
Effective heavy hole mass [28]	0.55 x m_0
Temperature, T	300 K
Initial carrier concentration	4.0x10^{23} m^{-3}

Piezoelectricity describes interaction between electrical and mechanical behaviour of the medium, expressed as

$$S = s^E T + dE$$
$$D = dT + \varepsilon^T E \qquad (16)$$

where *S, T, E, D* are strain, stress, electrical filed strength, and dielectric displacement respectively. *s, d, ε* are mechanical compliance, piezoelectric constant, and dielectric constant, where the superscripts to the symbols denotes the quantity kept constant under boundary conditions. For this case, as the mechanical-to-electrical conversion and the optical behaviour will be investigated, the electrical circuit connecting two ends of the rod is open, assuming there is no external electrical field the equation (16) is simplified to $D = dT$. The force is applied along the *c*-axis, the induced electrical charge $Q = d_{33} F$, where *F* is the force applied, d_{33} is the piezoelectric constant defined as the induced polarization per unit applied stress in direction 3 (*z* –axis). For the ZnO nanowire, piezoelectric constant d_{33} = 5.43 x 10^{-12} C/N [29]. It is assumed that the applied force ranges from 0 to 8 μN, considering nanowire dimension as 50 nm in diameter, 100 nm in length, the increment of the carrier density is calculated up to 1.38 x 10^{24} m^{-3}.

Results shown in Figure 3 display E_{st}' vs. wavelength for the axial forces applied on the ZnO nanowires. It is indicated that there is a peak value of emission along the wavelength spectrum. Furthermore different energy bandgaps result in various peak frequencies. For small diameter ZnO nanowires (<100 nm), the energy bandgap is around 3.3-3.4 eV, where the stimulated emission is peaked at around 375 nm according simulated results in Figure 3, this is in line with the measured photoluminescence spectra results in reference [16] [30] [18] [31]. The bandgap shifts up or down slightly depending on different diameters [27]. As the diameter of ZnO nanowires increases, the energy bandgap reduces into smaller values. The physics behind could be attributed to the surface-shrinking strain along the radial direction and the tensile strain along the *c*-axis direction. In the intrinsic state (under no external stress induced strain), surface effect causes the shrinking effect shortening the Zn-O bond parallel to the radial direction in the shell of nanowires. Significant in-plane surface Zn-O bond contraction was theoretically modelled appearing in the surface thickness of ~2 nm [32]. This surface effect will impact more on the small diameter nanowires than large diameter nanowires, as the small diameter wires have increased surface-volume ratios, leading to larger bandgap values. Bandgaps of 3.2 eV and 3.1 eV have also been used in the stimulated emission analysis, whose results are shown in the Figure 3. The electroluminescence of the thicker wires (800 nm in diameter) corresponding to smaller bandgap values have been experimentally shown in [15], at which the stimulated emission is peaked at around 400 nm, which matches with the theoretical observation in this work. In theory the bandgap value corresponding to the experimental results in the above reference is around 3.1 eV. It also reveals that as the force increases, the carrier density increases leading to higher emissions ascribed to extra induced piezoelectric charges. In the simulation, external mechanical strain induced bandgap change is neglected. The assumption is based

on that the axial force is mainly affecting the energy of the conduction band minimum state concentrated in the core (E_c), and the energy of the valence band minimum state localized on the surface is more sensitive to the radial bond length variation. The change in E_c under axial strain is much less than E_v [27]. As suggested in the equation (8), spontaneous emission shows similar trend but with much lower amplitude due to the absence of the injected photons. Comparing results in Figures 3a and 3b, it is seen that using the 3D confined DOS leads to the results much closer to the experimental observations. It also suggests that photo luminescence phenomenon exists in both the ZnO bulk films and nanostructures.

Considering the combined effect of the transmission coefficient shown in the Figure 2 and the stimulated emission results in the Figure 3, one is able to comment that as the incident wavelength increases, the absolute value of the complex refractive index reduces, leading to reduced stimulated emission peak. Macroscopically the optical transmission has the cut-off wavelength at around 400 nm. The physics behind could be elucidated that a smaller refractive index means that the optical wave has a shorter travelling time within the material, where less electro-photon interaction is expected, subsequently generating reduced stimulated emissions. Taking consideration of the low transparency for optical wavelength less that 400 nm, the thinner wires that more likely have stimulated emission peaks at shorter wavelengths will have much higher optical contrast for electroluminescence or photoluminescence applications. This will be very attractive for those applications requiring high contrast and high imaging resolutions. The theory above has been focused on the stimulated emission of the ZnO nanowires, it can also be applied on the ZnO thin films. The advantage of using nanowires is that the devices made of nanowires will have much higher imaging resolution than that of devices fabricated by thin films.

