Effect of AlN Nucleation Layer Thickness on Epitaxial GaN on Si

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Abstract

Growth of GaN thin films on Si(111) substrates using metal-organic chemical vapor deposition (MOCVD) with a low-temperature AlN nucleation layer. Abstract: GaN thin films were grown on Si(111) substrates by metal-organic chemical vapor deposition (MOCVD) using a low-temperature AlN nucleation layer. The influence of AlN nucleation layer thickness on the GaN epitaxial layer was investigated using high-resolution X-ray diffraction, spectroscopic ellipsometry, and atomic force microscopy. Measurements on AlN revealed that the surface roughness of AlN increases with increasing thickness. Measurements on GaN indicated that all GaN samples were under compressive strain in the vertical direction, which slightly weakened with increasing AlN thickness. The full width at half maximum (FWHM) of the GaN (0002) -scan slightly increased with increasing AlN nucleation layer thickness, while the FWHM of the GaN (10-12) -scan decreased with increasing thickness. The FWHM of the (10-12) -scan is correlated with the edge threading dislocation density of GaN. This demonstrates that a thicker AlN nucleation layer reduces the edge threading dislocation density and alleviates the compressive strain state along the c-axis.

Full Text

Effect of AlN Nucleation Layer Thickness on GaN Epitaxial Quality on Si(111)

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Abstract

GaN thin films were grown on Si(111) substrates using metal-organic chemical vapor deposition (MOCVD) with a low-temperature AlN nucleation layer. The influence of AlN nucleation layer thickness on the GaN epitaxial layer was investigated using high-resolution X-ray diffraction, spectroscopic ellipsometry, and atomic force microscopy. Measurements of the AlN layer revealed that its surface roughness increases with thickness. Characterization of the GaN films showed that all samples were under compressive strain in the vertical direction, which slightly decreased with increasing AlN thickness. The full width at half maximum (FWHM) of the GaN (0002) -scan increased slightly with AlN nucleation layer thickness, while the FWHM of the GaN (10-12) -scan decreased with thickness. The FWHM of the (10-12) -scan correlates with the edge-type threading dislocation density in GaN, indicating that thicker AlN nucleation layers reduce edge-type threading dislocation density and alleviate compressive strain along the c-axis.

Keywords: GaN; AlN nucleation layer; Si substrate; MOCVD

1. Introduction

GaN-based third-generation semiconductor buffer layers offer numerous advantages, including wide bandgap, high breakdown field, high thermal conductivity, corrosion resistance, and radiation hardness. In particular, AlGaN/GaN heterostructures exhibit high-density, high-mobility two-dimensional electron gas (2DEG), making wide-bandgap semiconductors ideal for microwave power devices. One factor limiting the quality and cost of GaN-based devices is the substrate material. While SiC substrates are commercially available, they remain expensive. Sapphire substrates are non-conductive, limiting their applications. In contrast, Si substrates are inexpensive and enable potential integration of GaN devices with existing Si-based electronics. Consequently, GaN growth on Si(111) has attracted significant attention in recent years, with continuously improving crystalline quality. However, Si substrates suffer from large lattice mismatch (17%) and thermal mismatch (56%) with GaN[1], leading to crack formation on the GaN surface when the epitaxial layer exceeds the critical thickness[2].

To achieve high-quality GaN on Si, researchers have explored various nucleation layers. Low-temperature GaN (LT-GaN) nucleation layers were initially used on sapphire and SiC substrates but are unsuitable for Si. The temperature ramp-up required for high-temperature GaN growth promotes decomposition of LT-GaN, and Ga metal reacts with Si to form alloys that roughen the substrate surface and degrade GaN crystalline quality[3,4]. Besides LT-GaN, other nucleation layers have been investigated, including porous Si[4,5], SiNx[6,7], 3C-SiC[8,9], AlAs[10,11], GaAs[12], -Al2O3[13], and AlN[14]. Since Al-N bonds form more readily than Si-N bonds, AlN nucleation layers can suppress the formation of polycrystalline SiNx, thereby improving GaN crystal quality. Additionally, AlN layers exhibit better thermal stability than LT-GaN. Therefore, AlN is commonly employed as the nucleation layer for GaN epitaxy on Si[15-19].

In this work, we investigate the influence of AlN nucleation layer thickness on the crystal quality and strain state of GaN epitaxial layers grown by metal-organic chemical vapor deposition (MOCVD), using high-resolution X-ray diffraction (HRXRD), atomic force microscopy (AFM), and spectroscopic ellipsometry.

