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Epitaxial growth of cubic GaN and AlN on Si(001)

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Abstract

Thermal treatment under propane at 1300-1400 °C has been used to prepare Silicon (001) wafers for subsequent growth of cubic GaN and AlN by Electron Cyclotron Resonance Plasma Assisted Molecular Beam Epitaxy (ECRMBE). Thermal treatment of Silicon wafers under propane, used in this experiment, produced a very thin (40 Å) layer of cubic SiC on the Silicon (001) surface. Despite an extremely low thickness of as-produced SiC layer, high quality cubic GaN has been successfully grown. The cubic form of AlN grown on the SiC(40Å)/Si(001) surface has also been observed despite a very high density of stacking faults.

1. Introduction

Silicon is one of the most attractive substrates for the future implementation of GaN and/or AlN -based devices, allowing integration of silicon based circuits on the same substrate. However, during the growth of GaN, one has to face serious problems: GaN can occur in either the hexagonal (wurtzite) or the cubic (zincblende) structures, and both polytypes often appear in the same epitaxial layer, leading to stacking faults. Moreover, GaN has a large lattice mismatch to substrates currently used in microelectronics like Si and GaAs (16.6% and 19.9% respectively). GaN films have been grown epitaxially on Si(001) by Electron Cyclotron Resonance Microwave Plasma-Assisted Molecular Beam Epitaxy (ECR-MBE) using a thick SiC buffer layer [1] [2]. Direct growth of GaN on a clean Si(001) 2x1 surface results in highly polycrystalline material; the case for which true epitaxy has been observed is for the growth on Si(001) surface covered by small crystallites of SiC formed during the Si(001) substrate annealing [3], and on the unreconstructed (i.e., 1x1) Si(001) surface [4] [5] . However, in the reflection high-energy electron diffraction (RHEED) image of an unreconstructed Si(001) surface [4] [5] one can clearly observe the spots characteristic of the presence of cubic SiC crystallites. Cubic GaN grown on the Si(001) surface covered by SiC crystallites has some misoriented domains [4] and the full width at half-maximum (FWHM) of the x-ray rocking curve of the (002) peaks of 4 and 1 µm thick films of GaN are as wide as 60 and 90 min. respectively [4].

In the present paper we report growth of cubic GaN and AlN on the Silicon (001) surface covered by a very thin (40 Å) epilayer of SiC. This thin epilayer of SiC is produced on the Silicon (001) surface by thermal treatment of Si(001) substrates under propane at 1300-1400 °C. The results described below clearly show that high quality cubic GaN can be successfully grown using this relatively simple procedure for the Silicon (001) surface preparation. The quality of as grown GaN is comparable to the quality of GaN grown on a thick SiC buffer layer obtained by CVD SiC epitaxy on Silicon [2].

Cubic AlN has been grown on Si(001) and Si(111) by Pulsed Laser Ablation [6]. To our best knowledge this is the first report of the use of thermal treatment of Silicon wafers under propane for the successful growth of cubic GaN and AlN by ECRMBE.

2. Experimental details

The GaN and AlN films were grown in a RIBER MBE 2300 chamber. The home-made 2.45 GHz ECR plasma source used in this experiment has been described elsewhere [7]. Molecular nitrogen was supplied to produce active nitrogen species via the plasma source. Conventional Knudsen effusion cells were used for the gallium and aluminum evaporation (Ga, Al 7N). The substrates used in this study were p-type boron-doped (15 Ohm/cm) Si(001) covered by a thin (40 Å) SiC layer. The SiC layer was obtained by thermal treatment of Si(001) substrates at

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1300-1400°C under propane [8].

Prior to the GaN and/or AlN growth the Si(001) substrates covered by a SiC(40Å) layer were outgassed in the MBE chamber at 850 °C for 30 minutes. The growth temperatures for GaN and AlN were respectively 640° and 720°C. A He-Cd laser was used for low temperature (9K) photoluminescence studies.