Further numerical calculation is performed for the relation between simulated emissions and vertically applied force. Results shown in Figure 4 explain that as the force increases, stimulated emission is enhanced. Figures 4a and 4b display results for bulk material and nanostructures respectively. As the photon energy is related to the wavelength, hence a shorter wavelength reflecting higher photon energy leads to reduced stimulated emission as implicated in the left half of the Lorentzian. The E_{St} vs F curves are quasi-linear, as explained from the theory of the basic piezoelectric induced charges. It is envisaged that more charges will participate the photon-electron interactions with the presence of externally applied forces. It is demonstrated from the results in Figures 4a and 4b that the ZnO nanostructures are much more sensitive to the applied forces than devices made in bulk materials such as films. Inspired by the reference [33], filter effect due to mechanical strains can be demonstrated with ZnO materials. Here in this work, simulation is performed for devices with varied energy bandgaps. Bandgaps ranging from 3.30 eV to 3.12 eV are designated in the numerical simulation, and results clearly show the filtering effect for both the bulk material and nanowires. In the Figure 5, it shows that the wavelength of the stimulated emission varies from about 375 nm to around 398 nm

when decreasing the bandgap from 3.30 eV to 3.12 eV. This can be explained that larger bandgap requires more photon energy to excite electrons transiting to lower energy states, i.e. shorter wavelength of the incident and emitted optical signals. The results qualitatively match with recent experiments reported in [34]. Modelling has been performed to mimic the images with adjustable intensity by vertically applying a mechanical force to the nanowires. Figure 6 displays simulated images with different forces showing enhanced intensity. The simulation shown in the Figure 6 (right) elucidates that as the applied force increases, more piezoelectric current will be induced; subsequently the emission intensity increases. It is also shown in Figure 6 that the emission spectrum can be tuned by the energy bandgap determined by the diameter of the nanowire. It is worth to emphasise that the bandgap variation can impact the emission spectrum according to calculation. Mechanical strain can also change the bandgap of the wire, which is regarded as a symmetric process, i.e. being independent of the direction of the applied force. However the piezoelectric induced charges have polarities (negative and positive) depending on the direction of applied force, namely an asymmetric process. Opposite applied force will generate charges with inverse polarity, which may influence the enhancement of the emission. Since the emission is determined by the distributions of electrons and holes.

Conclusion:

Quantum mechanics theory has been used to elucidate the electroluminescence or photoluminescence of ZnO nanowires. The results show that ZnO in the forms of both bulk and nanostructures can have stimulated emissions, wherein the bulk ZnO has much smaller quality factors on the wavelength spectrum than ZnO nanostructures. The physics behind is that in the nanostructures, electrons are confined and the density of states is governed by Lorentzians where the interaction time between photons and electrons are usually very short, leading to very sharp wavelength spectrum. For the imaging applications, ZnO nanostructures have the clear advantage of high resolution /contrast not only because of their small dimensions, but also due to their very high selectivity of incident optical wavelengths. According to the analysis, emission intensity can be adjusted by strain induced piezoelectric charges and energy bandgaps. More generated piezoelectric charges will result in increased charge density, hence increasing emission intensity. Again nanostructures demonstrate much superior performance to bulk materials in terms of the increase of emission intensity. The peak wavelength is tuneable by the energy bandgap E_g. Larger E_g corresponds to the emission peak at lower wavelength (high photon energy), and lower E_g corresponds to the emission peak at higher wavelength. This will help construct optical filters or prisms using nanowires array with controlled diameters.

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Figure captions:

Figure 1, Schematic diagram showing: (a), a nanowire being mechanically anchored on the bottom plane, and being applied a force F on the top face. Optical light shines on the bottom side, and light emits from the top side. (b), Schematic graph showing an electron transition from valence band to conduction band subjecting an incident photon of energy $\hbar\omega$. The Fermi-Dirac distribution of electron states in the conduction band is f_e, and in the valence band is f_h.

Figure 2, Calculated transmission coefficient for 100 nm ZnO film. It shows that as the length of the nanowires is less than 100 nm, emissions graphs will be riding on the transmission curve. For thicker films, due to the cut off frequency shift, the emissions graphs sit in the stop band, meaning a much higher imaging contrast.

