

Strain-related phenomena in GaN epilayers under MeV inert-gas ions irradiation

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Abstract

Single crystal GaN epilayers were irradiated with heavy inert-gas ions (2.3-MeV Ne⁸⁺, 5.3-MeV Kr¹⁹⁺) to fluences ranging from 1.0×10^{11} to 1.0×10^{15} ions/cm². The strain-related damage accumulation versus ion fluences was studied by using a high-resolution X-ray diffractometer (HRXRD) and an ultraviolet visible (UV-Vis) spectroscopy. Results show that damage accumulations are dominated by the nuclear energy loss mainly. When the ion fluence is less than ~ 0.055 dpa, lattice expansions and lattice strains markedly linearly increase with increasing ion fluences, accompanied by a slow enhancement in dislocation densities, distortion parameters and the Urbach energy for both ions irradiation. Above this fluence (~ 0.055 dpa), lattice strains present a slight increase, while a remarkable increase was observed in dislocation densities, distortion parameters and the Urbach energy with the ion fluences after both ions irradiation. The value of ~ 0.055 dpa is a threshold ion fluence for defect evolutions and lattice damages related to the strain. The mechanisms underlying the damage accumulation were discussed in detail.

Full Text

Preamble

Strain-Related Phenomena in GaN Epilayers Under MeV Inert-Gas Ion Irradiation

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Abstract

Single-crystal GaN epilayers were irradiated with heavy inert-gas ions (2.3-MeV Ne⁸⁺, 5.3-MeV Kr¹⁹⁺) to fluences ranging from 1.0×10^{11} to 1.0×10^{15} ions/cm². The accumulation of strain-related damage as a function of ion fluence was investigated using high-resolution X-ray diffractometry (HRXRD) and ultraviolet-visible (UV-Vis) spectroscopy. Results demonstrate that damage accumulation is dominated primarily by nuclear energy loss. When the ion fluence is below approximately 0.055 dpa, lattice expansion and lattice strain increase markedly and linearly with ion fluence, accompanied by a gradual enhancement in dislocation density, distortion parameters, and Urbach energy for both ion species. Above this fluence threshold (~ 0.055 dpa), lattice strain exhibits only a slight increase, while dislocation densities, distortion parameters, and Urbach energy show remarkable increases with ion fluence for both irradiation conditions. The value of ~ 0.055 dpa represents a threshold ion fluence for defect evolution and lattice damage related to strain. The underlying mechanisms of damage accumulation are discussed in detail.

Keywords: GaN; Gas-ion irradiation; HRXRD; UV-Vis spectra; Strains; Urbach energy

1. Introduction

Gallium nitride (GaN) with hexagonal structure exhibits strong covalent bonds between gallium (Ga) and nitrogen (N) atoms, with a Ga-N binding energy of approximately 8.92 eV per atom [1]. This property contributes to its high melting point, strong acid and alkali resistance, high thermal conductivity, excellent radiation resistance, and outstanding mechanical stability. Compared with other semiconductor materials (Si, Ge, InP, GaAs, ZnO) [2-5], GaN possesses superior electrical and optical properties, including a wide bandgap, high breakdown field (voltage), high electron mobility, and high saturated electron drift velocity. Consequently, GaN has attracted growing attention for its exceptional characteristics and is now regarded as a representative third-generation semiconductor material following Si and GaAs. It is widely used in optoelectronics, power electronics, and other fields, with promising potential for ultraviolet

detectors, short-wavelength light-emitting diodes (LEDs), laser diodes (LDs), high-electron-mobility transistors (HEMTs), heterojunction bipolar transistors (HBTs), and high-frequency, high-power, high-temperature electronic devices [6-9]. Notably, the significant radiation endurance of GaN, characterized by a high amorphization threshold, makes it particularly suitable for harsh environments with high irradiation fluences.

Therefore, GaN-based devices are commonly employed as detectors or lighting systems in demanding environments such as aviation, aerospace, nuclear industries, and nuclear power plants [10]. During service, these devices inevitably suffer radiation damage from cosmic rays or various energetic particles (protons, electrons, neutrons, swift heavy ions, highly-charged ions). For keV-energy ions, irradiation-induced damage in GaN materials is understood to transfer energy primarily through ion-atom nuclear collisions, quantified by nuclear energy loss. For MeV-energy ions, damage effects are considered to deposit most of their energy through electronic excitation and ionization of atoms along their trajectories, quantified by electronic energy loss [11-18].

