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Uniaxial Strain Effects on Optical Properties of c-plane Wurtzite GaN *

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We investigate the uniaxial strain effect in the c-plane on optical properties of wurtzite GaN based on $\boldsymbol{k}\cdot\boldsymbol{p}$ *theory, the spin-orbit interactions are also taken into account. The energy dispersions show that the uniaxial strain in the c-plane gives an anisotropic energy splitting in the* $k_x - k_y$ *plane, which can reduce the density of states. The uniaxial strain also results in giant in-plane optical polarization anisotropy, hence causes the threshold carrier density reduced. We clarify the relations between the uniaxial strain and the optical polarization properties. As a result, it is suggested that the compressive uniaxial strain perpendicular to the laser cavity direction in the c-plane is one of the preferable approaches for the efficient improvement of GaN-based laser performance.*

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In past decades, there has been considerable interest in applications of GaN and related ternary compounds for the optoelectronic devices in blue-green and near-ultraviolet emitters.[1−3] The high-brightness blue-green light-emitting diodes from the wurtzite (WZ) GaN semiconductor has been commercially applied,[4] laser diodes (LDs) were also reported.[5] Although these high-quality devices have been achieved, many basic aspects of material and device characteristics are still unknown.

It is well known that the strain is an effect way to alter the valence-band structures. From viewpoint of application, the strain effects have become an advantage for achieving lower threshold current density and higher differential quantum efficiency in zinc-blend GaAs-based lasers.[6] There are many experimental and theoretical studies on strain effect in the case of GaN-based layers.[7,8] According to their results, isotropic biaxial strains induced by the lattice mismatch in the c-plane (see Fig. 1(a)) neither effectively reduce the density of states (DOS)[9] nor the threshold current density.[10] This is because the biaxial strains in the c-plane preserve the original symmetry of the WZ GaN lattice so that no significant in-plane energy anisotropy occurs. However, an uniaxial strain in the c-plane can break the original C_{6v} symmetry of the WZ lattice into C_{2v} symmetry. Therefore, additional changes are expected, for example, in-plane polarization anisotropy can arise,[11−13] which has been confirmed experimentally.[14] Thus, it is important to achieve a further understanding to the properties of GaN under uniaxial strain.

In this Letter, using the 6×6 Hamiltonian on the basis of $\boldsymbol{k}\cdot\boldsymbol{p}$ theory,[15] we study the optical anisotropy in c-plane for GaN samples. The numerical calculations for the three valence-band dispersions are present. The relations between the uniaxial strain and the optical polarization are also clarified.

The Schrödinger equation for the periodic part $u_{v\boldsymbol{k}}(\boldsymbol{r})$ of the Bloch function and the energy $E_{v\boldsymbol{k}}(\boldsymbol{r})$ near the band edge can be written as[16]

$$H_{XYZ}u_{v\boldsymbol{k}}(\boldsymbol{r}) \cong \Big(H_0+\frac{\hbar^2k^2}{2m_0}+\frac{\hbar}{m_0}\boldsymbol{k}\cdot\boldsymbol{p}+H_{so}\Big)u_{v\boldsymbol{k}}(\boldsymbol{r}) = E_v(\boldsymbol{k})u_{v\boldsymbol{k}}(\boldsymbol{r}), \quad (1)$$

where

$$H_0 = \frac{P^2}{2m_0}+V(\boldsymbol{r}), \quad (2)$$

$$H_{so} = \frac{\hbar}{4m_0^2c^2}\nabla V\times\boldsymbol{P}\cdot\boldsymbol{\sigma}. \quad (3)$$

Here $V(\boldsymbol{r})$ is the periodic potential, H_{so} accounts for the spin-orbit interaction, and $\boldsymbol{\sigma}$ is the Pauli matrix. In the set of basis functions:

$$|Y_{11}\uparrow\rangle = \Big|-\frac{(X+iY)}{\sqrt{2}}\uparrow\Big\rangle,\ |Y_{1-1}\uparrow\rangle = \Big|\frac{(X-iY)}{\sqrt{2}}\uparrow\Big\rangle,$$

$$|Y_{10}\uparrow\rangle = |Z\uparrow\rangle,\quad |Y_{1-1}\downarrow\rangle = \Big|\frac{(X-iY)}{\sqrt{2}}\downarrow\Big\rangle,$$

$$|Y_{11}\downarrow\rangle = \Big|-\frac{(X+iY)}{\sqrt{2}}\downarrow\Big\rangle,\quad |Y_{10}\downarrow\rangle = |Z\downarrow\rangle.$$

