Electric potential and energy band in ZnO nanofiber tuned by local mechanical loading*

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Abstract Recent success in strain engineering has triggered tremendous interest in its study and potential applications in nanodevice design. In this paper, we establish a coupled piezoelectric/semiconducting model for a wurtzite structure ZnO nanofiber under the local mechanical loading. The energy band structure tuned by the local mechanical loading and local length is calculated via an eight-band $\mathbf{k} \cdot \mathbf{p}$ method, which includes the coupling of valance and conduction bands. Poisson's effect on the distribution of electric potential inversely depends on the local mechanical loading. Numerical results reveal that both the applied local mechanical loading and the local length exhibit obvious tuning effects on the electric potential and energy band. The band gap at band edges varies linearly with the applied loading. Changing the local length shifts the energy band which is far away from the band edges. This study will be useful in the electronic and optical enhancement of semiconductor devices.

Key words piezoelectric semiconductor (PS), local mechanical loading, strain engineering, energy band

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1 Introduction

Strain is a universal phenomenon and almost inevitable in the synthesis, fabrication, and applications of all types of materials^[1]. By changing the volume of crystal and lowering the crystal-symmetry, strain shifts the position of energy band and splits the degeneracies in energy band^[2], and thus enhances the performance of such materials. Since the electronic properties of semiconductor devices, such as energy band, can be modified by strain^[3–4], a useful mechanical

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technique known as strain engineering was put forward, which involves the deliberate application of controlled strain into the nanostructure devices to tailor their electronic properties^[5–6]. As nanostructures remain integrity when subject to a larger strain than their bulk counterparts, the strain engineering was treated as an effective way to improve the performance of nanostructure devices^[7]. Normally, strain is introduced by lattice mismatch^[8], impurity doping^[9], functional wrapping^[10] as well as direct mechanical applications^[5,11] in strain engineering. Thanks to strain engineering, tremendous achievements have been made, such as the turn of indirect band gap to direct band gap^[12], band gap opening^[13], enhancement of charge carrier mobility^[14], tune of the effective mass of carriers^[15], and transition of semiconductors to conductors^[16]. To our knowledge, among the vast research about tuning the energy band structure via strain, the tune mechanism of the wurtzite structure ZnO, which combines the semiconducting and piezoelectric properties, still remains unclear. To calculate the band structure of semiconductors, several methods have been proposed, such as the tight binding method^[17], the empirical pseudopotential method^[18], and the $\mathbf{k} \cdot \mathbf{p}$ method^[19–20], among which the $\mathbf{k} \cdot \mathbf{p}$ method is recognized as a useful method for calculating the energy band due to its cheap computational cost compared with other methods^[21]. The $\mathbf{k} \cdot \mathbf{p}$ method was initially put forward by Kane^[22] and Luttinger and Kohn^[23], and then it was utilized to calculate the band structure of bulk materials with strain effects by Bir and Pikus^[24], and subsequently it was successfully applied to solve the band structure of low-dimensional heterostructures^[25]. Since the fundamental electric and optical properties are mainly determined by the band structure near the direct band edges, the Hamiltonian near the band edges in the $\mathbf{k} \cdot \mathbf{p}$ method is important for the comprehensive understanding of the semiconductor properties^[26]. As for the above-mentioned wurtzite structure ZnO, the coupling of piezoelectric and semiconducting properties and their effects on the band structure in the theoretical model and analysis have not been taken into consideration thoughtfully in the previous studies. Thus, there is a great need to establish such a theoretical model considering the coupling of the piezoelectric and semiconducting properties to better understand the effect of strain on the band structure in the wurtzite structure ZnO.

In this paper, we study the tuning effects of the local mechanical loading and the local length on the electric potential and energy band structure in a wurtzite structure ZnO nanofiber with coupled piezoelectric/semiconducting properties. The article is organized as follows. In Section 2, we introduce a theoretical model for the piezoelectric semiconductor (PS) ZnO nanofiber under local mechanical loading. An eight-band $\mathbf{k} \cdot \mathbf{p}$ method is adopted for calculating the energy band. In Section 3, we compare the numerical results of electric potentials with those from the literature to verify the model. In Section 4, the effects of the local mechanical loading and local length on the energy band structures that approach or move away from band edges are studied in detail.