Regardless of whether through cascade collisions or excitation/ionization processes, once the deposited ion energy exceeds the displacement threshold energy of atoms in GaN, point defects—including vacancies and interstitials—are generated. This destroys the long-range order of GaN lattices and produces lattice strain. Corresponding changes in GaN's optical characteristics occur due to interactions between defects/disordered lattices and charge carriers, as optical properties are highly sensitive to the nature and concentration of point and extended defects.

With accumulating point defects, increasing disorder among lattice atoms intensifies distortion of lattice planes, accompanied by defect evolution related to strain. Irradiation-induced damage accumulation, lattice strains, defect evolution, and optical characteristic changes in GaN materials and devices have been extensively addressed by researchers [18-33]. For keV-energy ions, nuclear energy loss plays an important role in irradiation-induced damage in GaN. For MeV-energy ions, energy deposition processes depend not only on the kinetic energy of incident ions but also on their volumes [34]. Sometimes, irradiation damage from MeV-energy ions in GaN is also attributed primarily to nuclear energy loss rather than electronic energy loss. Therefore, clarifying the effects of different energy loss mechanisms in GaN under MeV-energy ion irradiation is an important issue. Moreover, inert gas ions do not bond with Ga and N atoms but do produce defects.

In this work, to investigate the predominant effects of electronic and nuclear energy loss from MeV-energy ions on the microstructures, lattice strains, and optical properties of GaN materials, we performed irradiation experiments on GaN films with 2.3 MeV $^{20}\text{Ne}^{8+}$ and 5.3 MeV $^{84}\text{Kr}^{19+}$ ions at various fluences. The specimens were analyzed using high-resolution X-ray diffractometry and ultraviolet-visible spectroscopy.

2. Experiment

The specimens used in this study were n-type wurtzite GaN layers grown on c-plane sapphire by metal-organic chemical vapor deposition (MOCVD) with a doping concentration of 1.0×10^{17} Si/cm³ and a thickness of approximately 3.0 μm. Irradiation experiments were conducted at the 320 kV high-voltage atomic physics experimental platform with an ECR ion source at the Institute of Modern Physics (IMP), China. Specimens were irradiated with 2.3-MeV ²⁰Ne⁸⁺ ions to successively increasing fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne⁸⁺ ions/cm², and with 5.3-MeV ⁸⁴Kr¹⁹⁺ ions to fluences of 1.0×10^{11} , 1.0×10^{12} , and 1.0×10^{13} Kr ions/cm², in a vacuum of approximately 5×10^{-5} Pa at ambient temperature. To avoid obvious heating effects from the ion beams, the ion flux was controlled below 10^{11} ions/cm²/s.

The projected ion ranges and electronic and nuclear stopping powers in GaN under these irradiation conditions were estimated using SRIM 2013 code [34]. The calculation results for ion ranges and energy loss are shown in Figs. 1a and 1b. [Figure 1: see original paper] reveals that the incident ion range is approximately 1.78 μm for 5.3-MeV Kr¹⁹⁺ ions and 1.68 μm for 2.3-MeV Ne⁸⁺ ions, both residing within the GaN epilayers. For 5.3-MeV Kr¹⁹⁺ ions in GaN, electronic and nuclear energy losses are of the same order of magnitude, with maximum values of 2.75 keV/nm and 2.49 keV/nm, respectively. For 2.3-MeV Ne⁸⁺ ions in GaN, electronic energy loss is about five times larger than nuclear energy loss, with maximum values of 2.15 keV/nm and 0.38 keV/nm, respectively.