Figure 3. Calculated stimulated emissions for difference forces applied to the nanowires. Three sets of curves correspond to three energy gaps ranging from 3.1 eV to 3.3 eV. (a), calculation using bulk DOS. (b), calculation using 3-D confined DOS.

Figure 4, calculated stimulated emissions for different photon energies, E_p. (a), calculation using bulk DOS. (b), calculation using 3-D confined DOS.

Figure 5, Stimulated emissions with various energy bandgaps, effectively forming an adjustable optical filter. Insert graph schematically shows an incident white light has been filtered to light with a narrow pass band, of which the peak can be adjusted by the means of applying mechanical axial forces. (a), calculation using bulk DOS. (b), calculation using 3-D confined DOS.

Figure 6, simulated emission spectrum tuned by the energy bandgap, and intensity enhancement with applied mechanical forces.

Highlights of "Piezophototronic effect enhanced luminescence of zinc oxide nanowires"

Yan Zhang, Lijie Li

1. A theoretical analysis of the stimulated emission of ZnO nanowires taking into consideration of the piezotronics effect has been conducted using the quantum mechanics theory.

2. It is revealed that extra piezoelectric charges induced by applied mechanical forces increase the overall charge density of the nanowire, subsequently enhancing the emission intensity.

3. Electronic bandgap varying with the diameter of the nanowire determines the peak value in the emitted optical spectrum.

Piezophototronic effect enhanced luminescence of zinc oxide nanowires

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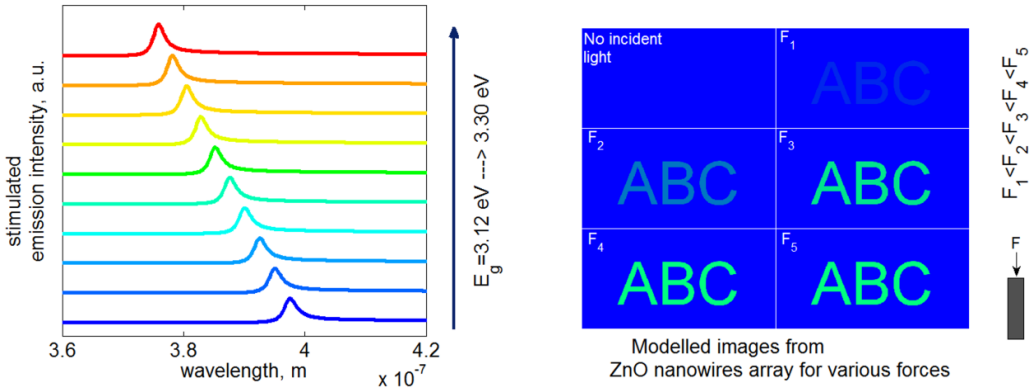
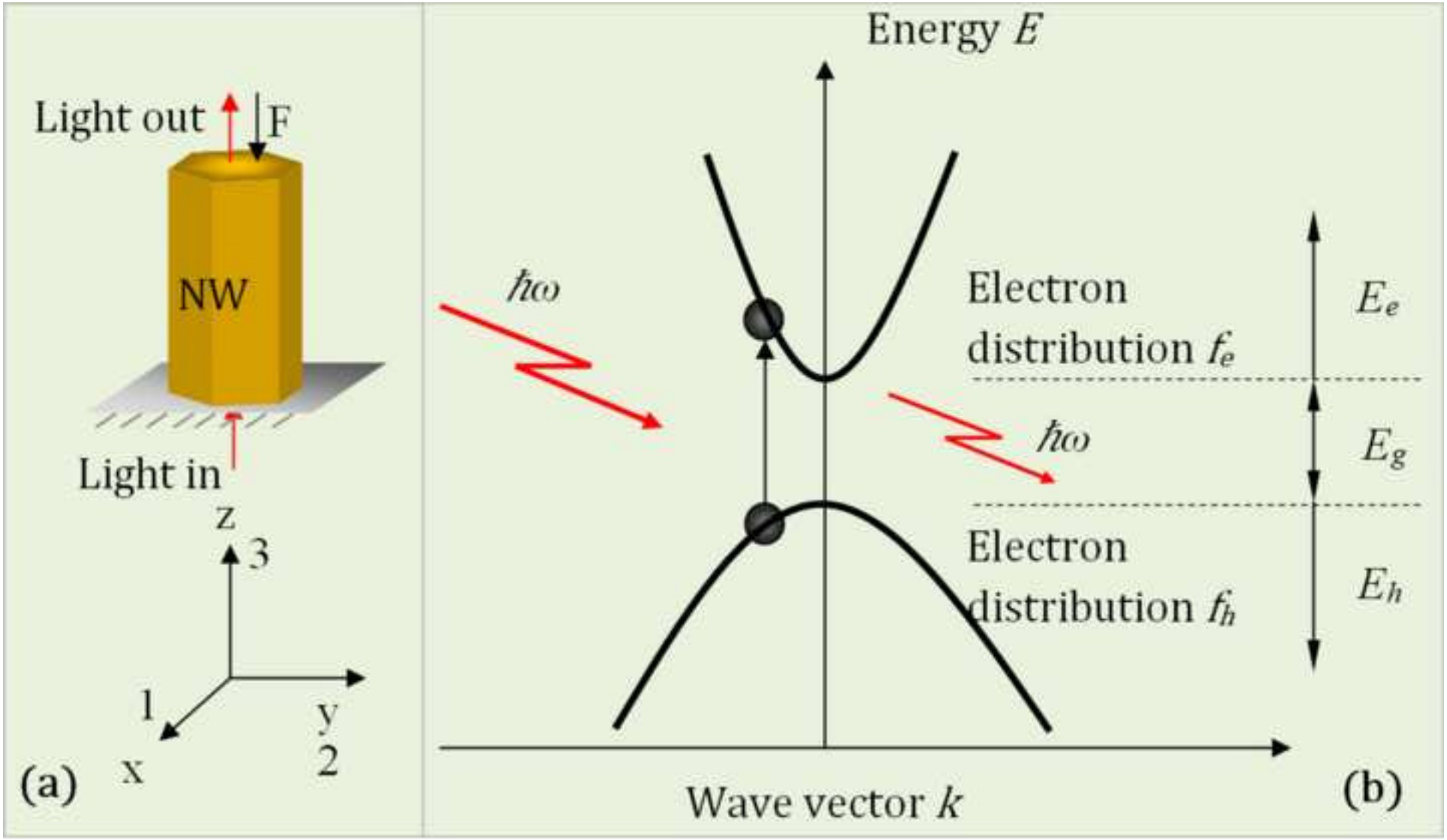