2 Electro-mechanical field and energy band in a PS nanofiber under local loading

2.1 Governing equation on electric potential

In this section, a theoretical model is established. As shown in Fig. 1(a), a ZnO nanofiber is placed on a polystyrene substrate and fixed to the substrate with silver paste at two positions on the nanofiber^[27]. When the substrate deforms, the nanofiber fixed on it will be mechanically loaded and driven to deform. As shown in Fig. 1(b), the local mechanical loading is located at the reference B - B and C - C (denoted as the plane B and the plane C). To simplify the problem, we put the silver paste on two symmetrical positions; that is to say, $L_2 = L_3$. The ZnO nanofiber utilized here is combined with both piezoelectric and semiconducting properties, and the c -axis of the nanofiber is as the same direction along x_3 .

Fig. 1 PS ZnO nanofiber under local mechanical loading $F^{[27]}$ (color online)

By considering the piezoelectric property of the ZnO nanofiber, the piezoelectric equations can be written as^[28]

$$\begin{cases} T_j = c_{ji}S_i - e_{nj}E_n, \\ D_m = e_{mi}S_i + \varepsilon_{mn}E_n, \end{cases} \quad (1)$$

where T_j , S_i , E_n , and D_m are the stress, the strain, the electric field, and the electric displacement, respectively; c_{ij} , e_{nj} , and ε_{mn} are the elastic, piezoelectric, and dielectric constants, respectively. Subscripts $i, j = 1, 2, \dots, 6$; $m, n = 1, 2, 3$. The strain and electric field under the applied local mechanical loading can be expressed as

$$S_{ij} = (u_{i,j} + u_{j,i})/2, \quad E_n = -\phi_{,n}, \quad (2)$$

where u and ϕ are the elastic displacement and the electric potential in the nanofiber, respectively.

For the local axial loading in the x_3 -direction, only the stress T_3 remains nonzero, and when Poisson's effect is considered by including the strains S_1 and S_2 , the piezoelectric equations possess the form as^[28]

$$\begin{cases} T_3 = \bar{c}_{33}S_3 - \bar{e}_{33}E_3, \\ D_3 = \bar{e}_{33}S_3 + \bar{\varepsilon}_{33}E_3, \end{cases} \quad (3)$$

where the coefficients containing the effect of strain in three directions are denoted as

$$\bar{c}_{33} = c_{33} - \frac{2c_{13}^2}{c_{11} + c_{12}}, \quad \bar{e}_{33} = e_{33} - \frac{2c_{13}e_{31}}{c_{11} + c_{12}}, \quad \bar{\varepsilon}_{33} = \varepsilon_{33} + \frac{2e_{31}^2}{c_{11} + c_{12}}. \quad (4)$$

For simplicity, the problem about the local axial loading can also be treated as a one-dimensional problem by ignoring Poisson's effect, namely, omitting the strains S_1 and S_2 . Thus, the coefficients in Eq. (4) reduce to

$$\bar{c}_{33} = c_{33}, \quad \bar{e}_{33} = e_{33}, \quad \bar{\varepsilon}_{33} = \varepsilon_{33}.$$

Poisson's effect on the distribution of electric potential in the ZnO nanofiber under the local mechanical loading will be discussed in Subsection 4.1.

The applied local loading generates a polarized electric field in the nanofiber due to its piezoelectric effect, and further the carriers including electrons and holes in the semiconducting nanofiber are redistributed by the polarized electric field. The drift current induced by the redistribution of carriers and the diffusion current caused by the concentration gradient in

x_3 -direction can be described by the electric current equations in physics of semiconductors as^[29]

$$J^p = qp\mu_p E - qD_p p_3, \quad J^n = qn\mu_n E + qD_n n_3, \quad (5)$$

where J^p and J^n are currents of holes and electrons, respectively; q is the elementary charge; μ_p and μ_n are the mobilities of holes and electrons, respectively; D_p and D_n are the diffusion coefficients of holes and electrons, respectively; p and n are the concentrations of holes and electrons, respectively. For a static problem, the electric currents are zero, namely, $J^p = 0$ and $J^n = 0$. The relationship between carrier concentration p or n and the electric potential ϕ is established by integrating Eq. (5), and with the condition that