Meanwhile, damage distribution and atom concentration in all GaN specimens were calculated from SRIM “quick calculations.” Displacement energies of 20.8 eV and 10.5 eV were adopted for Ga and N atoms, respectively [35]. Under 5.3-MeV Kr¹⁹⁺ irradiation at 1.0×10^{11} Kr¹⁹⁺ ions/cm², the calculated peak atomic displacement level is 2.5×10^{-4} dpa (displacements per atom) with an atom concentration of 1.6×10^{-2} appm. At 1.0×10^{12} Kr¹⁹⁺ ions/cm², the peak displacement damage and atom concentration increase to 2.5×10^{-3} dpa and 1.6×10^{-1} appm, respectively. At the highest fluence of 1.0×10^{13} Kr¹⁹⁺ ions/cm², the corresponding values are 2.5×10^{-2} dpa and 1.6 appm. For 2.3-MeV Ne⁸⁺ irradiation at fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne⁸⁺ ions/cm², the calculated peak displacement damage values are approximately 5.3×10^{-5} , 5.3×10^{-4} , 5.3×10^{-3} , 5.3×10^{-2} , and 5.3×10^{-1} dpa, respectively, with atom concentrations of approximately 2.57×10^{-2} , 2.57×10^{-1} , 2.57×10^1 , and 2.57×10^2 appm, respectively.

Following irradiation, all GaN specimens—including unirradiated and irradiated samples—were measured using high-resolution X-ray diffractometry (HRXRD) and ultraviolet-visible transmittance spectroscopy (UV-Vis). HRXRD measurements were performed using a D8 Discover X-ray diffractometer equipped with a four-crystal monochromator in Ge (220) configuration and one or two 200 m

slits before the detector. Monochromatic Cu $K\alpha_1$ X-rays ($\lambda = 0.15406$ nm) served as the incident beam. $\omega/2$ scans were performed on the (0002) lattice plane of all GaN specimens with a step size of 0.001° using the Ge (220) three-axis analyzing crystal set.

UV-visible transmittance spectra were acquired using a Lambda 900 UV/VIS/NIR Spectrometer from Perkin Elmer Inc., with tungsten and deuterium lamps as light sources. The spectral resolution was 1 nm, and transmittance spectra were recorded from 200 to 2500 nm.

3.1 HRXRD Analysis

[Figure 2: see original paper] shows $\omega/2$ scanning curves and strain distribution analysis of the GaN(0002) lattice plane irradiated with 5.3-MeV Kr^{19+} and 2.3-MeV Ne^{8+} ions at various fluences. The lattice constant c of the pristine specimen was measured to be 0.5188 nm, slightly larger than the standard value of 0.5185 nm. This difference is attributed to biaxial stress between the epitaxial GaN film and sapphire substrate [36, 37].

The $\omega/2$ scanning results for GaN irradiated with both ion species show identical trends. The diffraction peak shifts systematically to smaller angles as ion fluence increases, with concurrent peak broadening observed at higher fluences. Additionally, splitting of the main peak occurs and several satellite peaks appear beside the main peak at relatively high fluences. The appearance of these small peaks at lower angles results from expansion of the original lattice and generation of new crystal planes, while the disappearance of some small peaks is due to distortion of these new crystal planes or partial amorphization at higher fluences. Similar phenomena were observed in Ar-ion-irradiated GaN specimens [37]. These effects are attributed to defect creation in the crystal structure, leading to lattice expansion and variation in interplanar spacing. Lattice expansion can be calculated from Bragg's law, $2d \sin \theta = j\lambda$ ($\lambda = 0.15406$ nm, where θ is the diffraction angle from HRXRD curves). Furthermore, these effects are ascribed to buildup of lattice compression and lattice strain in GaN films through energy deposition from incident ions [37-39]. The broadening of diffraction peaks indicates increasing disordered regions and distorted lattice planes with increasing ion fluence in irradiated GaN films due to defect accumulation, thereby enhancing the amorphization rate.

It should be noted that a conflicting trend exists between lattice strain and dislocation density as functions of ion fluence. Based on data from the analysis and the aforementioned dislocation density values, we can conclude that dislocation density increases sharply during strain release.