Figure_1



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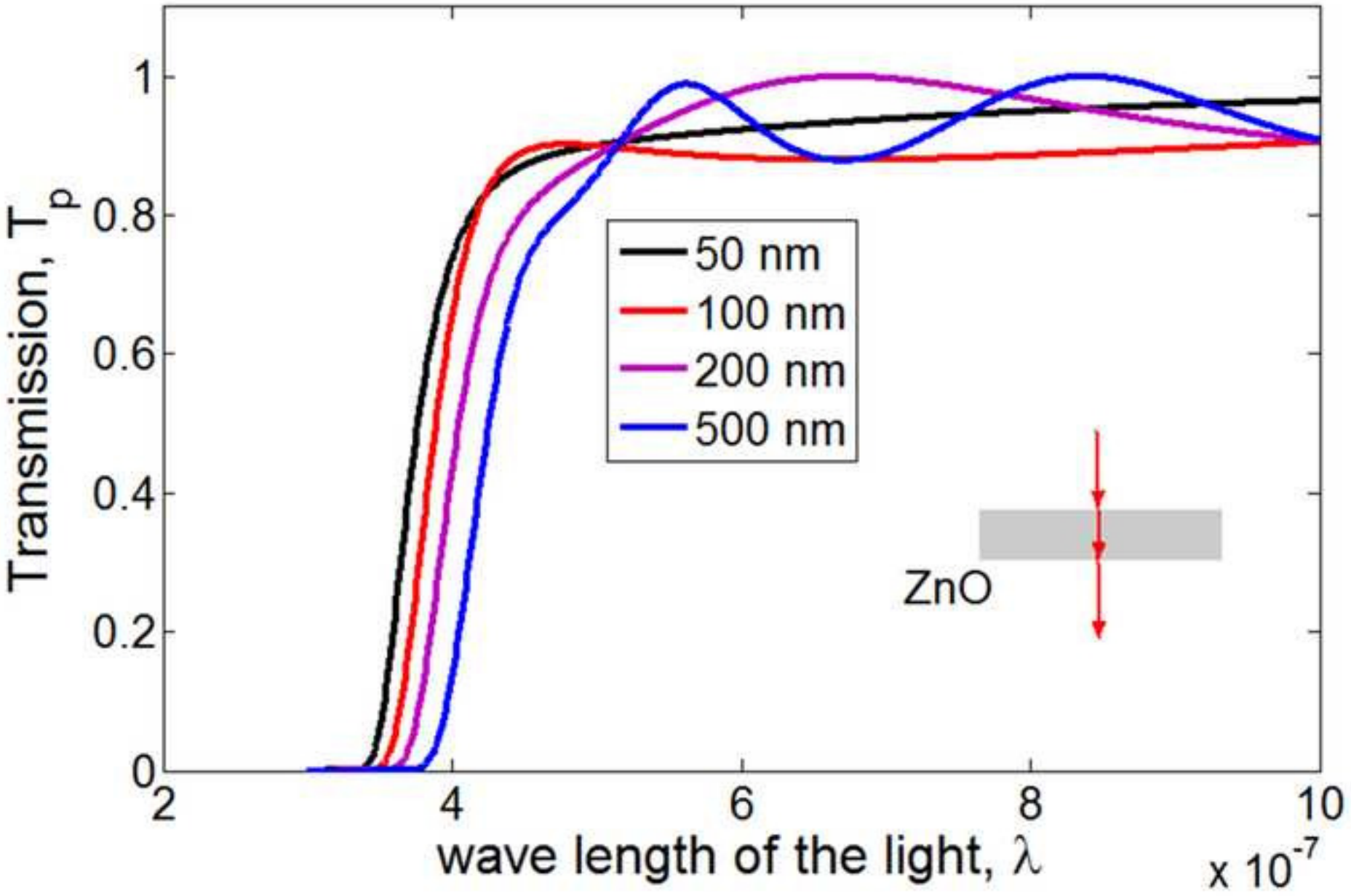