3. Results

Reflection high-energy electron diffraction (RHEED) observations prior to GaN growth give information about the structural quality of SiC(40Å)/Si(001) substrates. A three dimensional character of the SiC surface can be deduced from large spots observed in RHEED images in (100) and (110) directions. The GaN deposited at 640°C on the SiC(40Å)/Si(001) surface exhibits a three dimensional growth mode up to 0.2 µm thickness. However, at this stage of growth, RHEED observations in (100) and (110) directions show the beginning of appearance of two-dimensional diffraction rods. For a GaN epilayer thickness of about 1.5 µm the RHEED image shows a two-dimensional growth mode. The evolution of the film quality along the growth direction was also reflected by the width of X-ray diffraction scans. For GaN thickness of 0.25 µm, the X-ray rocking curve of a (002) scan exhibits a full width at half-maximum (FWHM) of about 55 minutes, and respectively 40 and 25 minutes for thickness of 1.3 and 1.7 µm. Lei et al. [4] reported the FWHM of 60 and 90 min. for respectively 4 µm and 1 µm thick samples grown on the unreconstructed 1x1 Si(001) surface. By introducing a very thin layer of SiC on the Si(001) by a simple treatment of the Silicon surface under propane we were able to considerably improve the quality of GaN films. Our results are comparable with those reported by Okumura et al. [2]. For 1 µm thick GaN grown on SiC Okumura reported a FWHM of 24 min. The epitaxial relationship of GaN and SiC to Si(001) deduced from RHEED pattern observation and X-ray diffraction in our samples is: GaN(001)[1 0 0]//SiC (001)[1 0 0]//Si (001)[1 0 0].

The local microstructure of our epilayers was characterized by High Resolution Transmission Electron Microscopy (HRTEM). Samples were prepared in cross-section using standard mechanical polishing and ion-milling techniques. Microscopy was performed with a JEOL 4000 EX microscope. The HRTEM image presented in Figure 1 gives more information about the quality of as-grown cubic GaN. The interface between the SiC layer and GaN is not flat, in agreement with the three dimensional character of the RHEED pattern of the SiC surface prior to GaN growth (as described above). Stacking faults propagating along the {111} planes appear to be the major form of strain relief in GaN as observed in growth of cubic GaN on GaAs and MgO substrates [9] [10] . In some cases stacking faults annihilate at their intersections and their density decreases away from the interface. Double stacking faults leading to appearance of micro-twins can also be observed in our GaN samples. The first stacking fault changes the stacking sequence from ABCABC to CBACBA, the second one re-induces the initial ABCABC sequence. These structural faults almost disappear for epilayer thickness of about 1.5 µm.

Figure 2 shows the low temperature (9K) photoluminescence spectrum of cubic GaN. Strong, near band-edge transitions dominate; the intensity of the so called yellow band observed between 500 and 700 nm is about 1000 times lower than the intensity of near band-edge emissions. In a logarithmic scale plot shown in inset in Figure 2 five peaks can be distinguished. We tentatively attribute the peaks at 3.254 eV, at 3.180 eV and at 3.085 eV to optical transition of cubic GaN. Peaks at respectively 3.471 and 3.392 eV can be attributed to some fraction of the wurtzite phase [11].

The Transmission Electron Microscopy (TEM) observations of AlN grown on SiC(40Å)/Si(001) substrate are shown in Figure 3. The AlN grows on SiC/Si(001) as a mixture of cubic and wurtzite phases. The electron diffraction pattern of the AlN/SiC/Si(001) sample presented in Figure 3 (a) indicates that the cubic form of AlN dominates, but its shape reveals a high degree of disorientation and a high density of stacking faults. The surface of an AlN layer about 700-800 Å thick is almost flat but the TEM image shown in Figure 3 (b) reveals a high density of stacking faults near the interface and close to the surface of the epilayer.

4. Conclusion

A 40 Å thick epilayer of cubic SiC obtained on a Si(001) surface by high temperature treatment of silicon substrates under propane has been used as starting surface for epitaxy of cubic GaN and AlN. Optical properties of as-grown cubic GaN are dominated by near band edge transitions. The AlN grows on the SiC(40Å)/Si(001) surface as a mixture of the cubic and hexagonal forms. The cubic form of AlN dominates despite a high density of stacking faults. Silicon covered by an epilayer of Silicon Carbide as thin as 40 Å, produced by thermal treatment of Silicon wafers under propane, appears to be a very promising substrate for successful growth of cubic Gallium Nitride; this is the most important result of our experiments. Thermal treatment of Silicon substrates under propane at 1300-1400 °C is a relatively simple procedure, much simpler than the growth of a thick SiC buffer layer on Si(001) by CVD.

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References

[1] M. J. Paisley, Z. Sitar, J. B. Posthill, R. F. Davis , *J. Vac. Sci. Technol. A* ***7***, 701-705 (1989).

[2] H Okumura, S Misawa, T Okahisa, S Yoshida, *J. Cryst. Growth* ***136***, 361-365 (1994).

[3] U. Rossner, A. Barski, J. L. Rouviere, A. Bourret, J. Massies, C. Deparis, N. Grandjean, *Mater. Sci. Eng. B* ***29***, 74 (1995).

[4] T. Lei, T. D. Moustakas , R. J. Graham , Y. He, S. J. Berkowitz , *J. Appl. Phys.* ***71***, 4933-4943 (1992).

[5] T. D. Moustakas, T. Lei, R. J. Molnar, *Physica B* ***185***, 36-49 (1993).

