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Band Gap and Phase Stability in $(Al_xGa_{1-x})_2O_3$ Alloy Films

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Gallium oxide is a transparent semiconductor (E_g = 4.8 eV) that exhibits n-type conductivity; it has been proposed for a variety of uses ranging from "solar-blind" conductive coatings to chemical sensing. An intriguing possibility is development of transparent, high power transistors based on carrier accumulation at an epitaxial Ga_2O_3–$(Al_xGa_{1-x})_2O_3$ alloy interface. Using pulsed laser deposition, composition-spread $(Al_xGa_{1-x})_2O_3$ thin films were fabricated on sapphire and silicon substrates, with x varying smoothly across the surface. Position-dependent X-ray diffraction revealed [-201]-oriented Ga_2O_3 on c-plane sapphire, and unoriented Ga_2O_3 on silicon with native oxide. Alloy $(Al_xGa_{1-x})_2O_3$ films on sapphire remain in the β-Ga_2O_3 phase for $x < 0.30$ then relax to the α-Al_2O_3 phase, whereas films on silicon remain in the β-Ga_2O_3 phase for $x < 0.35$ and then relax into the cubic γ-Al_2O_3 phase. Photoemission spectroscopy shows core and valence levels shifting to higher binding energy and decreasing work function, while spectroscopic ellipsometry reveals the absorption edge moving to higher photon energy, consistent with a widening band gap.

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