To further confirm strain changes induced by defect evolution, we estimated the dislocation density parameter (δ) from HRXRD curves using an equation relating diffraction peak shape and broadening to dislocation density within a crystal lattice [43]. This analysis provides insight into strain changes induced by defect evolution within the crystal structure. The equation is:

$$\delta = \frac{1}{D^2} \quad (3)$$

where D is the thickness of the diffracting layer of GaN(0002) lattice planes. By fitting the HRXRD experimental curves, the full width at half maximum (FWHM) and Bragg angle of the GaN(0002) diffraction peak were determined. Using the empirical Scherrer equation, D was obtained. For the unirradiated GaN specimen, D was approximately (178.6558 ± 7.146) nm. After Kr^{19+} ion irradiation at 1.0×10^{11} , 1.0×10^{12} , and 1.0×10^{13} Kr ions/ cm^2 , the corresponding diffracting layer thicknesses were approximately (135.3325 ± 6.7666) nm, (115.1562 ± 4.6062) nm, and (59.3774 ± 2.9688) nm, respectively. For Ne^{8+} ion irradiation at fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne ions/ cm^2 , the corresponding D values were approximately (171.2225 ± 6.489) nm, (168.0248 ± 8.4012) nm, (112.5115 ± 4.5004) nm, (23.9323 ± 1.1966) nm, and (22.8045 ± 1.1402) nm, respectively.

The dislocation density parameter (δ) at various fluences for both ion irradiations was calculated accordingly. For the unirradiated GaN specimen, δ was approximately $(3.1330 \pm 0.1253) \times 10^{-5}$ lines/ nm^2 . After Kr^{19+} ion irradiation, δ values were approximately $(5.4600 \pm 0.2184) \times 10^{-5}$, $(7.5409 \pm 0.3770) \times 10^{-5}$, and $(28.363 \pm 1.134) \times 10^{-5}$ lines/ nm^2 for 1.0×10^{11} , 1.0×10^{12} , and 1.0×10^{13} Kr ions/ cm^2 irradiation, respectively. As irradiation fluence increased successively to 1.0×10^{12} Kr^{19+} / cm^2 , the average dislocation density increased slowly from $(3.1330 \pm 0.1253) \times 10^{-5}$ to $(7.5409 \pm 0.3770) \times 10^{-5}$ lines/ nm^2 . Above this fluence, the average dislocation density rose rapidly to $(28.363 \pm 1.134) \times 10^{-5}$ lines/ nm^2 .

For Ne^{8+} ion irradiation at fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne ions/ cm^2 , the corresponding average dislocation densities were approximately $(3.4109 \pm 0.1705) \times 10^{-5}$, $(3.5420 \pm 0.1416) \times 10^{-5}$, $(7.8996 \pm 0.3949) \times 10^{-5}$, $(175.2 \pm 7.031) \times 10^{-5}$, and $(192.3 \pm 9.011) \times 10^{-5}$ lines/ nm^2 . When irradiation fluence increased successively to 1.0×10^{13} Ne^{8+} / cm^2 , the average dislocation density increased slowly from $(3.1330 \pm 0.1253) \times 10^{-5}$ to $(7.8996 \pm 0.3949) \times 10^{-5}$ lines/ nm^2 . At 1.0×10^{14} Ne^{8+} / cm^2 , the average dislocation density sharply increased to $(1.752 \pm 0.07031) \times 10^{-3}$ lines/ nm^2 . As fluence further rose to 1.0×10^{15} Ne^{8+} / cm^2 , the average dislocation density increased gently to $(1.923 \pm 0.09011) \times 10^{-3}$ lines/ nm^2 . Generally, similar changes in dislocation density were observed for both ion-irradiated GaN films as ion fluence increased.

To provide further insight into structural changes induced by MeV-energy ion irradiation and understand the overall strain behavior of GaN films under different conditions, distortion parameters (g) were calculated from HRXRD curves based on a specific formula [45]:

$$g = \frac{\beta}{\tan \theta} \quad (4)$$

where β is the full width at half maximum (FWHM) of the GaN(0002) diffraction peak and θ is the Bragg diffraction angle of the GaN(0002) main peak. For the unirradiated GaN specimen, the distortion parameter was approximately $(3.216 \pm 0.128)\%$. After Kr^{19+} ion irradiation at 1.0×10^{11} , 1.0×10^{12} , and 1.0×10^{13} Kr ions/ cm^2 , the corresponding distortion parameters were approximately $(4.046 \pm 0.202)\%$, $(4.648 \pm 0.185)\%$, and $(9.007 \pm 0.450)\%$, respectively. For Ne^{8+} irradiation at fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne ions/ cm^2 , the distortion parameters were approximately $(3.319 \pm 0.165)\%$, $(3.373 \pm 0.168)\%$, $(3.493 \pm 0.139)\%$, $(13.11 \pm 0.655)\%$, and $(13.15 \pm 0.526)\%$, respectively.