[6] WT Lin, LC Meng, GJ Chen, et al., *Appl. Phys. Lett.* ***66***, 2066-2068 (1995).

[7] U. Rossner, D. Brun-Le Cunff, A. Barski, B. Daudin, *J. Vac. Sci. Technol. A* ***14***, 2655 (1996).

[8]N. Becourt, Ph. D. Thesis, Montpellier, unpublished (1993).

[9] S. Strite , J. Ruan , Z. Li , A. Salvador , H. Chen , David J. Smith , W. J. Choyke , H. Morkoc , *J. Vac. Sci. Technol. B* ***9***, 1924-1929 (1991).

[10] R. C. Powell, N.-E. Lee, Y.-W. Kim, J. E. Greene , *J. Appl. Phys.* ***73***, 189-204 (1993).

[11]O. Brandt, H. Yang, and K. H. Ploog, Semiconductor Heteroepitaxy, Growth, Characterization and Device Applications, Montpellier, France 4-7 July 1995, Published by World Scientific Co. Pte. Ltd.

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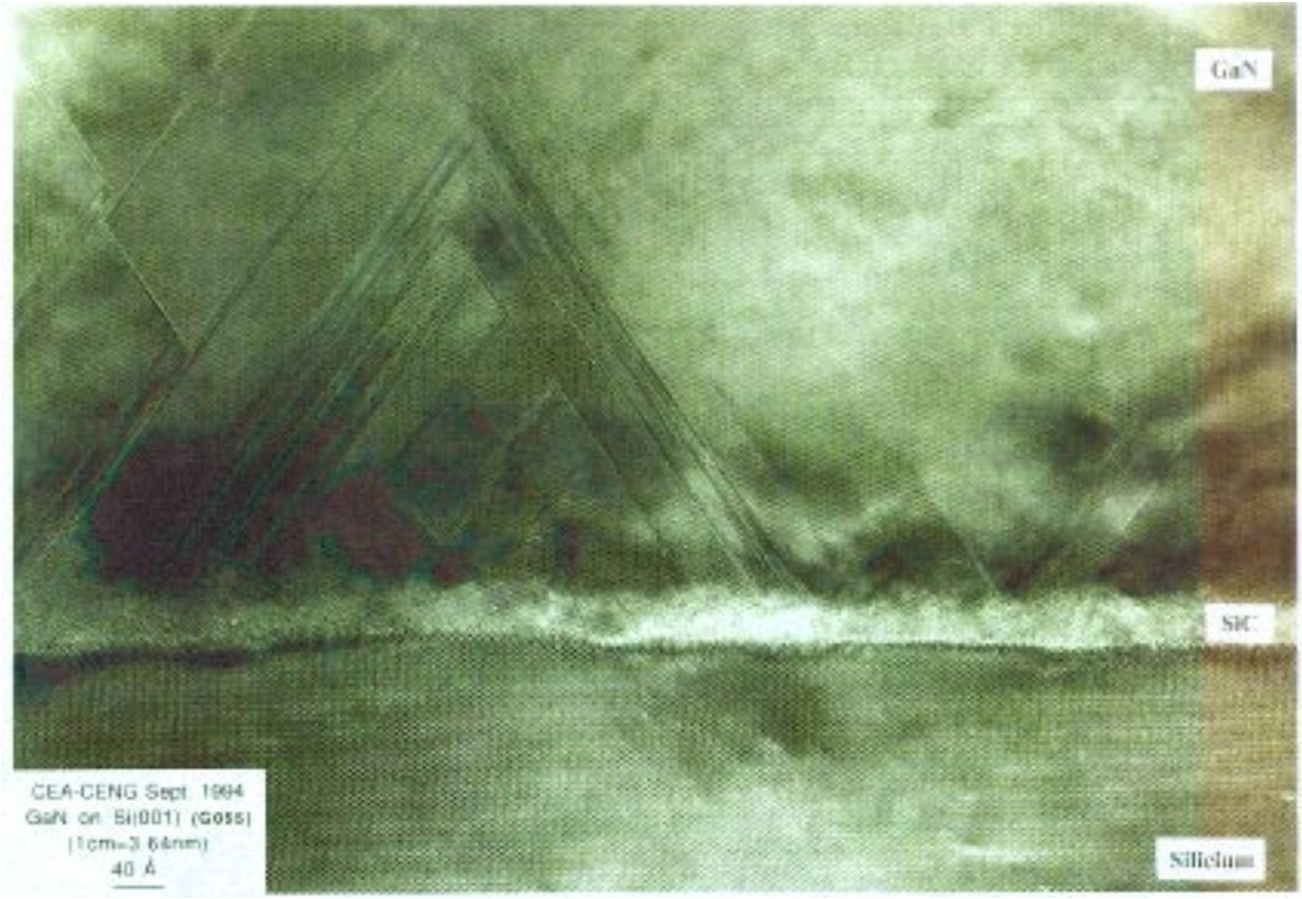

Figure 1. HRTEM image of cubic GaN grown on a SiC(40Å)/Si(001) substrate.