$$p|_{x=0} = p_0, \quad n|_{x=0} = n_0, \quad \phi|_{x=0} = 0,$$

we get

$$p(x) = p_0 e^{-\frac{q}{\kappa_0 T} \phi(x)}, \quad n(x) = n_0 e^{\frac{q}{\kappa_0 T} \phi(x)}. \quad (6)$$

Finally, the electrostatic equation which describes the relationship between charges and electric displacements can be written as^[29]

$$D_3 = q(p - n + N_D^+ - N_A^-), \quad (7)$$

where N_A^- and N_D^+ are the acceptor and donor doping concentrations, respectively, and their relationship with the initial hole and electron concentration is written as $N_D^+ = n_0$ and $N_A^- = p_0$. Based on Eqs. (3), (6), and (7), the governing equation about the electric potential ϕ in the ZnO nanofiber under the local loading can be derived as

$$\hat{\varepsilon} \phi_{,33} + q(p_0 \exp(-q\phi/(k_0 T)) - n_0 \exp(q\phi/(k_0 T)) + n_0 - p_0) = 0, \quad (8)$$

where (p_0, n_0) are initial carrier concentrations without any mechanical loading; k_0 is the Boltzmann constant; T is the Kelvin temperature set as $T = 300$ K; $\hat{\varepsilon} = e_{33}^2/c_{33} + \varepsilon_{33}$.

Along with the governing equation (8), the boundary conditions are set as zero electric displacements at the two end points where $x_3 = -(L_1/2 + L_2)$ and $x_3 = L_1/2 + L_2$. And the continuity conditions about electric potential and electric displacement are satisfied at both reference planes B and C . The governing equation (8), boundary conditions, and continuity conditions are numerically solved via the finite element method, and then the distribution of electric potential along the nanofiber is obtained.

2.2 Eight-band $\mathbf{k} \cdot \mathbf{p}$ method for energy band

To study the effect of the local loading on the energy band, an eight-band $\mathbf{k} \cdot \mathbf{p}$ method is used^[20]. The basis that constitutes the 8×8 Hamiltonian matrix can be written as^[20]

$$(|S \uparrow\rangle, |X \uparrow\rangle, |Y \uparrow\rangle, |Z \uparrow\rangle, |S \downarrow\rangle, |X \downarrow\rangle, |Y \downarrow\rangle, |Z \downarrow\rangle)^T. \quad (9)$$

The 8×8 Hamiltonian matrix $\mathbf{H}$ in block matrix form owns the expression as

$$\mathbf{H} = \begin{pmatrix} \mathbf{G}(\mathbf{k}) & \mathbf{\Gamma} \\ -\mathbf{\Gamma}^* & \mathbf{G}^*(\mathbf{k}) \end{pmatrix}, \quad (10)$$

where both $\mathbf{G}(\mathbf{k})$ and $\mathbf{\Gamma}$ are 4×4 square matrices, and the superscript asterisk means the complex conjugate. The matrix $\mathbf{G}$ consisting of a series of 4×4 square matrices can be written as^[20]

$$\mathbf{G} = \mathbf{G}_1 + \mathbf{G}_2 + \mathbf{G}_{\text{SO}} + \mathbf{G}_{\text{CR}} + \mathbf{G}_{\text{ST}}. \quad (11)$$