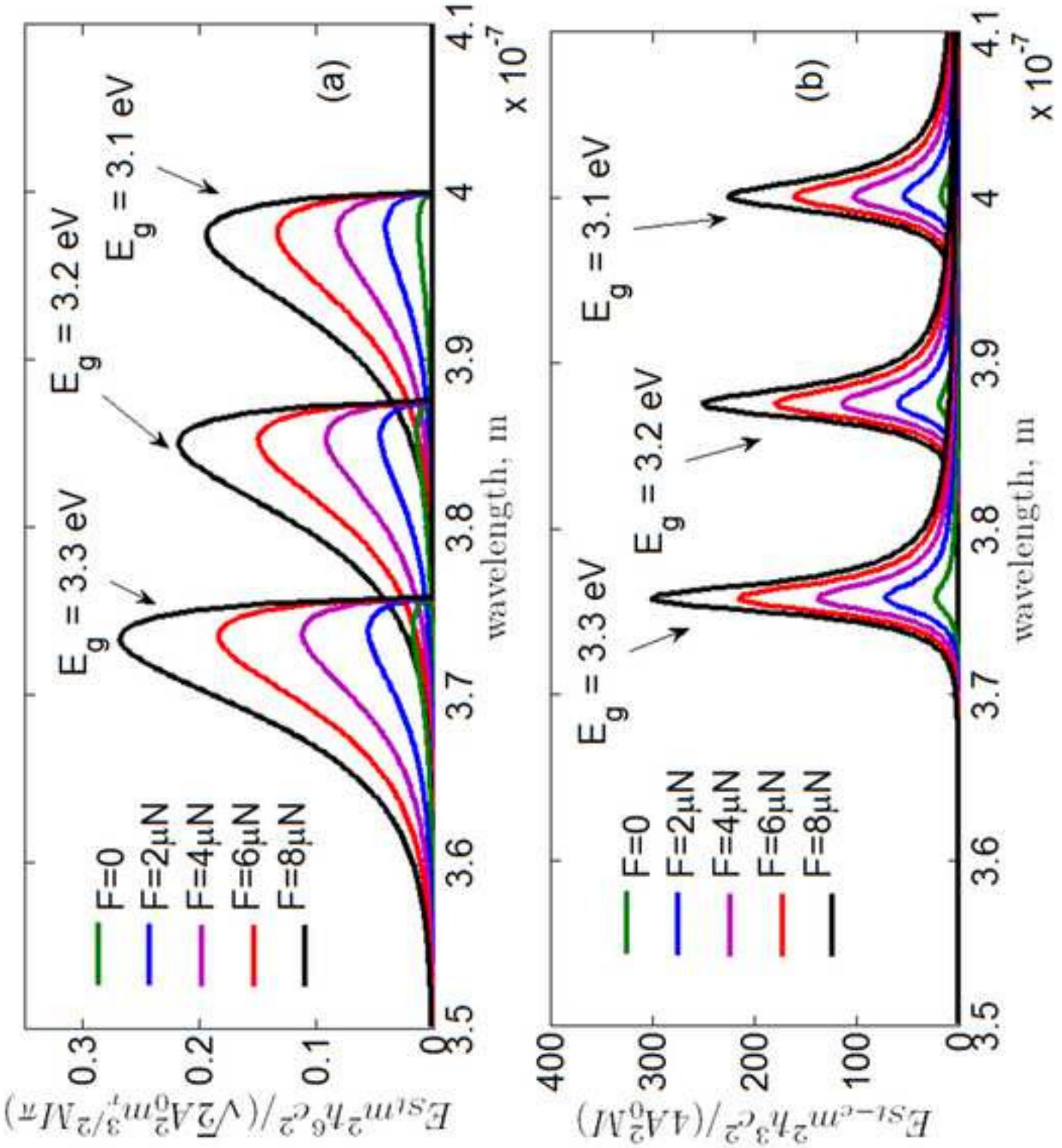


Figure_3

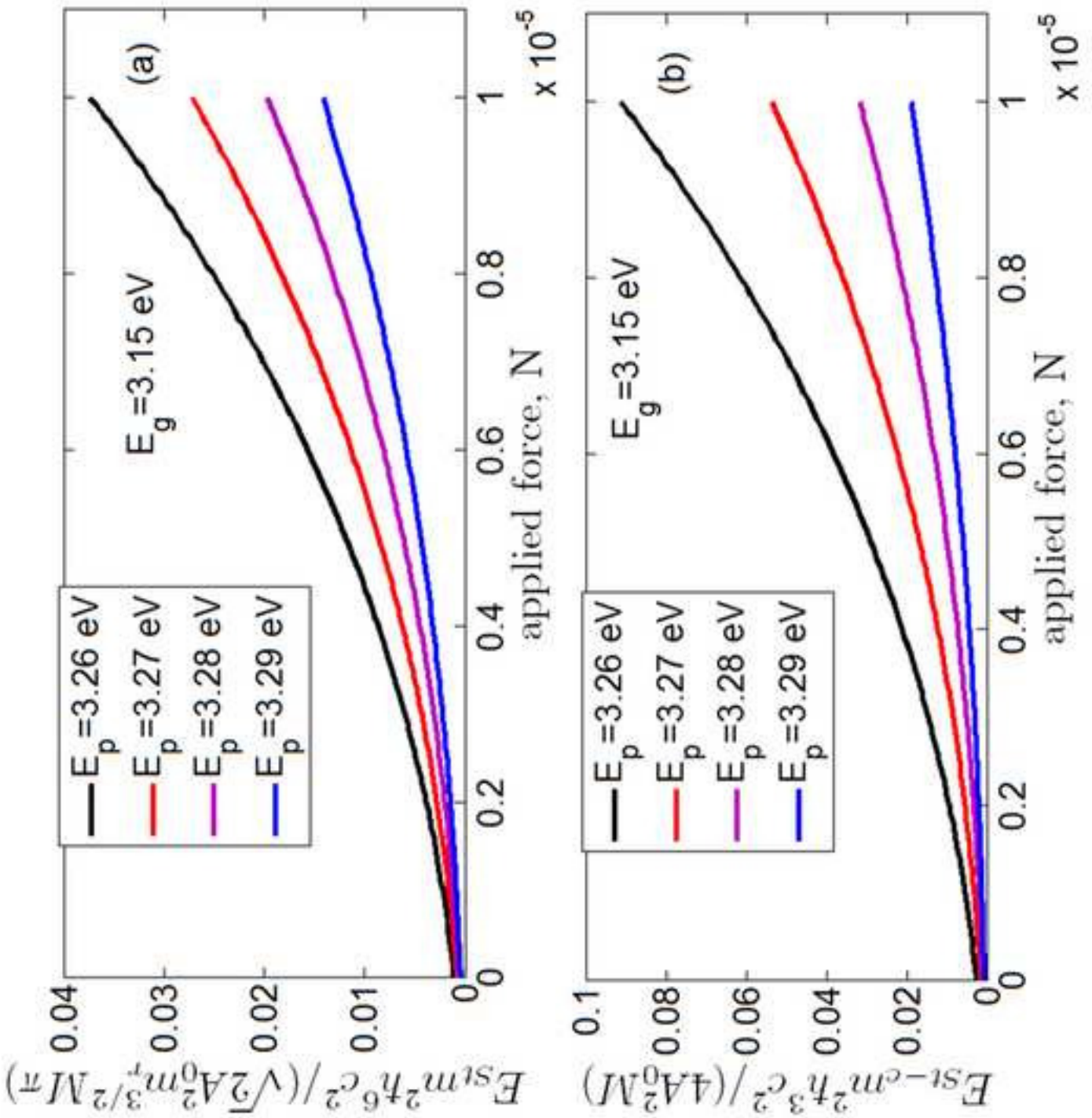