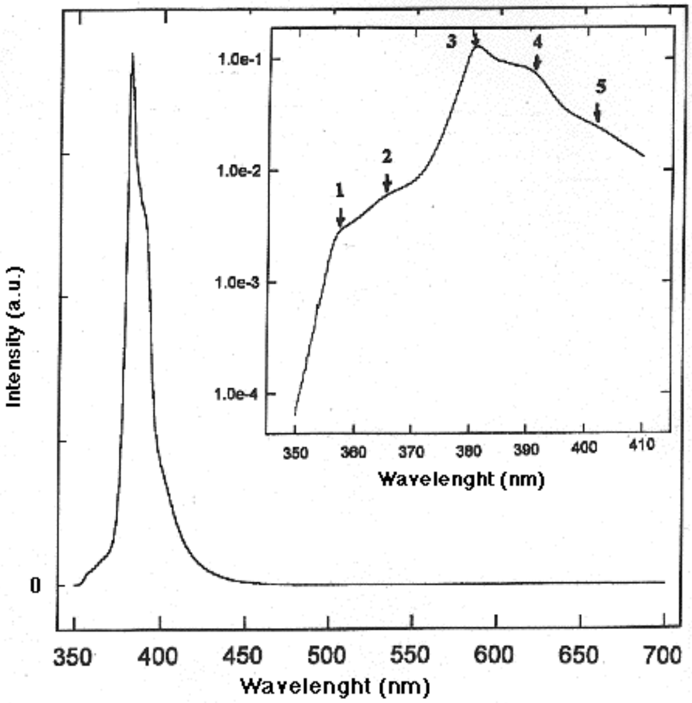

Figure 2. Low temperature (9K) photoluminescence spectrum of cubic GaN. In the inset is shown the photoluminescence (9K) spectrum in the near-bandedge part of the emission. Peaks labeled 1 to 5 are respectively at : 3.471 eV (357.2 nm); 3.392 eV (365.6 nm); 3.254 eV (381.1 nm); 3.180 eV (389.9 nm) and 3.085 eV (402 nm).

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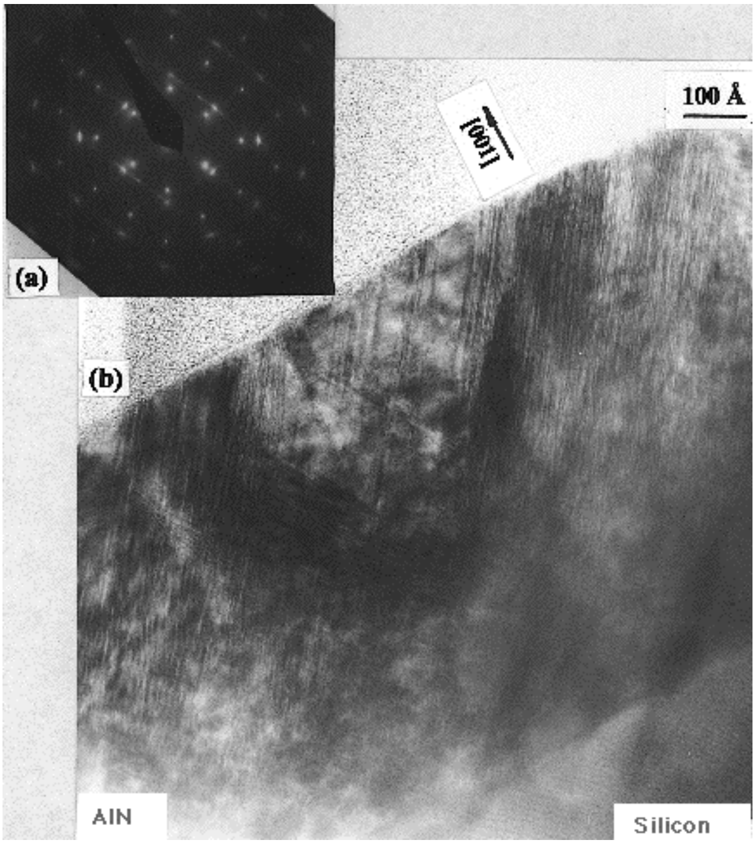

Figure 3. TEM image of AlN grown on a SiC (40Å)/Si(001) substrate. (a) electron-diffraction pattern of an AlN/SiC/Si(001) layer, (b) TEM observation of an AlN/SiC/Si(001) sample in the [1 -1 0] direction.

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