Among these 4×4 matrices, $\mathbf{G}_1$ can be denoted as^[20]

$$\mathbf{G}_1 = \begin{pmatrix} E'_c & iP_2k_1 & iP_2k_2 & iP_1k_3 \\ -iP_2k_1 & E'_v & 0 & 0 \\ -iP_2k_2 & 0 & E'_v & 0 \\ -iP_1k_3 & 0 & 0 & E'_v \end{pmatrix}, \quad (12)$$

where E'_c and E'_v are the conduction band (CB) edges and valence band (VB) edges, respectively, when the local loading is applied on the nanofiber; P_1 and P_2 are defined as the Kane parameters^[20]. The CB edges and the VB edges can be written as^[20]

$$\begin{cases} E'_c = E_v + E_g + \Delta_{CR} + \Delta_{SO}/3 + V_{\text{ext}}, \\ E'_v = E_v + V_{\text{ext}}, \end{cases} \quad (13)$$

where E_v is treated as the average VB edge on the Kelvin temperature; E_g is the band gap energy without strain; Δ_{CR} and Δ_{SO} are the crystal-field split energy and the spin-orbit split-off energy, respectively. V_{ext} is treated as any additional scalar potential energy. We know that when the nanofiber is applied with the external local loading, the electric potential energy, written as $-q\phi$, will be introduced in the whole nanofiber. Obviously, the electric potential energy can be treated as an additional potential energy, and thus the CB edges and VB edges can be written as

$$\begin{cases} E'_c = E_v + E_g + \Delta_{CR} + \Delta_{SO}/3 - q\phi, \\ E'_v = E_v - q\phi. \end{cases} \quad (14)$$

Another matrix $\mathbf{G}_{ST}$ which reveals the dependence of the Hamiltonian matrix $\mathbf{H}$ on strains is written as^[20]

$$\mathbf{G}_{ST} = \begin{pmatrix} a_2(S_1+S_2)+a_1S_3 & 0 & 0 & 0 \\ 0 & l_1S_3+m_1S_2+m_2S_3 & n_1S_6 & n_2S_5 \\ 0 & n_1S_6 & m_1S_1+l_1S_2+m_2S_3 & n_2S_4 \\ 0 & n_2S_5 & n_2S_4 & m_3(S_1+S_2)+l_2S_3 \end{pmatrix}, \quad (15)$$

where the parameters l_i, m_i , and n_i ($i = 1, 2, 3$) in Eq. (15) can be found in Ref. [20]. Other matrices without considering strain can also be found in Ref. [20].

The parameters about the wurtzite ZnO nanofiber mentioned above are listed in Table 1.

Table 1 Material parameters for wurtzite ZnO nanofiber

Parameter	c_{11} /GPa	c_{12} /GPa	c_{13} /GPa	c_{33} /GPa	e_{31} /(C·m ⁻²)	e_{33} /(C·m ⁻²)	ϵ_{33}
Value	209.7 ^[30]	121.1 ^[30]	105.1 ^[30]	210.9 ^[30]	-0.537 ^[30]	1.32 ^[30]	9.16 ^[30]
Parameter	E_{g0} /eV	Δ_{CR} /eV	Δ_{SO} /eV	E_v /eV	a_1 /eV	a_2 /eV	
Value	3.34 ^[31]	0.043 ^[32]	0.016 ^[32]	0	-3.9 ^[33]	-4.13 ^[33]	

3 Verification of numerical results

In this study, the nonlinear property in the electric current of Eq. (5), shown as the product of carrier concentration and electric field, is considered and numerically solved via the finite element method. If we replace the first carrier concentration p or n in Eq. (5) with the initial carrier concentrations p_0 and n_0 , the electric current equations can be linearized, and the electric

potential can be obtained with the analytical solution for a small axial force^[34]. To verify the nonlinear model in this paper, we first set the length $L_1 = L_2 = L_3 = 1\,200\text{ nm}$, and the axial local force $F = 4.25\text{ nN}$ (the axial stress T_3 can be calculated as $T_3 = F/A_1$, where A_1 is the cross section of the ZnO nanofiber^[34]), $n_0 = 1 \times 10^{21}\text{ m}^{-3}$, and $p_0 = 1 \times 10^{11}\text{ m}^{-3}$. The material parameters can be found in Table 1. It can be seen from Fig. 2(a) that the numerical results about the electric potential along the x_3 -direction are almost the same as the analytical linear results in Ref. [34] when the local force is relatively small.