Figure_4

Figure_5

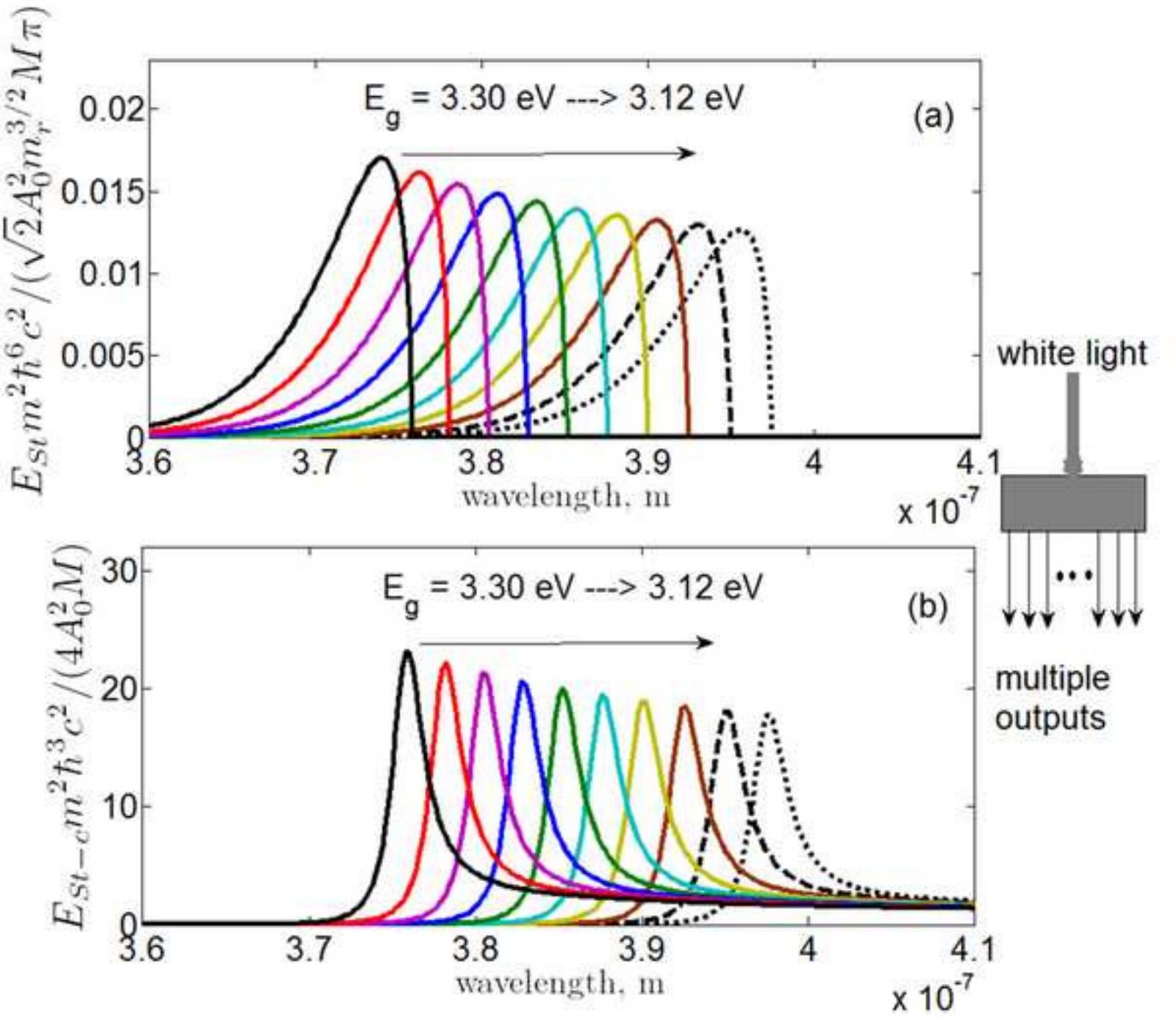
