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# Understanding the Growth Mechanism of β-$(Al_xGa_{1-x})_2O_3$ by Atom Probe Tomography

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$(Al_xGa_{1-x})_2O_3$ is a promising material for high power electronics and optoelectronics due to its wide band gap, tunable between 4.8 eV (β-$Ga_2O_3$) and 8.7 eV (α-$Al_2O_3$) [1]. $(Al_xGa_{1-x})_2O_3$, being a potential new material, different growth techniques such as molecular beam epitaxy (MBE), pulsed laser deposition, mist chemical vapor deposition etc. [1] have been introduced to obtain high quality crystal growth. The growth mechanism of this material plays an important role in obtaining high crystal quality which in turn helps researchers to fabricate improved performance devices. Atom Probe Tomography (APT) is a powerful nanoscale analyzing tool that yields elemental information down to sub-nanometer resolution providing structural and compositional details of the material [2]. Here we have employed APT to understand the growth mechanism of β-$(Al_xGa_{1-x})_2O_3$ using plasma assisted MBE (PAMBE) system. Information thus obtained is crucial in explaining material growth and determining crystal quality for device implementations.

β-$(Al_xGa_{1-x})_2O_3$ samples with two different Al molar concentration of x = 0.2 (Fig. 1a) and 0.5 (Fig. 2a) were grown on β-$Ga_2O_3$ by PAMBE. Focused ion beam (FIB) milling technique was employed to prepare the APT needles. The needles were then investigated in CAMECA LEAP 5000X HR using a UV laser with pulse energy of 20 pJ, detection rate of 0.005 atoms/pulse and base temperature of 50 K. Typically, ternary alloys are subjected to alloy fluctuations during growth that degrades the crystal quality. To investigate if there is alloy inhomogeneity and understand it's origin, we have selected a series of volume starting from the $Ga_2O_3$ substrate to the bulk of β-$(Al_xGa_{1-x})_2O_3$ and performed 2D compositional distribution of Al. All the data for the composition reported here are in at.%, not in molar %. In both cases, Ga distribution within the substrate was found to be homogeneous (Fig. 1b-I and 2b-I). For all the volumes selected in bulk $(Al_{0.2}Ga_{0.8})_2O_3$, the composition fluctuation of Al was observed to be 1-2 at. % which is relatively insignificant. However, for $(Al_{0.5}Ga_{0.5})_2O_3$, the variation in Al composition was observed up to 10-12 at. % for all the volumes selected (Fig. 2b II-VI). This variation in Al composition was seen in well-patterned crests (higher composition) and troughs (lower composition) that implies phase separation of the alloy. The compositional trend of Al shows up right from the interface in both cases (Fig 1b II and Fig 2b II) indicating the initiation of inhomogeneity as the growth starts. The frequency distribution analysis for the series of bulk volumes were performed using 150 atom bin size. The Pearson coefficient (μ) of Al were found to be 0.8, 0.2 and 0.2, respectively. Also μ values resulted in P values < 0.0001 at 95% confidence level during the null-hypothesis testing. These higher μ and very low P values confirm the existence of statically significant extent of Al segregation. These Al segregations imply clearly a phase separation in the alloy which is not at the same phase as the substrate. We hypothesize that the surface mobility difference of Ga and Al is responsible for the inhomogeneity in β-$(Al_xGa_{1-x})_2O_3$. Both Ga and Al atoms arbitrarily move on the surface, but with higher surface mobility of Ga atoms than that of Al atoms, a lot of Ga atoms can easily drift to form islands and enhance their size [3]. Because of lower surface mobility of Al atom, less Al atoms contribute to the islands formation and enlargement and are distributed more arbitrarily throughout the surface that makes the surface inhomogeneous.

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Here we investigated the growth of β-$(Al_xGa_{1-x})_2O_3$ with varying Al concentration using APT. Our future goal is to study the influence of growth temperature and other parameters on the Al inhomogeneity. The understandings on how the growth of β-$(Al_xGa_{1-x})_2O_3$ proceeds at lower and higher Al concentration is going to be helpful for the realization of β-$(Al_xGa_{1-x})_2O_3$ based devices.