Note that when the lengths L_2 and L_3 gradually reduce to zero, the local loading will degenerate into an end loading. We set $L_1 = 1\,200\text{ nm}$ unchanged, and make $L_2 = L_3 = 1\text{ nm}$ to approximate the end loading case studied in Ref. [35], which can be treated as $L_2 = L_3 = 0$. The comparison between the result with that from Ref. [35] for $T_3/c = 5 \times 10^{-5}$ ($c = \bar{c}_{33}$ and $T_3 = 5 \times 10^{-5}\bar{c}_{33}$) is shown in Fig. 2(b). It is indicated that when the length $L_2 = L_3$ approaches zero, the distribution of the electric potential between the plane B and the plane C converges to that with the end loading in Ref. [35] (the external force is applied on the two ends of the fiber). In conclusion, the numerical results in this paper are reliable since they are in accordance with the analytical linear results and can degenerate to the results of the case with the end loading.

Figures 2(c) and 2(d) further study the applicability of the analytical linear theory^[34] and the nonlinear theory. First, Fig. 2(c) intuitively shows that, for a large axial force $F = 500\text{ nN}$, there is an obvious difference between linear and nonlinear numerical results since the electric potential field in the nonlinear theory loses its antisymmetry, while in the linear result it still remains its antisymmetry. Figure 2(d) exhibits the minimum electric potential $\phi_{\min}$ at $x_3 = -600\text{ nm}$ and the maximum electric potential $\phi_{\max}$ at $x_3 = 600\text{ nm}$ for both linear and nonlinear numerical results. Clearly, the maximum and minimum electric potentials remain the same for both linear and nonlinear numerical results when the axial force is less than 10 nN . This indicates that the linear theory with analytical solutions^[34] can be used with the axial force less than 10 nN , while the nonlinear theory can be adopted for any force.

4 Electric potential and energy band under local loading

We have studied that the local loading can make a difference to both the mechanical and electric parameters of the nanofiber^[34]. Moreover, the local lengths L_1 and $L_2 = L_3$ may also affect such parameters since the length of the interaction zone between the carrier and the polarized electric field can affect the electric potential in the nanofiber. Thus, in this section, we study the distribution of electric potential with different local lengths under the local loading. Considering that the energy band of VB and CB can be influenced by electric potential, we show how the local loading and local length tune the energy band.

4.1 Effect of local loading on distribution of electric potential

Figure 3 shows the effect of local length $L_2 = L_3$ on the distribution of the electric potential between the plane B and the plane C under different values of local tensile/compressive loadings. Here, we set $L_1 = 1\,200\text{ nm}$. It is indicated that for a smaller local loading such as $T_3/c = \pm 1 \times 10^{-4}$, the distribution of electric potential gradually converges to the result when length $L_2 = 1\text{ nm}$ as L_2 reduces from 600 nm to 1 nm . At the same time, for a larger local loading such as $T_3/c = \pm 5 \times 10^{-4}$, various lengths L_2 make little difference in the distribution of electric potential. From Fig. 2(b), it can be concluded that an extreme small end length $L_2 = 1\text{ nm}$ can be treated as the limitation of the local loading, namely, the end loading, where external loadings are applied on the two ends of the nanofiber. We can conclude in Figs. 3(a) and 3(c) that for a smaller local loading, the value of electric potential for length L_2 larger than 1 nm is smaller than that with $L_2 = 1\text{ nm}$. That is to say, for a smaller local loading, the distribution of electric potential with a longer length L_2 does not reach the limitation of local loading. At the

Fig. 2 (a) Numerical result versus analytical linear result in Ref. [34] with $F = 4.25$ nN; (b) local loading result degenerating to end loading result in Ref. [35]; (c) numerical versus linear calculation results with $F = 500$ nN; (d) linear and numerical electric potential $\phi_{\min}$ at $x_3 = -600$ nm and $\phi_{\max}$ at $x_3 = 600$ nm (color online)

same time, a larger external local loading makes the carrier redistribute much more dramatical, and thus even a longer L_2 can make the distribution of electric potential reach the limitation of local loading and makes L_2 cause little difference in the electric potential. It also demonstrates that the end loading, which is the limitation of local loading, can reach the largest electric potential distribution in the nanofiber under the same loading.