The distortion parameters clearly increase with ion fluence, confirming the production of disordered structures in irradiated GaN films. The dislocation density parameter (δ) and distortion parameters (g) exhibit the same trend with respect to ion fluence for both irradiations. As irradiation fluence increased successively to 1.0×10^{12} Kr^{19+} / cm^2 , the average distortion parameter increased slowly from $(3.216 \pm 0.128)\%$ to $(4.648 \pm 0.185)\%$. Above this fluence, it rose rapidly to $(9.007 \pm 0.450)\%$. For Ne^{8+} ion irradiation, when fluence increased successively to 1.0×10^{13} Ne^{8+} / cm^2 , the average distortion parameter increased slowly from $(3.216 \pm 0.128)\%$ to $(3.493 \pm 0.139)\%$. At 1.0×10^{14} Ne^{8+} / cm^2 , it sharply increased to $(13.11 \pm 0.655)\%$. As fluence further rose to 1.0×10^{15} Ne^{8+} / cm^2 , it increased gently to $(13.15 \pm 0.526)\%$.

It is worth noting that during the period when distortion parameters rise remarkably, lattice strains undergo a transition from rapid to mild increase. This can be attributed to lattice stress release through migration and rearrangement of dislocations and stacking faults, as strain energy can be consumed by material deformation, cracking, and fracture.

3.2 UV-Vis Spectrum

Bandgap energy is a vitally important optical parameter of semiconductor materials such as GaN. To investigate the effects of irradiation-induced lattice strain on bandgap energy, we performed UV-Vis transmittance spectrum analysis on irradiated GaN films. [Figure 4: see original paper] shows the UV-Vis transmittance spectra of GaN films irradiated by 5.3-MeV Kr^{19+} and 2.3-MeV Ne^{8+} ions at various fluences. The transmissivity of GaN films decreases with increasing ion fluence for both ion species, due to enhanced absorption and scattering from irradiation-induced defects. Simultaneously, a wide interference band appears due to the interface between the GaN film and Al_2O_3 substrate. Moreover, the shape of the optical absorption edge in GaN films gradually becomes more oblique with increasing ion fluence, which can be ascribed to the introduction of

absorption structures within the bandgap. Specifically, this alteration in band-edge absorption of irradiated GaN films is attributed to the introduction of additional electronic energy states [46], likely resulting from structural changes induced by irradiation, such as the creation of various defects. These observations highlight the complex interplay between lattice stress, irradiation, and the optical and electronic properties of GaN films, with significant implications for the performance and reliability of GaN-based devices.

Tauc's formula [47] was used to estimate optical bandgap energy (E_g):

$$\alpha h\nu = A(h\nu - E_g)^n \quad (5)$$

where α is the absorption coefficient calculated from the UV-Vis transmittance curve, $h\nu$ is photon energy computed by $h\nu = 1240/\lambda$, A is a constant related to refractivity, reduced mass, and absorption edge width, and n is the optical transition phase. For direct bandgap semiconductor materials like GaN, n is chosen as $1/2$.

Using this formula, the optical bandgap energy of GaN films was deduced from $(\alpha h\nu)^2$ versus $(h\nu)$ plots. The bandgap energy of the unirradiated GaN specimen was approximately (3.3562 ± 0.1667) eV. After Kr^{19+} ion irradiation at 1.0×10^{11} , 1.0×10^{12} , and 1.0×10^{13} Kr ions/cm², the corresponding bandgap energies were approximately (3.2645 ± 0.1632) eV, (3.2372 ± 0.1618) eV, and (2.9394 ± 0.1469) eV, under lattice strains of approximately 0.005%, 0.06%, and 0.32%, respectively. For Ne^{8+} ion irradiation at fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne ions/cm², the corresponding bandgap energies were approximately (3.3513 ± 0.1675) eV, (3.3245 ± 0.1662) eV, (3.2916 ± 0.1645) eV, (2.9258 ± 0.1629) eV, and (2.8645 ± 0.1617) eV, under lattice strains of approximately 0, 0.008%, 0.06%, 0.44%, and 0.68%, respectively.

