Atomic layer deposition of Sc$_2$O$_3$ for passivating AlGaN/GaN high electron mobility transistor devices

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Polycrystalline, partially epitaxial Sc$_2$O$_3$ films were grown on AlGaN/GaN substrates by atomic layer deposition (ALD). With this ALD Sc$_2$O$_3$ film as the insulator layer, the Sc$_2$O$_3$/AlGaN/GaN metal-insulator-semiconductor high electron mobility transistors showed excellent electrical performance with a high $I_{on}/I_{off}$ ratio of over $10^8$ and a low subthreshold slope of 75 mV/dec. The UV/NH$_4$OH surface treatment on AlGaN/GaN prior to ALD was found to be critical for achieving these excellent figures. In addition, the Sc$_2$O$_3$ dielectric is found to be negatively charged, which facilitates the enhancement-mode operation. While bare Sc$_2$O$_3$ suffers from moisture degradation, depositing a moisture blocking layer of ALD Al$_2$O$_3$ can effectively eliminate this effect. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4770071]

Gallium-nitride based high electron mobility transistors (HEMTs) are promising for high frequency switches and high power devices. However, typical AlGaN/GaN HEMTs rely on Schottky gates, which suffer from high gate leakage and impose a limit on the maximum gate bias that can be applied to the device. Applications for power electronics require low leakage in the off-state and large voltage swings, and thus it is necessary to fabricate devices with a gate dielectric, i.e., metal-insulator-semiconductor (MIS)-HEMTs. Atomic layer deposition (ALD) of high-$k$ dielectrics, such as HfO$_2$ and Al$_2$O$_3$, is a promising technique for depositing gate dielectrics due to its precise control of the film thickness. These ALD oxides have very low leakage, and their high-$k$ dielectric constant ensures an effective channel modulation by the gate, even with relatively large dielectric thickness. In addition, the accurate thickness control allowed by ALD enables ultra-smooth conformal films without pinholes.

Scandium oxide (Sc$_2$O$_3$) is another high-$k$ oxide material that has also been reported to form a good gate dielectric for AlGaN/GaN MIS-HEMTs and to mitigate current collapse. Sc$_2$O$_3$ has a dielectric constant of 14 and a band gap of 6.3 eV with high conduction and valence band offsets. Crystalline Sc$_2$O$_3$ exists in a cubic bixbyite crystal structure with a mismatch of 9% in its (111) orientation parallel to the GaN (0001) plane. In early reports, the Sc$_2$O$_3$ was mainly prepared by molecular beam epitaxy (MBE) in a high-vacuum chamber, and a heteroepitaxy of Sc$_2$O$_3$ on GaN with a relationship of (111) $\times$ [110]$_{\text{Sc}_2\text{O}_3}//(0001) \times [1120]_{\text{GaN}}$ was achieved under certain growth conditions. The heteroepitaxy was considered to be beneficial for good electrical properties, as it tends to minimize the density of surface dangling bonds that could be a source for surface states on the GaN.

However, despite the high quality of MBE films, MBE is difficult to scale up due to cost and technical reasons. In this letter, we report promising electrical performance of ALD Sc$_2$O$_3$ thin films on AlGaN/GaN devices. These Sc$_2$O$_3$ films are partly epitaxial, polycrystalline films with some mis-oriented grains. The fabricated devices have excellent sub-threshold slopes and high $I_{on}/I_{off}$ ratios. The proposed ALD of Sc$_2$O$_3$ dielectrics on GaN-based transistors is very promising, as it combines the excellent properties of Sc$_2$O$_3$ dielectrics with the large-scale of ALD equipment.