2. Experimental Details

The GaN samples were prepared using a Veeco D180 metal-organic chemical vapor deposition (MOCVD) system. Two-inch Si(111) substrates (n-type, resistivity 1-15 $\Omega \cdot$cm, thickness 430 m) were cleaned prior to growth to remove surface contaminants. The cleaning process consisted of ultrasonic cleaning in acetone and absolute ethanol for 8 minutes each to remove organic contaminants, followed by cleaning in Solution No. 1 (NH3$\cdot$H2O:H2O2:H2O) to remove acidic contaminants, and finally cleaning in Solution No. 2 (HCl:H2O2:H2O = 1:2:7) to remove alkaline contaminants. Immediately before loading into the reactor, the substrates were rinsed with diluted HF solution. Trimethylgallium (TMGa) and trimethylaluminum (TMAl) served as Ga and Al sources, respectively, while high-purity ammonia (NH3) was used as the N source. No intentional doping was performed. The substrates underwent high-temperature pretreatment at 1100°C for 10 minutes to remove native SiO2, followed by annealing to 980°C for AlN nucleation layer growth. The TMAl flow rate was maintained at 200 sccm, growth pressure at 100 torr, and NH3 flow at 4 slm. Three different AlN nucleation layer thicknesses were obtained by varying the growth time. To minimize experimental uncertainties, two samples were grown for each AlN thickness: one for characterization and another for subsequent GaN epitaxy. After growth, AlN nucleation layer thickness was measured using an MD2000D spectroscopic ellipsometer, and surface morphology was characterized with a Veeco Dimension 3100 atomic force microscope (AFM). GaN epitaxial layers were then grown on these AlN nucleation layers under identical conditions.

GaN epitaxy was performed at 1000°C and 200 torr, yielding an approximately 2.5 m thick layer. The grown GaN samples were characterized using a Bruker D8 Discover high-resolution X-ray diffraction (XRD) system. Double-crystal -scans and triple-crystal -2 rocking curves were measured. The full width at half maximum (FWHM) of the (0002) and (10-12) reflections obtained from -scans was used to evaluate GaN crystal quality. The -2 scans provided the primary and secondary diffraction peak positions of the GaN (0002) plane, enabling calculation of the c-axis lattice constant and vertical strain state.

3. Results and Analysis

[Figure 1: see original paper] presents the measured AlN thicknesses. AlN layers grown for 10, 20, and 30 minutes exhibited thicknesses of 38 nm, 66 nm, and 108 nm, respectively. Linear fitting closely matches the measured trend, indicating an AlN growth rate of 2.3 nm/min under the conditions of 200 sccm TMAl flow, 4 slm NH3, and growth times between 10-40 minutes.

[Figure 2: see original paper] shows the relationship between AlN surface roughness and thickness.

Experiments revealed that AlN surface roughness (RMS) increases with growth time. Previous studies have shown that AlN experiences compressive stress during initial epitaxy on Si, which gradually transitions to tensile stress[4]. Compressive stress facilitates AlN adatom migration, whereas tensile stress reduces it[3,4]. Under tensile stress, island growth mode is promoted, leading to increased AlN surface roughness (RMS). [Figure 3: see original paper] displays the surface morphology of AlN layers grown for different durations, with a scan area of 2 m × 2 m. The RMS roughness values for 10, 20, and 30 minute growth times were 1.86 nm, 2.33 nm, and 6.73 nm, respectively. The images show that AlN nucleation islands grow larger and begin to coalesce with increasing growth time.

[Figure 4: see original paper] illustrates the relationship between AlN thickness, GaN -scan FWHM values for the (0002) and (10-12) planes, and surface roughness. The GaN (0002) FWHM values for AlN thicknesses of 38 nm, 66 nm, and 108 nm were 752 arcsec, 760 arcsec, and 796 arcsec, respectively, while the corresponding GaN (10-12) FWHM values were 1412 arcsec, 1398 arcsec, and 1366 arcsec. The (0002) FWHM increases with AlN nucleation layer thickness, which is generally associated with screw-type threading dislocation density[20]. GaN has a mosaic structure, and screw-type threading dislocations are related to tilt between GaN crystallites[21]. Increased AlN thickness roughens the AlN surface, degrading GaN orientation and likely enhancing crystallite tilt, thereby increasing screw-type threading dislocation density. Conversely, [Figure 6: see original paper] shows that the (10-12) FWHM decreases with AlN thickness. As noted earlier, thicker AlN promotes island growth mode, increasing surface roughness and island density. Since GaN nucleates on the top surfaces of AlN islands[22], higher AlN island density provides more GaN nucleation sites. GaN nucleation also proceeds via island growth[23], and higher island density enables more edge-type threading dislocations to bend and annihilate during coalescence[28].

