

Band Gap Shift of GaN under Uniaxial Strain Compression

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ABSTRACT

The band-gap shift of GaN:Mg epilayers on (0001)-oriented sapphire was studied as a function of uniaxial strain compression along the *c*-axis using time-resolved, optical absorption measurements in shock wave experiments. For longitudinal stresses ranging from 4 to 14 GPa, the band gap shift is approximately 0.026 eV/GPa. Combining this result with the known behavior of wurtzite GaN under hydrostatic pressure and biaxial stress, a new set of deformation potentials has been estimated: $a_{cz}D_1 = -10.2$ eV, $a_{ct}D_2 = -7.9$ eV, $D_3 = 1.33$ eV and $D_4 = -0.74$ eV. A slow band gap shift is also observed following the immediate band gap increase upon impact. This phenomenon can be explained by a time-dependent screening of the piezoelectric field.

INTRODUCTION

In recent years, much attention has been devoted to the study of the properties of GaN-based III-V semiconductors. The effect of strain on the optical properties of wurtzite GaN thin films and quantum-well structures is of great interest. Strain is always present in such heterostructures due to the large differences in lattice parameters and expansion coefficients between the substrate and III-nitride epilayers. In addition to its role in band-gap engineering, strain influences the electrical and optical properties of the devices through the piezoelectric effect [1-3]. The values of the deformation potentials for wurtzite GaN are important for device modeling. However, the values found in the literature are scattered over a relatively large range [4-7]. In this study, we present band-gap measurements of GaN:Mg under uniaxial strain compression along the *c*-axis using time-resolved, optical absorption spectroscopy in shock-wave experiments. This unique method enables us to obtain the hydrostatic deformation potential along the *c*-axis ($a_{cz}D_1$) directly.

EXPERIMENTAL DETAILS

The samples used in this work were thin (4 μm), semi-insulating, Mg-doped GaN epilayers on *c*-cut sapphire substrates (420 μm) grown by metalorganic chemical vapor deposition. Shock waves were generated by the impact of an optically transparent sapphire impactor onto the sample. The impactor was mounted on a projectile that was accelerated by a light gas gun. The GaN:Mg sample was backed by a sapphire buffer window. The transmitted light was collected by a UV-transparent lens and focused into an optical fiber. This light was spectrally dispersed by a spectrometer (ARC SpectraPro 150, 600 grooves/mm grating blazed at 300 nm), temporally dispersed by an electronic streak camera (Imacon 500) and digitally recorded on a charge-coupled device (CCD) detector as a series of transmission spectra, each separated in time by 20

ns. The shock wave produced a constant stress at the center of the sample for a duration of 130 to 270 ns, depending on the lateral dimensions of the sample. All relevant experiment data were collected within this time window. The steady-state stress reached in GaN was determined by the projectile velocity and the shock response of *c*-cut sapphire, which could be calculated very accurately (1-2%). Details of the experimental configuration can be found in Ref. 8.

RESULTS AND DISCUSSION

Absorption spectra of GaN:Mg samples shocked to different stresses along the *c*-axis are shown in Figure 1. The absorption coefficient α is obtained as a function of photon energy $\hbar\omega$ using

$$\alpha = \ln\left(\frac{I_0 - I_b}{I - I_b}\right) / d, \quad (1)$$

where I is the intensity transmitted through the sample (GaN + sapphire substrate), I_0 is the intensity transmitted through the reference sample (sapphire substrate), I_b is the background intensity recorded with the streak camera shutter closed, and d is the thickness of the GaN epilayer. Only the tail region of the band-edge absorption ($\alpha < 0.8 \times 10^4 \text{ cm}^{-1}$) was observed. The energy shifts of the direct band gap are plotted in Figure 2 as a function of longitudinal stress. The band-gap energy was defined to be the energy at which $\alpha = 0.288 \times 10^4 \text{ cm}^{-1}$. Since the shape of the absorption edge does not change much upon shock compression, the shift of the edge measured at a constant value of α yields the band-gap shift [13]. The band-gap shift, ΔE_g , was taken to be the difference between the shocked band gap (120 ns after impact) and the unshocked band gap.

