Effect of different substrates and growth conditions on nucleation and properties of κ- and β-Ga_2O_3 thin films grown by MOVPE

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Gallium Oxide (Ga_2O_3) is a wide-bandgap semiconductor that has been proposed for the next generation of high-power electronics devices and UVC solar-blind photodetectors. It can crystallize in different phases (α, β, γ, δ, and κ), with the monoclinic β being the thermodynamically stable and most investigated one. However, the metastable polymorphs have recently gained attention due to their higher crystallographic symmetry and peculiar physical properties. For example, the orthorhombic κ phase has a spontaneous polarization and ferroelectric behavior that could in principle be exploited for fabrication of heterostructures with a 2D electron gas.
In this work we studied the growth of Ga_2O_3 thin films using water and trimethyl-gallium as precursors with metal-organic vapour phase epitaxy (MOVPE) on sapphire and GaN/sapphire templates, at growth temperatures (T_g) of 610 °C and 650 °C.
In a previous work (1) we showed that by controlling the precursor supersaturation in the gas phase (i.e., the growth rate), it is possible to nucleate either κ- or β−Ga_2O_3. This is somewhat surprising as the β phase is normally reported to nucleate at much higher T_g. The structural properties of Ga_2O_3 were studied by XRD and HR-TEM. X-ray diffraction on films deposited on c-oriented sapphire indeed showed the co-existence of both phases at moderate supersaturation, while phase-pure β−Ga_2O_3 was achieved at extremely low supersaturation and T_g as low as 610 °C on sapphire. On the other hand, no phase-pure β−Ga_2O_3 was obtained under the same conditions on the GaN template. TEM investigation showed that films grown at 650 °C on sapphire contained both phases: pure κ up to a thickness of about 200 nm, followed by formation of 20-100 nm inclusions of β phase. Attention is focused on the strain of metastable κ-Ga_2O_3 phase due to i) substrate mismatch and ii) presence of β-Ga_2O_3 inclusions. Formation and effects of inclusions of β-Ga_2O_3 in mixed-phase material were also studied by TEM.
We shall discuss the obtained results considering the different lattice mismatch and interface energy between Ga_2O_3 films and Al_2O_3 or GaN, as well as the effective precursor supersaturation at different substrate sites.

References

[1] M. Bosi, L. Seravalli, P. Mazzolini, F. Mezzadri, R. Fornari, Thermodynamic and Kinetic Effects on the Nucleation and Growth of ε/κ- or β-Ga 2 O 3 by Metal–Organic Vapor Phase Epitaxy, Cryst. Growth Des. 21 (2021) 6393–6401; https://doi.org/10.1021/acs.cgd.1c00863.