AlN thickness also affects the strain state of GaN. Vertical strain in GaN is reflected in the lattice constants, which were measured using triple-crystal -2 scans. [Figure 5: see original paper] shows the -2 scan results, with the first peak corresponding to the GaN (0002) diffraction and the second peak to the GaN (0004) diffraction (the second-order reflection of (0002)). The c-axis lattice constant, which equals the (0001) interplanar spacing d0001, can be calculated from the two peak angles using Equation (1)[23]:

000100020004242sin()2sin()d

where is the X-ray wavelength (CuK 1 = 0.154186 nm), 0002 and 0004 are the measured Bragg diffraction angles, and Δ is the zero-point error of the XRD system, which was determined to be -0.03° using this equation.

[Figure 6: see original paper] shows the calculated c-axis lattice constant as a function of AlN thickness and surface roughness. The c-axis lattice constants for AlN nucleation layers of 38 nm, 66 nm, and 108 nm were 0.5179 nm, 0.5181 nm, and 0.5182 nm, respectively. The unstrained GaN lattice constant is 0.5185 nm. The strain state for each sample was calculated using Equation (2)[24], yielding values of -0.11%, -0.077%, and -0.057%, all negative, confirming that the GaN epitaxial layers were under compressive strain in the vertical direction.

The measurements demonstrate that increasing AlN nucleation layer thickness expands the c-axis lattice constant and reduces vertical strain, indicating that thicker AlN layers help alleviate compressive strain along the GaN c-axis. 00epiccec

4. Conclusion

This study investigated the influence of AlN nucleation layer thickness on GaN epitaxial layer crystal quality. As growth time increased, both AlN thickness and surface roughness increased. The increased AlN surface roughness led to higher screw-type threading dislocation density, likely due to enhanced tilt and degraded orientation of GaN crystallites. Conversely, increasing AlN thickness reduced edge-type threading dislocation density, possibly because higher surface roughness indicates greater AlN island density. Since GaN nucleates on the top surfaces of AlN islands, higher AlN island density provides more GaN nucleation sites. GaN grows in an island mode, and the coalescence of these islands promotes bending and annihilation of edge-type threading dislocations. Furthermore, increasing AlN thickness reduced compressive strain along the GaN c-axis, demonstrating that thicker AlN layers help relieve compressive strain in GaN epitaxial layers.

References

[1] XING Yan-hui, HAN Jun, DENG Jun, etal. Properties of the InGaN: Mg with roughened surface and high hole concentration and its light-emitting diode application[J]. Journal of Optoelectronics • Laser, 2011,22(5):666-668

[2] Srinivasan R, Redwing J M. Growth stresses and cracking in GaN films on (111)Si grown by metal-organic chemical-vapor deposition. I. AlN buffer layers[J]. Appl. Phys. Lett,2005,98:0235141-0235149

[3] XING Yan-hui, LI Ying-zhi, HAN Jun, etal. Scanning electron acoustic microscopy and electron backscattering diffraction study of GaN/Al2O3 heteroepitaxial layer film[J]. Journal of Optoelectronics•Laser. 2012,23(10): 1909-1912

[4] Zhang B S, Wu M, Shen X M, etal. Influence of high-temperature AlN buffer thickness on the properties of GaN grown on Si(111)[J]. J. Cryst. Growth,2003, 258(1):34-40

[5] Matoussi A, Boufaden T, Missaoui A. Porous silicon as an intermediate buffer layer for GaN growth on (100) Si[J]. Microelectron. J, 2001,32(12) :995-998.

[6] Kang T W, Park S H, Kim T W. Improvement of the crystallinity of GaN epitaxial layers grown on porous Si (100) layers by using a two-step method [J] J. Mater. Res, 2000, 15(12): 2602-2605.

[7] Masao Tamura, Maximo López-lópez, Tokuo Yodo. Effects of the substrate tilting angle on the molecular beam epitaxial growth of GaAs on Si(110)[J]. J. Vac. Sci. Technol. B, 2000, 19(4):1567-1571

[8] Nakada Y, Aksenvo I, Okumura H. GaN heteroepitaxial growth on silicon nitride buffer layers formed on Si (111) surfaces by plasma-assisted molecular beam epitaxy[J] Appl. Phys. Lett, 1998,73(6):827-830.

[9] Sanchez-Garcia M A, Ristic J, Calleja E, etal. Characterization of GaN quantum discs embedded in AlxGa1-xN nanocolumns grown by molecular beam epitaxy[J] Phys. State Sol. A, 2002, 68(12):192-198

[10] Park C I, Kang J H, Kim K C, etal. Characterization of GaN thin film growth on 3C-SiC/Si(111) substrate using various buffer layers[J] J. Crystal Growth,2001, 224(1):190-194

[11] Strittmatter A, Bimberg D, Krost A, etal. Structural investigation of GaN layers grown on Si(111) substrates using a nitridated AlAs buffer layer[J] J. Crystal Growth, 2000, 221(1):293-296.