Deformation potentials

For wurtzite semiconductors [7], the three valence bands HH (Γ_9^V), LH (Γ_7^V) and CH (Γ_7^V) have energy maxima given by

$$E_0^{HH} = \Delta_1 + \Delta_2 + \lambda_\epsilon + \theta_\epsilon, \quad (2)$$

$$E_0^{LH} = (\Delta_1 - \Delta_2 + \theta_\epsilon) / 2 + \lambda_\epsilon + \sqrt{[(\Delta_1 - \Delta_2 + \theta_\epsilon) / 2]^2 + 2\Delta_3^2}, \quad (3)$$

$$E_0^{CH} = (\Delta_1 - \Delta_2 + \theta_\epsilon) / 2 + \lambda_\epsilon - \sqrt{[(\Delta_1 - \Delta_2 + \theta_\epsilon) / 2]^2 + 2\Delta_3^2}, \quad (4)$$

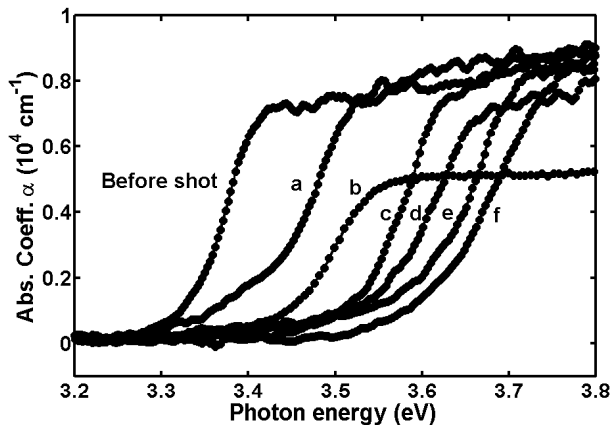


Figure 1. Absorption spectra of GaN:Mg (T=300 K) unshocked and after shocked to (a) 2.96 GPa, (b) 4.59 GPa, (c) 6.80 GPa, (d) 8.96 GPa, (e) 11.54 GPa and (f) 13.71 GPa along the *c*-axis.

with

$$\lambda_{\varepsilon} = D_1 \varepsilon_{zz} + D_2 (\varepsilon_{xx} + \varepsilon_{yy}), \quad (5)$$

$$\theta_{\varepsilon} = D_3 \varepsilon_{zz} + D_4 (\varepsilon_{xx} + \varepsilon_{yy}), \quad (6)$$

where Δ_1 is the crystal-field splitting of the Γ_9 and Γ_7 orbital states, Δ_2 and Δ_3 are parameters that describe the spin-orbit coupling, ε_{ij} are components of the strain tensor, and D_i are valence-band deformation potentials. Here we use the convention that a positive (negative) value of ε_{ij} indicates a tensile (compressive) strain. For the conduction band, the minimum energy is given by

$$E_0^C = \Delta_1 + \Delta_2 + E_g + a_{cz} \varepsilon_{zz} + a_{ct} (\varepsilon_{xx} + \varepsilon_{yy}), \quad (7)$$

where E_g is the band gap in the absence of strain, and a_{cz} and a_{ct} are the conduction-band deformation potentials.

In the present study involving shock compression along the c -axis, the following *uniaxial strain* relations hold: $\varepsilon_{zz} = \sigma_{zz}/C_{33}$ and $\varepsilon_{xx} = \varepsilon_{yy} = 0$, where C_{ij} are the elastic constants and σ_{ij} are components of the stress tensor. In this work, we use the stiffness coefficients given in Ref. 9, $C_{11} = 390$ GPa, $C_{12} = 145$ GPa, $C_{13} = 106$ GPa and $C_{33} = 398$ GPa. Using equations (1)-(7), we calculated that the slopes for A -, B -, and C - band gap shifts versus ε_{zz} under uniaxial strain are $a_{cz}-D_1-D_3$, $a_{cz}-D_1$ and $a_{cz}-D_1-D_3$, respectively. Assuming D_3 is positive [4-7], the lowest band-gap shift arises from the B valence band; thus, the slope of the band-gap shift versus ε_{zz} is equal to $a_{cz}-D_1$. For shock stresses above 10 GPa, the band-gap shifts deviate from linearity (Fig. 2). A reduction in the band gap may be caused by strong piezoelectric fields produced at these higher stresses. In the present study, the experimental data are fit linearly below 10 GPa, resulting in

$$E_B = 0.0256 \sigma_{zz} \text{ eV/GPa} = -10.2 \varepsilon_{zz} \text{ eV}. \quad (8)$$

Hence, $a_{cz}-D_1 = -10.2$ eV. With the exception of the theoretical calculations given in Refs. 10-11, our value for $a_{cz}-D_1$ is lower (more negative) than those found by other groups.

Analyzing the band-gap shift of wurtzite GaN under hydrostatic pressure and biaxial stress, we are able to obtain further information on the other deformation potentials (details will be published elsewhere). Combining these results with the present study, a new set of deformation potentials has been estimated: $a_{cz}-D_1 = -10.2$ eV, $a_{ct}-D_2 = -7.9$ eV, $D_3 = 1.33$ eV and $D_4 = -0.74$ eV.