Figure 4 shows Poisson's effect on the distribution of electric potential for different local loadings and local lengths. It is shown clearly in Fig. 4(a) that, with the same length L_2 , when Poisson's effect is considered or the three normal strains are included other than only considering the strain S_3 , the electric potential changes more rapidly, so does it in Fig. 4(b). From Eq. (3), we obtain the expressions with and without considering Poisson's effect as

$$\phi_{,3} = \begin{cases} (T_3 - c_{33}S_3)/e_{33} & \text{without Poisson's effect,} \\ (T_3 - \bar{c}_{33}S_3)/\bar{e}_{33} & \text{with Poisson's effect.} \end{cases} \quad (16)$$

Since it has been known that both $\bar{c}_{33}$ and $\bar{e}_{33}$ are smaller than c_{33} and e_{33} , respectively, it is no wonder that the gradient of electric potential with Poisson's effect is greater than that without Poisson's effect. Therefore, the electric potential changes more rapidly when considering Poisson's effect. It also reveals that for a larger local loading, there is little difference whether Poisson's effect is considered or not, as shown in Fig. 4(b). Thus, we conclude that Poisson's effect should be considered for a small local loading and can be ignored for a large local loading.

Fig. 3 Effects of local length $L_2 = L_3$ on distribution of electric potential between planes B and C under local loading: (a) $T_3/c = 1 \times 10^{-4}$; (b) $T_3/c = 5 \times 10^{-4}$; (c) $T_3/c = -1 \times 10^{-4}$; (d) $T_3/c = -5 \times 10^{-4}$ (color online)

Fig. 4 Poisson's effect on distribution of electric potential for (a) $T_3/c = 1 \times 10^{-4}$ and (b) $T_3/c = 5 \times 10^{-4}$ (color online)

In order to unify the narrative within the full-text, Poisson's effect is considered in the following calculation.

4.2 Effect of local loading and local length L_2 on energy band

In this subsection, we analyze how the local length L_2 affects the VB edges and CB edges under different local loadings. The middle length L_1 is set as $L_1 = 1200$ nm, and the doping

concentrations are $N_D^+ = 1 \times 10^{21} \text{ m}^{-3}$ and $N_A^- = 1 \times 10^{11} \text{ m}^{-3}$. At band edges, wave vector $k_j = 0$ ($j = 1, 2, 3$).

Figures 5 and 6 show the effect of local length L_2 on the VB edges and CB edges under different local tensile/compressive loadings, in which the VB includes heavy hole (HH), light hole (LH), and spin-orbit split-off (SO) band. The variety tendency of VB and CB edges is in accordance with the observation in Ref. [19]. Results show that with the reduction of L_2 , VB edges and CB edges gradually converge to the situation where $L_2 = 1 \text{ nm}$, namely, the end loading, which is treated as the limitation of the local loading. Yet unlike the smaller local loading $T_3/c = \pm 1 \times 10^{-4}$, for a larger local loading $T_3/c = \pm 5 \times 10^{-4}$, the VB and CB band edges' convergence is not that obvious since the VB edge lines almost superpose together for $L_2 = 300 \text{ nm}$ and $L_2 = 600 \text{ nm}$. This is because the larger local tensile/compressive loading makes electric potential distribution easy to reach the limitation of local loading while the smaller local tensile/compressive loading is difficult to reach the limitation. It also shows that to increase the band energy, we can also change the local loading to end loading besides increasing the value of mechanical loading.

Fig. 5 Effects of local length L_2 on VB and CB edges under different local tensile loadings (color online)

Figure 7 shows the effect of local loading on the VB edges and CB edges at the reference planes B and C , where the local loading T_3/c ranges from -5×10^{-4} to 5×10^{-4} . The length L_1 is set as 1200 nm . It can be seen clearly that the VB and CB edges at the reference planes B and C change rapidly around $T_3/c = 0$ while changing slowly away from $T_3/c = 0$. This is in accordance with the analysis in Figs. 5 and 6 that the smaller local loading makes the

Fig. 6 Effects of local length L_2 on VB and CB edges under different local compressive loadings (color online)

energy band change more obviously while the larger local loading makes it change more slowly. Besides, results also show that the interval, where energy band changes more rapidly with the local loading, becomes narrower and narrower when reducing the length L_2 , that is to say, compared with the end loading, the local loading can expand the interval where energy band is sensitive to the applied loading.