The bandgap energy of GaN films clearly decreases with increasing ion fluence, accompanied by increased lattice strain. After Kr^{19+} ion irradiation, the value gradually decreased from (3.3562 ± 0.1667) eV to (2.9394 ± 0.1469) eV. As ion fluence increased to 1.0×10^{12} Kr ions/cm², the optical bandgap energy decreased to (3.2372 ± 0.1618) eV with a rapid strain increase from 0.005% to 0.06%. Above this fluence, the value sharply decreased to (2.9394 ± 0.1469) eV under a strain of approximately 0.32%. Similar changes were observed in Ne^{8+} -irradiated GaN specimens, with bandgap energy decreasing from (3.3562 ± 0.1667) eV to (2.8645 ± 0.1617) eV. At fluences below 1.0×10^{13} Ne⁸⁺/cm², the bandgap energy slowly decreased to (3.2916 ± 0.1645) eV after lattice strain rapidly increased to 0.06%. Above this fluence, the bandgap energy rapidly decreased to (2.9258 ± 0.1629) eV while strain increased to 0.44% from 0.06%. As irradiation fluence further increased to 1.0×10^{15} Ne ions/cm², the value slowly decreased to (2.8645 ± 0.1617) eV under a gradual strain increase from 0.44% to 0.68%.

Ion interaction with GaN films creates various defects in the bandgap, resulting in reduced optical bandgap energy. Defect generation establishes localized states between the valence and conduction bands, reducing bandgap energy [48]. At lower fluences, slow bandgap reduction occurs due to single defect generation and strain accumulation. At relatively higher fluences for both ions, the significant bandgap reduction is attributed to creation of dislocations, lattice distortions, and stacking faults due to strain release. These results generally agree well with HRXRD analysis.

The exponential shape of the optical absorption edge from UV-Vis spectra reflects structural disorder in dielectrics and semiconductors [49-51]. Research groups have investigated disordered and amorphous materials using Urbach energy obtained from UV-Vis spectral absorption edges [52-55]. Urbach energy successfully characterizes total structural disorder in ion- and neutron-irradiated crystals, glasses, thin films, and nanoparticles [53-55], enabling qualitative and quantitative assessment of atomic disorder levels from spectral curve shapes. Similarly, lattice disorders in crystalline semiconductors (GaN) induced by ion irradiation can be characterized by Urbach energy, which can be deduced from absorption spectra.

The absorption coefficient (α) can be obtained from UV-Vis spectra and characterized using the equation [48]:

$$\alpha(\nu) = \alpha_0 e^{h\nu/E_u} \quad (6)$$

where E_u is the Urbach energy (Urbach band tail), calculated by plotting absorption coefficient ($\ln\alpha$) versus photon energy ($h\nu$). E_u characterizes static and dynamic disorder in materials and represents the state-density-tail length at the energy band boundary, located at the onset of sharp transmittance drops in UV-Vis curves.

Based on the UV-Vis curves, the energy band boundary of the unirradiated GaN specimen is approximately 3.28 eV. For Kr^{19+} -irradiated GaN specimens, the energy band boundary values are approximately 3.12 eV, 2.97 eV, and 2.78 eV, corresponding to 1.0×10^{11} , 1.0×10^{12} , and 1.0×10^{13} $\text{Kr}^{19+}/\text{cm}^2$, respectively. For Ne^{8+} -irradiated GaN specimens at fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne ions/ cm^2 , the corresponding values are approximately 3.28 eV, 3.26 eV, 3.23 eV, 2.59 eV, and 2.42 eV, respectively.