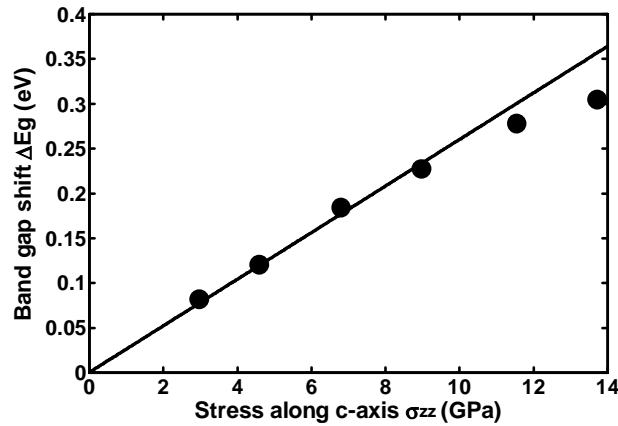


Figure 2. The band gap shift of GaN:Mg as a function of longitudinal shock stress σ_{zz} . The solid line is the linear fit to the experimental data below 10 GPa.

Time-dependence of band-gap shift

After the initial abrupt increase upon impact, the band-gap increases at a slower rate. Figure 3 shows the time dependence of the band-gap for a sample shocked to 13.7 GPa. The slow time-dependent behavior may be related to strong piezoelectric fields caused by the shock compression along the c -axis of GaN. It is well known that an applied electric field shifts the fundamental optical absorption edge to lower energies (Franz-Keldysh effect). The slow increase of the band gap shift after impact implies that the piezoelectric field decreases with time, due to screening by charge carriers. The rate of the band-gap shift (shown as the dotted line in Fig. 3) is plotted as a function of stress σ_{zz} (Fig. 4). It is clear that this rate increases with stress. A least-squares fit to the data revealed that the rate is approximately proportional to the square of the stress σ_{zz} . This fit is shown as the solid line in Fig. 4. It is reasonable to postulate that for higher shock stresses, larger piezoelectric fields would be produced, resulting in a faster screening process.

CONCLUSIONS

The band-gap shift of GaN:Mg has been studied as a function of uniaxial compression along the c -axis using time-resolved, optical absorption measurements in shock-wave experiments. The hydrostatic deformation potential $a_{cz}-D_1$ (parallel to the c -axis), has been determined independently from $a_{ct}-D_2$ (perpendicular to the c -axis). Based on experimental results, a set of deformation potentials has been obtained: $a_{cz}-D_1 = -10.2$ eV, $a_{ct}-D_2 = -7.9$ eV, $D_3 = 1.33$ eV and $D_4 = -0.74$ eV. Meanwhile, a “slow” band-gap shift is also observed, following the immediate band-gap increase upon impact. The rate of the slow shift increases with stress. This time-dependent behavior may be due to screening of the strain-induced piezoelectric fields by charge carriers.

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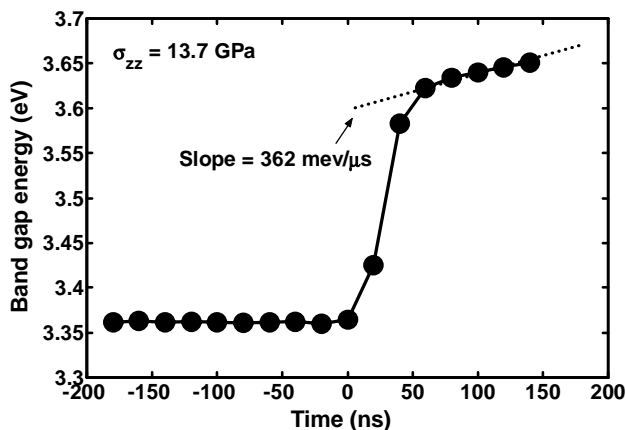


Figure 3. The band gap energy of GaN:Mg as a function of shock time when shocked to 13.7 GPa.

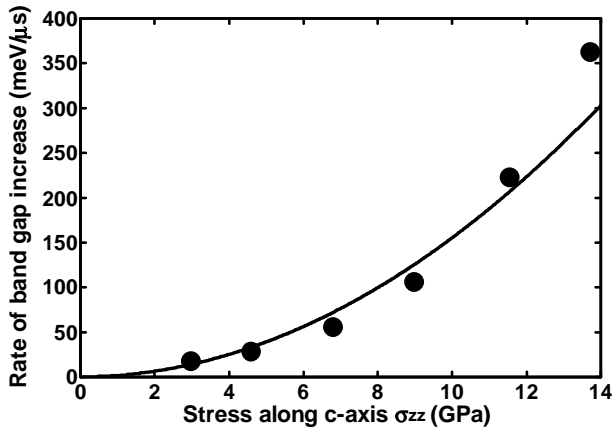


Figure 4. The rate of band gap increase (eV/ μ s) as a function of shock stress σ_{zz} .

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