Figure 8 shows the band gap under various local loadings at the reference plane B . The band gap is calculated by subtracting the valance band value HH from conduction band value E_c . It is indicated that the band gap of wurtzite structure ZnO varies linearly with the applied compressive or tensile local loading under different local lengths L_2 , which is in accordance with the observation in Ref. [19]. Besides, by comparing with the end loading, the local loading tunes the band gap in a wider scale which can be utilized in the case where the larger band gap is required.

Figure 9 shows the effect of local length L_2 on energy band that deviates from band edges with different k_3 at the reference plane B . The variety of VB with different k_3 is also in accordance with the observation in Ref. [19]. It is seen clearly from Fig. 9 that reducing length L_2 shifts VB and CB along the positive direction of vertical axis for the local tensile loading, or along the negative direction of vertical axis for the local compressive loading. When moving the loading from the ends inside, the reduction of the energy band due to a tensile loading enhances, or the increase in the energy band due to a compressive loading enhances. It is also indicated that both the maximum VB and minimum CB are located at the band edges where $k_j = 0$ ($j = 1, 2, 3$).

Fig. 7 Effects of local loading on the VB and CB edges at reference planes *B* and *C* under various L_2 (color online)

4.3 Effect of local length L_1 and local loading on electric potential and energy band

In this subsection, we analyze the effect of local length L_1 and local tensile/compressive loading on the electric potential and energy band. Here, we set $L_2 = L_3$ remaining unchanged as $L_2 = L_3 = 600$ nm, and let L_1 vary from 600 nm to the very limitation $L_1 = 1$ nm. It is easy to find that as L_1 gradually reduces to zero, the distribution of electric potential in the nanofiber will be infinitely close to the situation where the nanofiber is free of local loading.

Figure 10 shows the effect of local length L_1 on electric potential distribution under the local tensile/compressive loading $T_3/c = \pm 1 \times 10^{-4}$, among which Figs. 10(a) and 10(c) represent the electric potential distribution between the reference planes *A* and *B*, Figs. 10(b) and 10(d)

Fig. 8 Band gap under various local loadings at reference plane *B* (color online)

Fig. 9 Effects of local length L_2 on energy band that deviates from band edges with different k_3 at reference plane *B* (color online)

represent the electric potential distribution between the reference planes *C* and *D*, noted as electric potential on the left/right, respectively. To show the distribution of electric potential more obviously and conveniently, we move the electric potential on the left/right to the interval of $[-600 \text{ nm}, 0 \text{ nm}]$ and $[0 \text{ nm}, 600 \text{ nm}]$ from their different original intervals due to the variety of L_1 . Obviously, both electric potential distributions on the left and right tend to zero everywhere with the reduction of L_1 , namely to the situation where the nanofiber is free of the external loading, and this is in accordance with the physical mechanism that it obeys. Also, it indicates that the local tensile loading makes the electric potential change more dramatically on the left

Fig. 10 Effects of local length L_1 on the electric potential distribution under different local loadings. Electric potential distribution under tensile loading: (a) between reference planes A and B ; (b) between reference planes C and D . Electric potential distribution under compressive loading: (c) between reference planes A and B ; (d) between reference planes C and D (color online)

and more slightly on the right while the local compressive loading does the opposite. Besides, since the larger local loading gives rise to stronger carrier redistribution, it is easy to predict that the larger local loading will bring stronger electric potential distribution while the smaller local loading will bring weaker effects, and no corresponding images will be given here in order to save pages of the article. That is to say, the local length L_1 can also tune the distribution of electric potential to a large extent under different local loadings.