[12] Strittmatter A, Krost A, Stra-Xburg M, etal. Low-pressure metal organic chemical vapor deposition of GaN on silicon(111) substrates using an AlAs nucleation layer[J] Appl. Phys. Lett,1999,74(9) :1242-1244.

[13] Yang J W, Sun C J, Chen Q, etal. High quality GaN-InGaN heterostructures grown on (111) silicon substrates[J] Appl. Phys. Lett, 1996, 69(23):3566-3568.

[14] Kobayashi N P, Kobayashi J T, Dapkus P D, etal. GaN growth on Si(111) substrate using oxidized AlAs as an intermediate layer Appl. Phys. Lett, 1997,71(24):3569-3571.

[15] Gagnon J C, Tungare M, WENG Xiao-jun, etal. In situ stress measurements during GaN growth on ion-implanted AlN/Si substrates[J]. Journal of Electronic Materials. 2012, 41(5):865-872

[16] Yushamdan Y, Yusoff M Z, Ainorkhilah M,etal. The investigation of porous AlxGa1-xN layers on Si (111) substrate with GaN/AlN as buffer layer[J]. Advanced Materials Research.2012, 364(1):164-168

[17] Medjdoub F, Zegaoui M, Ducatteau D, etal. High-performance low-leakage-current AlN/GaN HEMTs grown on silicon substrate[J]. IEEE Electron Device Letters.2011,32(7):874-876

[18] Yusoff M Z, Hassan Z, Azzafeerah M, etal. Structural characterization of AlN and AlGaN layers grown on GaN/AlN/Si 111 by plasma-assisted MBE[A]. ISBEIA 2011 - 2011 IEEE Symposium on Business, Engineering and Industrial Applications[C]. Malaysia : IEEE Computer Society, 2011,554-557

[19] Arulkumaran S, Vicknesh S, Selvaraj S L,etal. High vertical breakdown strength in with low specific on-resistance AlGaN/AlN/GaN HEMTs on silicon[J]. Physica Status Solidi - Rapid Research Letters. 2011,5(1):37-

[20] Watanabe A, Takeuchi T, Hirosawa K. Growth of single crystalline GaN on a Si substrate using AlN as an intermediate layer [J] J. Cryst. Growth, 1993, 128(1):391-396.

[21] Zheng X H, Wang Y T, Feng Z H. Method for measurement of lattice parameter of cubic GaN layers on GaAs (001) [J]. J. Cryst. Growth, 2003,250(1):345-348

[22] XING Yan-hui, HAN Jun, DENG Jun, etal. Improved properties of light emitting diode by rough p-GaN grown at lower temperature[J]. Acta Phys. Sin. ,2010,59(2):1233-1236

[23] XU Zhen-jia. Semiconductor Detection and Analysis [M].Beijing: Science Press(second edition).2007

[24] HAN Jun, FENG Lei, XING Yan-hui, etal. Investigation of effects of source flux on the properties of p-GaN flim grown by MOCVD[J]. Journal of Optoelectronics・Laser. 2012, 23(4): 708-711

[25] Krost, Dadgar, Blasing. Evolution of stress in GaN heteroepitaxy on AlN ⁄Si(111): From hydrostatic compressive to biaxial tensile[J]. Appl. Phys. Lett, 2004, 85(16):3441-3443

[26] Chen J, Zhang S M, Zhang B S. Influences of reactor pressure of GaN buffer layers on morphological evolution of GaN grown by MOCVD[J]. J.Cryst.Growth,2003, 256(1):248-253

[27] Wu M F, Vantomme A, Pattyn H. Comprehensive Rutherford backscattering and channeling study of ion-beam-synthesized ErSi1.7 layers [J] . J. Appl. Phys, 1996, 80 (10):5713-5717.

[28] Feng Lei, HAN Jun, XING Yan-hui, etal. Optimized growth and composition investigation of AlGaN materials with high Al composition[J]. Journal of Optoelectronics・Laser, 2012, 23(9): 1754-1760.

[29] SHAO Hui-min, ZHANG Shi-lin, XIE Sheng, etal. Research of AlGaN/GaN PIN solar-blind ultraviolet photodetector with back-illumination[J]. Journal of Optoelectronics・Laser, 2011, 22(7): 984-986

[30] DALAI Mu-ren, YAN Zu-wei, SHI Lei. Effects of hydrostatic pressure and external electric field on the impurity binding energy in strained GaN/AlxGa1-xN spherical quantum dots[J]. Optoelectronics Letters, 2012,8(3):0224-0228

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