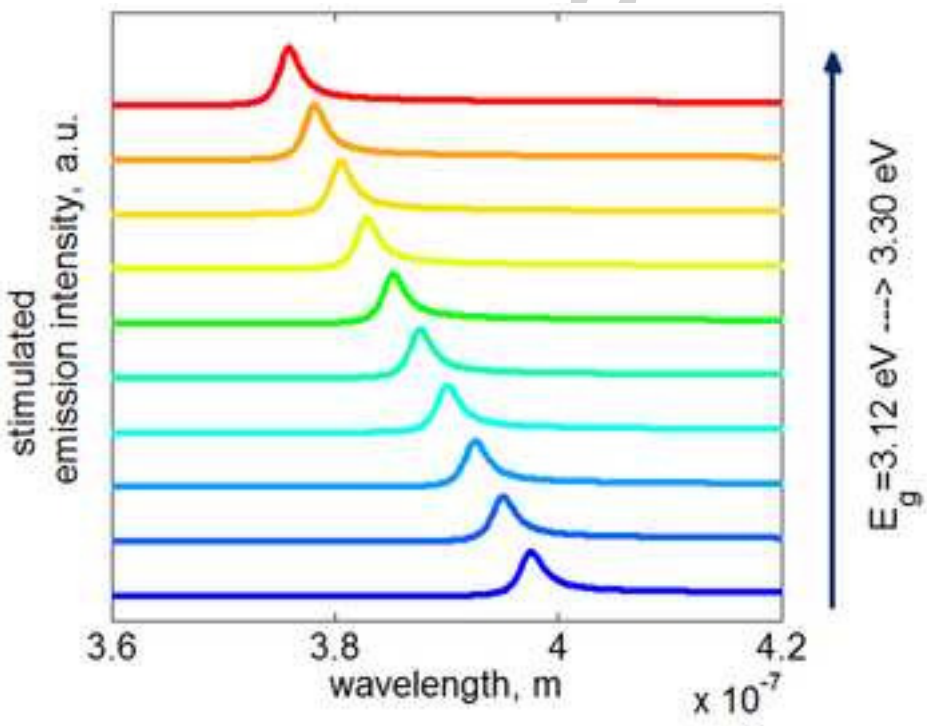
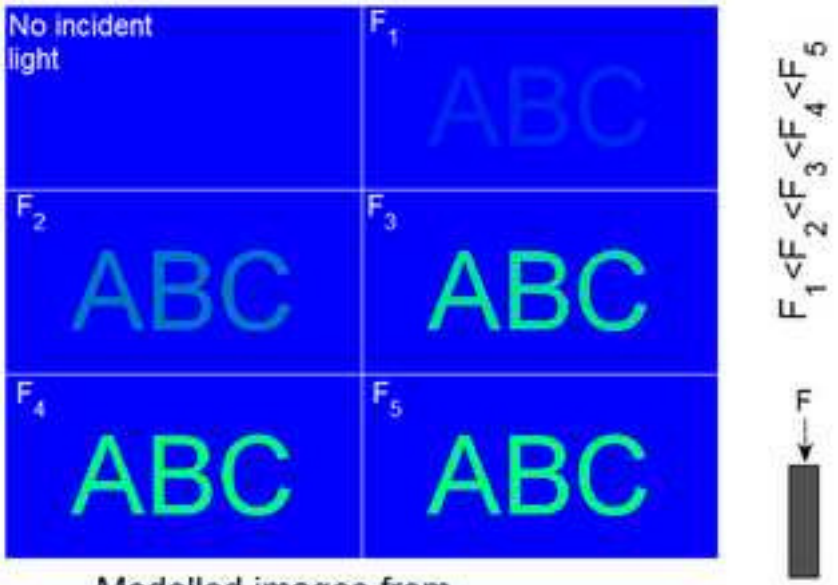


Figure_6





Modelled images from
ZnO nanowires array for various forces