The ALD of Sc$_2$O$_3$ was carried out in a home-built tubular reactor. Scandium tris(N,N'-diisopropylacetamidinate) and H$_2$O were used as scandium and oxygen sources, respectively. The scandium precursor was kept in a sealed bubbler in an oven heated to 160 °C, and was delivered into the reaction chamber with N$_2$ carrier gas. Si(100) and (111) wafers were used for characterizing the Sc$_2$O$_3$ growth. Each Si wafer was treated with UV light for 5 min and then dipped into a dilute H$_2$O solution for 30 s before being loaded into the deposition chamber. The Sc$_2$O$_3$ deposition was performed at substrate temperatures from 300 °C to 360 °C. The growth rate was 0.03 nm/cycle at 300 °C, and increased to 0.07 nm/cycle at 360 °C. Detailed descriptions of the deposition process can be found in our previous report. Transmission electron microscopy (TEM) was used to examine the crystallinity of the as-deposited Sc$_2$O$_3$ films. As shown in Figure 1, the top-view and cross-sectional-view TEM images clearly show the polycrystalline structure of the Sc$_2$O$_3$ films deposited on a Si$_N_x$ TEM grid and a Si(111) substrate, respectively. The corresponding electron diffraction patterns (not shown here) matched well with the Sc$_2$O$_3$ bixbyite cubic phase. In addition, we noticed that epitaxial growth of Sc$_2$O$_3$ on Si (111) has been achieved by MBE, whereas polycrystalline films were deposited by our ALD method. This difference might be due to the formation of an ultra-thin layer of...
SiO$_2$ during the initial growth, and a similar phenomenon was observed in ALD growth of LaLuO$_3$ on Si (111) in our previous studies.

Sc$_2$O$_3$ was deposited on AlGaN/GaN substrates, which were later processed into HEMT devices for characterizing the electrical and transport properties. The AlGaN/GaN substrates were grown by metal-organic chemical vapor deposition (MOCVD) on sapphire single crystals, and the structure was composed of 0.8 nm of Fe-doped insulating GaN, 1.2 nm unintentionally doped GaN, 1 nm AlN, 17 nm AlGaN (28% Al), and finally a 2 nm GaN capping layer. The cross-sectional TEM image in Figure 2(a) shows that a highly textured polycrystalline Sc$_2$O$_3$ film was grown on AlGaN/GaN with a preferred growth orientation of (111). The majority of the Sc$_2$O$_3$ micro-grains were oriented in the direction (111)$_{\text{Sc}_2\text{O}_3}$//(0001)$_{\text{GaN}}$, e.g., the highlighted grains “A” and “B” in Figure 2(a). There were also a few grains showing a tilted orientation, e.g., the grain “C” in Figure 2(a). We also noticed that the slight difference in the lattice texture of the grains “A” and “B,” which suggested a relationship of in-plane rotation between the two grains. The TEM image also showed no observable interfacial layer between Sc$_2$O$_3$ and GaN. The preferred growth orientation was further examined by selective area electron diffraction (ED), as shown in Figure 2(b). Rather than diffraction rings, the ED pattern only shows scattered Sc$_2$O$_3$ diffraction spots, within which the spots with stronger intensity belong to Sc$_2$O$_3$(222) and (4-40). This again supported that the grains were highly oriented, and the preferred growth orientation had a relationship of (111) $\times [\bar{1}10]_{\text{Sc}_2\text{O}_3}//(0001)_{\text{GaN}}$ to the substrate. In addition, we also noticed a few relatively weak spots, circled in the ED pattern, that correspond to the misaligned micro-grains as shown in the TEM image (Figure 2(a)).

Sc$_2$O$_3$/AlGaN/GaN MIS-HEMT devices were fabricated for characterizing the electrical properties. The HEMT devices were fabricated on the same AlGaN/GaN substrate mentioned above. Ti/Al/Ni/Au ohmic metals were patterned, deposited, and annealed at 870 °C to form ohmic source/drain contacts. Then, mesa isolation was performed by etching with a Cl$_2$/BCl$_3$ plasma before deposition of the gate dielectric. In order to study the effect of surface treatment before the Sc$_2$O$_3$ deposition, some of the devices were first exposed to UV in air for 5 min, and then immersed in NH$_4$OH (aqueous, 15%) for 10 min, while some other samples were only treated with UV. Then 20 nm of Sc$_2$O$_3$ was deposited on top of the device samples at a temperature of 330 °C by 400 ALD cycles. After the Sc$_2$O$_3$ deposition, Ni/Au/Ni gates were deposited by e-beam evaporation and patterned by liftoff. Finally, the devices were annealed in forming gas at 400 °C for 30 s in order to improve the subthreshold slope and Ion/Ioff behavior.