The Hamiltonian can be written in the following form:[15]

$$H = \begin{vmatrix} F & -K^* & -H^* & 0 & 0 & 0 \\ -K & G & H & 0 & 0 & \Delta \\ -H & H^* & \lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F & -K & H \\ 0 & 0 & \Delta & -K^* & G & -H^* \\ 0 & \Delta & 0 & H^* & -H & \lambda \end{vmatrix}, \quad (4)$$

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where

$$
\begin{aligned}
&F = \Delta_1 + \Delta_2 + \lambda + \theta,\ G = \Delta_1 - \Delta_2 + \lambda + \theta,\\
&\lambda = \frac{\hbar^2}{2m_0}[A_1 k_z^2 + A_2(k_x^2 + k_y^2)] + D_1\epsilon_{zz}\\
&\quad + D_2(\epsilon_{xx} + \epsilon_{yy}),\\
&\theta = \frac{\hbar^2}{2m_0}[A_3 k_z^2 + A_4(k_x^2 + k_y^2)] + D_3\epsilon_{zz}\\
&\quad + D_4(\epsilon_{xx} + \epsilon_{yy}),\\
&K = \frac{\hbar^2}{2m_0}A_5(k_x + ik_y)^2 + D_5(\epsilon_{xx} - \epsilon_{yy} + 2i\epsilon_{xy}),\\
&H = \frac{\hbar^2}{2m_0}A_6 k_z(k_x + ik_y) + iD_6(\epsilon_{xz} + i\epsilon_{yz}),\\
&\Delta = \sqrt{2}\Delta_3. \qquad (5)
\end{aligned}
$$

The conduction-band wave function of a bulk WZ semiconductor can be written as

$$\Psi^{c\eta}(\boldsymbol{k}, \boldsymbol{r}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} |S\eta\rangle, \qquad (6)$$

where $\eta = \uparrow$ or $\downarrow$, and S is a spherically symmetric wave function. The complete Bloch wave functions for the valence band are given by

$$\Psi^{v}(\boldsymbol{k}, \boldsymbol{r}, \epsilon) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} |u_v\rangle. \qquad (7)$$

$|u_v\rangle$ is the periodic parts which can be written as

$$
\begin{aligned}
|u_v\rangle = {} & a|Y_{11}\uparrow\rangle + b|Y_{1-1}\uparrow\rangle + c|Y_{10}\uparrow\rangle\\
& + d|Y_{1-1}\downarrow\rangle + e|Y_{11}\downarrow\rangle + f|Y_{10}\downarrow\rangle, \qquad (8)
\end{aligned}
$$

where v denotes the heavy-hole (HH), light-hole (LH), or crystal- field split-off (CH) bands, and the coefficient vector $[a, b, c, d, e, f]^t$ is given by the normalized eigenvector of the valence Hamiltonian.

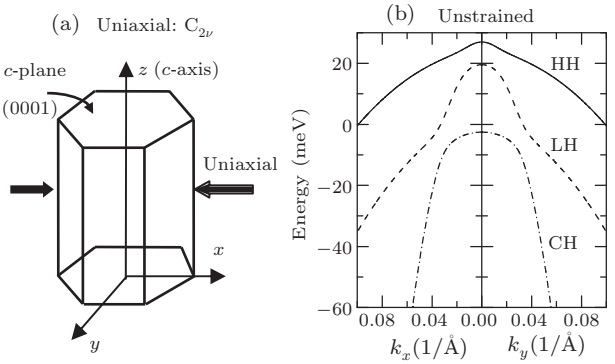


Fig. 1. (a) Calculated valence-band dispersion relations for no strained GaN crystal. (b) Direction of the uniaxial strain in the c-plane.

The squared magnitudes of the optical matrix elements can be expressed as

$$|M_x|^2 = \left|\frac{(-a+b)}{\sqrt{2}}P_2\right|^2 + \left|\frac{(d-e)}{\sqrt{2}}P_2\right|^2, \qquad (9)$$

$$|M_y|^2 = \left|\frac{(-a-b)}{\sqrt{2}}P_2\right|^2 + \left|\frac{(-d-e)}{\sqrt{2}}P_2\right|^2. \qquad (10)$$

The unit of matrix element is $P_2 = \langle S|P_x|X\rangle = \langle S|P_y|Y\rangle$, $P_1 = \langle S|P_z|Z\rangle$.

