Investigation of doping-defect interaction in Si doped $(Al_xGa_{1-x})_2O_3$ integrating atom probe tomography and first principal calculation

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N-type doping is critical in ultra-wide bandgap $(Al_xGa_{1-x})_2O_3$ for achieving the theoretically predicted performance limit of high frequency devices. First principal density functional theory (DFT) result suggests that Si would be the most efficient donor among other group IV elements as it continues to act as a shallow donor at the highest range of Al content (85%) [1]. Although n-type doping in $(Al_xGa_{1-x})_2O_3$ using Si were reported experimentally, the dopant chemistry and defect interaction with varying alloy composition has not been established yet. A fundamental understanding on how dopant Si affects the structural chemistry of the films by defects formations and interacting with those defects when the alloy composition is varying needs in depth theoretical and experimental efforts.

The dopant interaction in $(Al_xGa_{1-x})_2O_3$ with Al content, x = 0.10-100% was studied by atom probe tomography (APT). Statistical radial distribution function (RDF) analysis on APT data was used to analyze the nearest neighbor chemistry to explain dopant interaction in $(Al_xGa_{1-x})_2O_3$. RDF analysis in layers with low Al (x = 0-20%) indicated Si is substituting in Ga sites and presence of V_{Ga}. This result implies the potential V_{Ga}-Si defect complex formation. At high Al (x = 60-100%), results suggested Al site occupancy with possible V_{Al}-Si complexes which would possibly results in dopant compensation in $(Al_xGa_{1-x})_2O_3$. First principal DFT calculation will be performed to verify the hypothesis developed from APT RDF analysis. The formation energy of V_{Ga}, V_{Ga}-Si, V_{Al} and V_{Al}-Si will be calculated in $(Al_xGa_{1-x})_2O_3$ layers with low (x = 10%) and high (x = 80%) Al content layers. The theoretical DFT verification of composition dependent cationic site preference for dopant Si atoms as well as formation of dopant-defect complex at different Al compositions would provide a conclusive evidence for the hypothesis presented based on APT analysis. The dominant defect types responsible for dopant compensation as the alloy composition varies will be unambiguously identified.

A detail understanding on how dopant Si affects the doped $(Al_xGa_{1-x})_2O_3$ matrix at low and high Al content in terms of preferential cationic site occupancy and formation of the dominant type of defect complex will be presented. This information would be beneficial for growing high quality films with efficient n-type doping and realizing high frequency devices.

Reference:

[1] J. B. Varley *et. al.*, Appl. Phys. Lett. **116**, 172104 (2020).