Figure 11 shows the effect of local length L_1 on VB and CB edges under the local tensile/compressive loading, among which Figs. 11(a) and 11(b) represent VB edges on the left, Figs. 11(c) and 11(d) represent VB edges on the right, and Figs. 11(e) and 11(f) represent CB edges on the left/right. In the same way as mentioned above in Fig. 10, we replace the different original intervals with $[-600 \text{ nm}, 0 \text{ nm}]$ and $[0 \text{ nm}, 600 \text{ nm}]$. As the length L_1 reduces, the energy band pictures of HH, LH, SO, and E_c clearly indicate the convergence of energy band to the situation where $L_1 = 1 \text{ nm}$, shown by the almost horizontal lines in Fig. 11. Both VB and CB edges are away from the limitation $L_1 = 1 \text{ nm}$ for the larger local loading while VB and CB edges are close to the limitation for the smaller local loading for the same length L_1 , whether it is a local tensile or compressive loading. Similar to the variation tendency of electric potential, the local tensile loading makes both VB and CB edges change more dramatically on the left and more slightly on the right while the local compressive loading does the opposite.

Figure 12 shows the effect of local loading on the VB edges and CB edges at the plane $x_3 = 0$. Different from the foregoing analysis, here we choose the plane $x_3 = 0$ to study the energy band tuned by the local loading due to the variety of L_1 . Seen clearly, the almost horizontal lines in

Fig. 11 Effects of local length L_1 on VB and CB edges under different local tensile/compressive loadings (color online)

Fig. 12 represent the limitation of local loading, also noted as the situation free of loading. As the increasing of L_1 or as the deviation to the situation free of loading, the effect of both VB and CB tuned by the local loading becomes stronger. As mentioned above, this is due to the fact that the potential distribution induced by the larger length L_1 is far from the situation free of loading while smaller length L_1 is close to the situation free of loading.

Figure 13 shows the band gap under various local loadings at the plane $x_3 = 0$, where the band gap is calculated as shown in Fig. 8. Results show that the band gap varies linearly with the applied local loading under different local lengths L_1 . As studied in Subsection 4.2, the case here indicates that a longer local length L_1 corresponds to a wider tunable energy range by the applied loading, showing the tuning effect of band gap via the mechanical loading.

Figure 14 shows the effect of local length L_1 on energy band that deviates from band

Fig. 12 Effect of local loading on VB and CB edges at plane $x_3 = 0$ (color online)

Fig. 13 Band gap under various local loadings at plane $x_3 = 0$ (color online)

edges with different wave vector components k_3 at the reference planes B and C , among which Figs. 14(a) and 14(b) represent VB on the left, Figs. 14(c) and 14(d) represent VB on the right, and Figs. 14(e) and 14(f) represent CB on the left/right, respectively. The variety of both VB and CB with the increase of k_3 is in accordance with the observation in Ref. [19]. Under the local tensile loading, decreasing L_1 makes both VB and CB shift along the negative direction of vertical axis at the reference plane B , and makes VB and CB at the reference plane C shift along the positive direction of vertical axis. The local compressive loading does the opposite. Again, results show that both the maximum VB and minimum CB are located at the band edges where $k_j = 0$ ($j = 1, 2, 3$).

5 Conclusions

In this paper, we have established a theoretical model for investigating the electric potential and energy band in a wurtzite structure ZnO nanofiber under a local loading, considering the coupling of piezoelectric and semiconducting properties. We analyze the distribution of electric potential induced by the local loading and fiber lengths. The tuning effects of energy band structure by the local loading and local length are studied based on an eight-band $\mathbf{k} \cdot \mathbf{p}$ method, which includes the coupling of VB and CB. Numerical results show that Poisson's effect cannot be ignored for a smaller external loading while it makes no difference for a relatively large external loading. For VB and CB at band edges, calculation reveals that both the local loading

Fig. 14 Effects of length L_1 on energy band that deviates from band edges with different k_3 at reference planes B and C (color online)

and local length exhibit good tuning effect, and the energy band reaches its extreme value at the end loading compared with the local loading. And the band gap at band edges shows a linear change with the applied local loading. For VB and CB away from band edges, the local length shifts the energy band upward or downward along the vertical axis, and both the values of VB maximum and CB minimum are located at the band edges. We believe that this study can be utilized in the electronic and optical enhancement of semiconductor devices.

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