In general, the polarization degree ρ is defined as

$$\rho = \frac{|M_x|^2 - |M_y|^2}{|M_x|^2 + |M_y|^2}. \qquad (11)$$

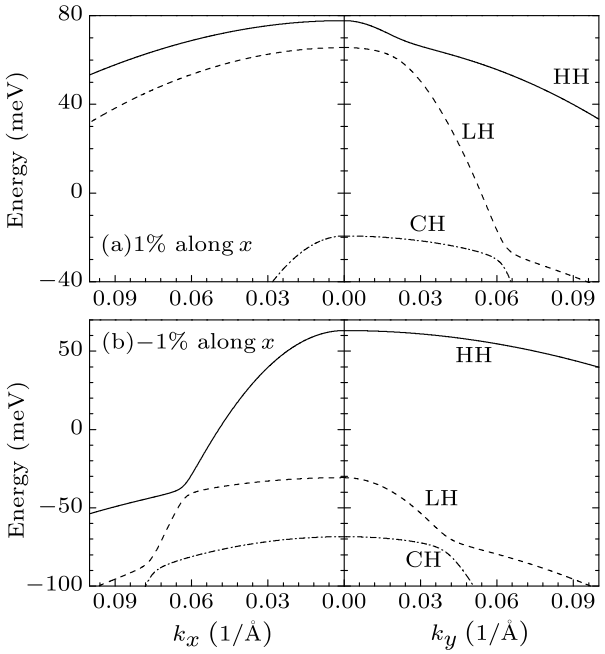


Fig. 2. Calculated Valence-band dispersion relations for (a) 1.0% tensile strained GaN crystal, and (b) −1.0% compressive strained GaN crystal in x direction.

We study the strain effect on the electronic band structure of WZ GaN. The original data of material parameters are taken from Ref. [15]. We give the electronic structure near the valence-band maximum (VBM) without strain for comparison in Fig. 1(b). As expected, there is no anisotropic energy splitting in the $k_x - k_y$ plane for the three valence-bands. Figures 2 and 3 show the valence-bands structure of uniaxial strained WZ GaN. The energy dispersion relations are no longer symmetric in the $k_x - k_y$ plane due to the symmetry is broken from C_{6v} to C_{2v}. Since the CH band is far away from the top of valence-bands, the following discussions are limited to HH and LH bands. Under the 1.0% tensile strain along x (y) direction, both the HH and LH bands along the y (x) direction move to the lower-energy side, as shown in Fig. 2(a) (Fig. 3(a)). The −1.0% compressive strain along the x (y) direction makes the LH band along the k_y (k_x)

but the HH band along the k_x (k_y) direction move to lower-energy side, as shown in Fig. 2(b) (Fig. 3(b)). Therefore, the density of states can be reduced by uniaxial strained in either x or y direction. Furthermore, the compressive uniaxial strains in x and y directions separate the LH band much away from the HH band compared to the tensile uniaxial strain, which is also advantage to reduce the DOS. Therefore, the compressive uniaxial strain plays a more remarkable role in reducing the DOS around the VBM. This is useful for realizing the population inversion.

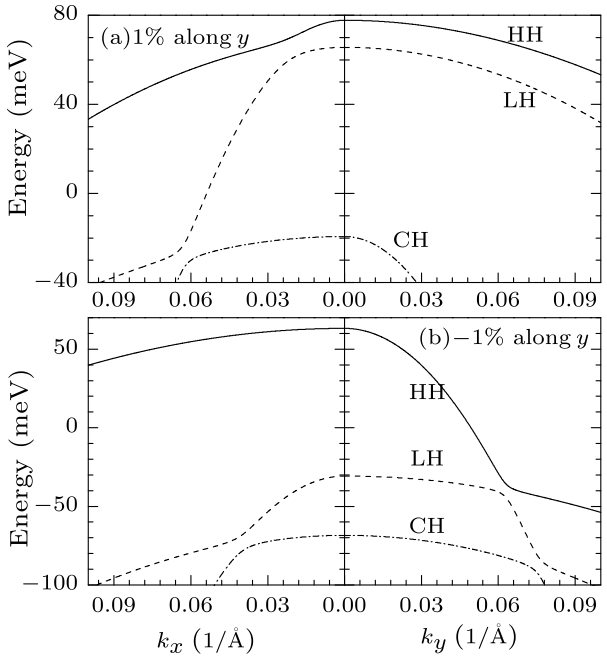


Fig. 3. Calculated valence-band dispersion relations for (a) 1.0% tensile strained GaN crystal, and (b) −1.0% compressive strained GaN crystal in y direction.