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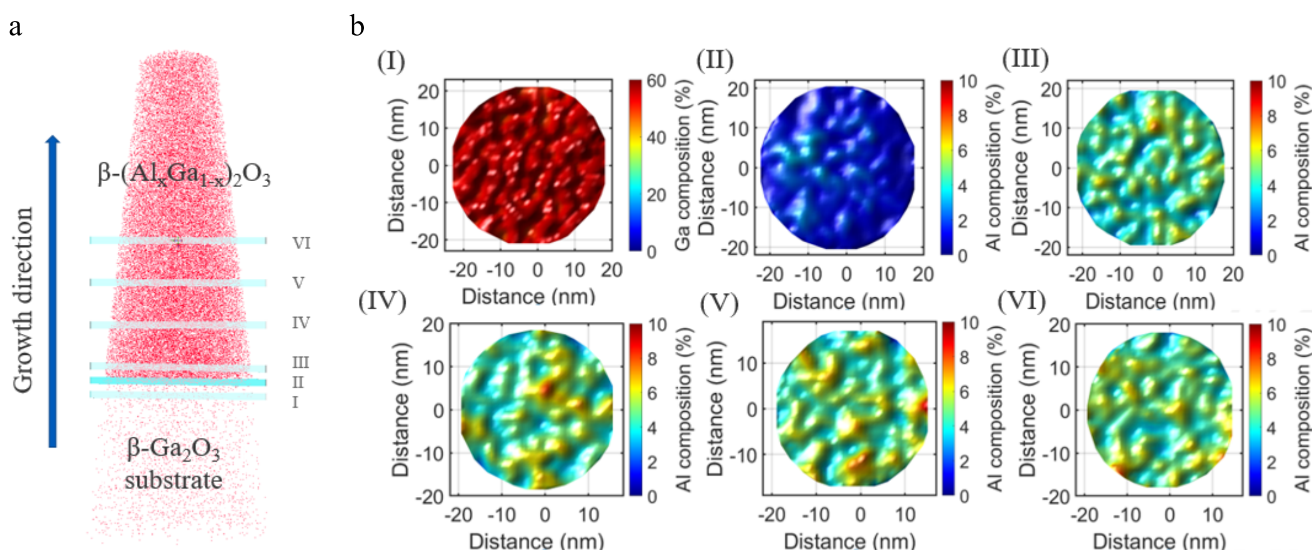


**Figure 1.** (a) 3D elemental map of $(Al_{0.2}Ga_{0.8})_2O_3$; Al atoms are shown in red dots (b) 2D atomic distribution of (I) Ga in β-$Ga_2O_3$, (II) Al in interface and (III-VI) Al in bulk β-$(Al_xGa_{1-x})_2O_3$.

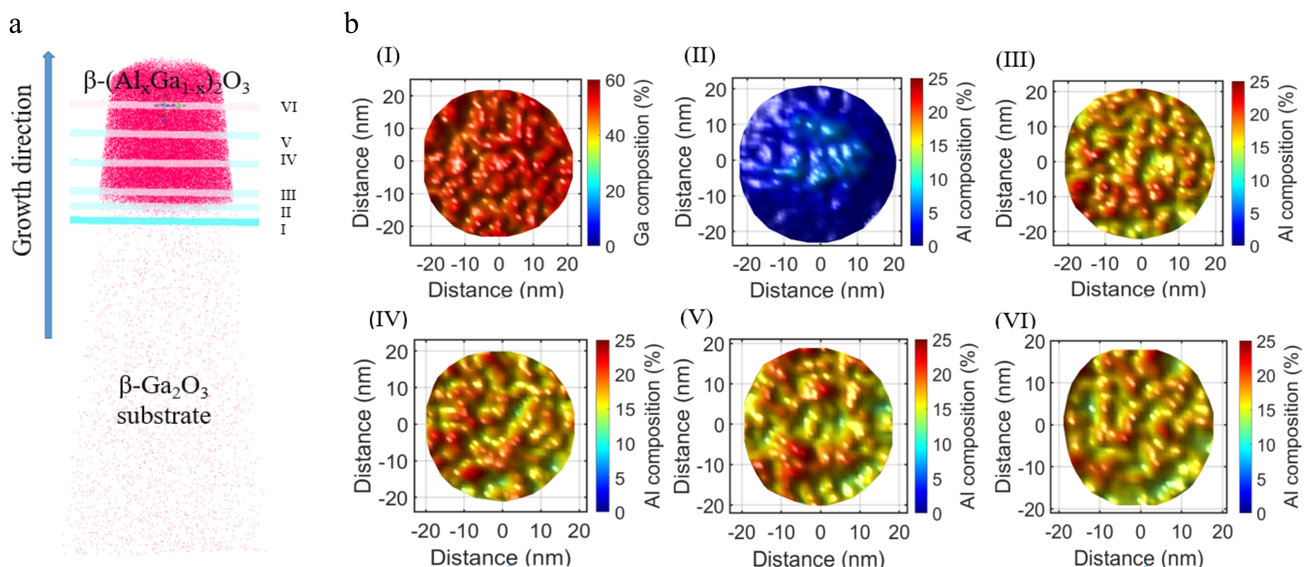


**Figure 2.** (a) 3D elemental map of $(Al_{0.5}Ga_{0.5})_2O_3$; Al atoms are shown in red dots (b) 2D atomic distribution of (I) Ga in β-$Ga_2O_3$, (II) Al in interface and (III-VI) Al in bulk β-$(Al_xGa_{1-x})_2O_3$.

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