Near the energy band boundary, E_u can be computed from $\ln\alpha$ versus $h\nu$ plots. The Urbach energy of the unirradiated GaN film is approximately (0.1735 ± 0.0086) eV. After Kr^{19+} ion irradiation at 1.0×10^{11} , 1.0×10^{12} , and 1.0×10^{13} Kr ions/ cm^2 , the Urbach energy values are (0.3056 ± 0.0152) eV, (0.3075 ± 0.0153) eV, and (0.3307 ± 0.0165) eV, under lattice strains of approximately 0.005%, 0.06%, and 0.32%, respectively. For Ne^{8+} ion irradiation, Urbach energy values are

(0.2887 ± 0.0144) eV, (0.2953 ± 0.0147) eV, (0.3122 ± 0.0156) eV, (0.3401 ± 0.0170) eV, and (0.3526 ± 0.0176) eV, corresponding to fluences of 1.0×10^{11} , 1.0×10^{12} , 1.0×10^{13} , 1.0×10^{14} , and 1.0×10^{15} Ne⁸⁺/cm², with lattice strains of approximately 0, 0.008%, 0.06%, 0.44%, and 0.68%, respectively.

Urbach energy clearly increases with lattice strain and ion fluence after GaN films are irradiated with both ion species at various fluences, due to disorder creation and localized state formation from irradiation [56, 57]. However, as Kr¹⁹⁺ ion fluence increases to 1.0×10^{12} Kr ions/cm², Urbach energy slowly increases from (0.1735 ± 0.0086) eV to (0.3075 ± 0.0153) eV while strain rapidly increases from 0.005% to 0.06%. When irradiation fluence further increases to 1.0×10^{13} Kr ions/cm², Urbach energy significantly increases to (0.3307 ± 0.0165) eV while strain slowly increases to 0.32% from 0.06%. Ne⁸⁺-irradiated GaN specimens show similar behavior. At fluences below 1.0×10^{13} Ne⁸⁺/cm², Urbach energy slowly increases from (0.1735 ± 0.0086) eV to (0.3122 ± 0.0156) eV after lattice strain rapidly increases to 0.06%. Above this fluence, the value sharply increases to (0.3401 ± 0.0170) eV while strain slowly increases to 0.44%. As fluence further increases to 1.0×10^{15} Ne⁸⁺/cm², Urbach energy mildly increases to (0.3526 ± 0.0176) eV under a strain of 0.68%. These results generally coincide with findings from other research groups [58, 59].

When irradiation fluence exceeds a certain value, the significant increase in Urbach energy is ascribed to production of dislocations, lattice distortions, and stacking faults due to strain release. This result agrees well with average distortion parameters and dislocation density deduced from HRXRD curves. Based on the analysis and computed data (average distortion, dislocation density, bandgap energy, and Urbach energy), we conclude that severe lattice damage occurs and defect concentration increases remarkably during strain release processes, leading to significant decreases in optical bandgap energy and obvious increases in Urbach energy.

4. Conclusions

An investigation of strain-related defect evolution and band-edge characteristics of GaN films irradiated with 2.3-MeV Ne⁸⁺ and 5.3-MeV Kr¹⁹⁺ ions at various fluences was performed using HRXRD and UV-Vis spectroscopy. Results revealed that damage accumulation and lattice strains are caused mainly by nuclear energy loss, while electronic energy loss contributes less to GaN crystal damage. Moreover, lattice strain comprises two main components: defect-induced strain and incident-ion-induced strain, with defect-induced strain being the principal contribution.

When ion fluence is below ~ 0.055 dpa, defects in GaN are primarily simple point defects whose concentration is approximately linearly proportional to total nuclear energy loss. This results in rapid enhancement of lattice strains with

ion fluence. Simultaneously, dislocation density, distortion parameter, and Urbach energy generally show slow increases with ion fluence for both irradiations. When irradiation fluence exceeds ~ 0.055 dpa, lattice strains increase slowly while dislocation density, distortion parameter, and Urbach energy increase rapidly with ion fluence. This is attributed to saturation of point defect concentration and formation of more complex defects (dislocations, stacking faults) due to strain release. It is suggested that ~ 0.055 dpa represents a threshold value for defect evolution from point defects to complex defects and for stress release in GaN materials. These results may provide references for full utilization of GaN-based devices in radiation environments.

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