Without the strain, the HH and LH bands are $|X+Y\rangle$ and dominant $|X-Y\rangle$ states, respectively. The $|Z\rangle$ character, which is yielded from the CH band, is very little at the VBM. Thus, the following discussions are limited to the TE mode. Figure 4 shows the strain effect on the optical polarization degree. As expected, in the absence of the strain in c-plane, the polarization degree for the three bands are zero. With the increasing of uniaxial compressive along y (x), the C-HH transition rapidly becomes $|Y\rangle$ ($|X\rangle$) character, while C-LH transition rapidly becomes $|X\rangle$ ($|Y\rangle$) character. Namely, they become different polarization direction. If we introduce the tensile uniaxial strain along the x (y) direction, the HH band also rapidly becomes $|Y\rangle$ ($|X\rangle$) character. However, the LH band experiences a change from $|X\rangle$ ($|Y\rangle$) character at 0.23% tensile strain to $|Y\rangle$ (($|X\rangle$)) character at 1.0% tensile strain. These are consistent with Figs. 2 and 3. We should also notice that with a further increasing of the tensile strain in the x or y directions, the polarization characters of HH and LH bands are no longer in different directions, but become identical at 1.0% tensile strain. This is different from the situation with the compressive strain and the results in Ref. [12]. Taking the laser cavity in the y direction as an example, the optical polarization for the electric field is in the x direction, when we introduce a compressive uniaxial strain along the x direction or a tensile uniaxial strain along the y direction, the orbital component at the VBM becomes almost $|X\rangle$ character, which is beneficial to reduce the threshold carrier density. However, considering the reduction of the DOS, the useful uniaxial strain is the compressive strain in the x direction. Here, the useful strain for the laser cavity in the x direction is the compressive strain in the y direction. Therefore, it is efficient and advantageous to improve the GaN LDs performance by introducing a compressive strain perpendicular to the laser cavity direction in the c-plane.

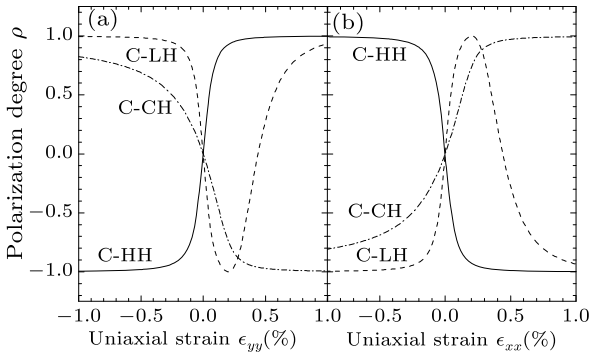


Fig. 4. Polarization degrees response for the C-HH, C-LH, C-CH optical transition as a function of the uniaxial strain (a) in x direction, (b) in y direction.

In conclusion, we have theoretically studied the uniaxial strain effect on optical anisotropy of WZ GaN crystal based on $\boldsymbol{k}\cdot\boldsymbol{p}$ theory. The valence-bands dispersions are given for compressive and tensile uniaxial strain in both x and y directions. The results show that the valence-band energies are no longer symmetric in k_x-k_y plane under uniaxial strain, which can cause the DOS reduced. Furthermore, the energy difference between HH and LH band become large due to the compressive strain effect. The in-plane polarization anisotropy has also been observed under the uniaxial strain in the c-plane, and it is advantageous to reduce threshold carrier density by introducing an compressive strain parallel to the polarization or an tensile one perpendicular to it. As a result, an uniaxial compressive strain in the direction perpendicular to the laser cavity direction can cause the DOS and the threshold carrier density reduced, which is very useful for the performance of LDs based on GaN-based crystal.

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