Ambient moisture was found to have a noticeable impact on the electrical performance of the Sc$_2$O$_3$ devices as shown both in C-V (red curves in Figure 3) and I-V measurements (blue and green curves in Figure 4). Compared with the measured results in vacuum, the capacitance measured in air is higher and the threshold voltage is positively shifted. This is likely because the ambient water molecules diffuse through the grain boundaries of the Sc$_2$O$_3$ layer and reach the AlGaN surface and these molecules respond to AC signals through a process of ionization and deionization. Therefore, to avoid the effect of moisture, we performed our measurements in vacuum unless specified.

We also investigated the effect of the surface treatment of UV and UV/NH$_4$OH on AlGaN/GaN prior to the Sc$_2$O$_3$ deposition. Both UV and UV/NH$_4$OH treated Sc$_2$O$_3$/AlGaN/GaN HEMTs showed excellent transfer characteristics: the Ion/Ioff ratio of over $10^8$ and subthreshold slope of 75 mV/dec for the HEMTs with the NH$_4$OH treatment (Figure 4); while the HEMTs with the UV treatment showed slightly worse results with a subthreshold slope of 80 mV/dec and an Ion/Ioff ratio of $8 \times 10^7$ (not shown here). The electron mobility was
determined to be 2050 cm²/Vs, which is slightly higher than that of the AlGaN/GaN Schottky HEMTs, i.e., 2000 cm²/Vs. The threshold voltage for transistors with Sc₂O₃ dielectric is lower than for other high-k dielectrics. Additionally, Q-point pulsed I-V measurements were performed on the Sc₂O₃ HEMTs with and without the NH₄OH treatment, and the results are shown in Figure 5. The devices with NH₄OH treatment showed much less current collapse compared with the devices with only UV treatment. These results suggest that the surface treatment of AlGaN/GaN is crucial for obtaining good electrical properties, and the UV/NH₄OH pretreatment provides a better quality of the interface between oxide and AlGaN/GaN.

To prevent the effect from moisture, Gao et al. suggested adding a fluorocarbon layer as the moisture blocking layer. Here, we propose adding a thin layer of ALD Al₂O₃ on top of the Sc₂O₃ as the moisture blocking layer, since ALD Al₂O₃ is known to have low water permeability. We made capacitors with 10 nm Sc₂O₃ capped with 10 nm Al₂O₃ by in situ ALD. As the blue curves shown in Figure 3, the capacitors do not show any variation in 1 MHz C-V measurements whether in air or in vacuum. At the same time, the I_on/I_off ratio remains almost the same (Figure 4). This shows that the Sc₂O₃ surface can be effectively passivated by ALD Al₂O₃. Q-point pulsed I-V measurements on Al₂O₃/Sc₂O₃ HEMTs show almost the same results as Sc₂O₃ HEMTs, suggesting that the quality of the interface between Sc₂O₃ and AlGaN/GaN, rather than the top surface of Sc₂O₃, is the main determinant of the current collapse behavior. In addition, by integrating the 1 MHz C-V curves (Figure 6), one can obtain the carrier concentration in the channel. The Sc₂O₃ dielectric layer was found to be effective in helping to deplete carriers in the channel, which is necessary for enhancement-mode operation, while adding Al₂O₃ under the gate can increase the carrier concentration. This allows for reducing the carrier concentration from 8 × 10¹² cm⁻² with pure Al₂O₃ to 5 × 10¹² cm⁻² with pure Sc₂O₃ on a HEMT structure that has a carrier concentration of 6.5 × 10¹² cm⁻² without any gate oxide, resulting in reduced turn-on voltages. Coupled with the excellent subthreshold slope and high I_on/I_off ratio, Sc₂O₃ based oxides are very promising for AlGaN/GaN HEMTs for power applications.

In summary, we found that polycrystalline, partially epitaxial Sc₂O₃ films on GaN can be grown by ALD. This Sc₂O₃ layer provides a good interface with AlGaN/GaN, as the HEMT devices made from it showed a high I_on/I_off ratio of over 10⁸ and a low subthreshold slope of 75 mV/dec. The UV/NH₄OH surface treatment was found to be critical for achieving these excellent figures. While bare Sc₂O₃ suffers from moisture, adding a fluorocarbon layer or ALD Al₂O₃ on top of Sc₂O₃ provides a moisture-blocking layer.
from moisture degradation, depositing a moisture blocking layer of ALD Al₂O₃ can effectively eliminate this effect. The Sc₂O₃ dielectric is found to be negatively charged, which facilitates the enhancement-mode operation.

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