Development of β-(AlxGa1-x)2O3/Ga2O3 Heterostructures

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Abstract—The β-(AlxGa1-x)2O3/Ga2O3 heterostructure is a promising element of advanced designs to fully exploit the excellent material properties of β-Ga2O3 for power devices. However, β-(AlxGa1-x)2O3 growth is challenging because of the different crystal structure of the corundum-phase Al2O3 and the monoclinic phase β-Ga2O3. Existing growth conditions have resulted in an Al composition lower than x= 25% achieved in Molecular Beam Epitaxy (MBE) growth. A recent development of a metal-oxide catalyzed epitaxy (MOCATAXY) growth condition enabled a tremendous expansion of the growth window, pushing the growth temperature more than 200 °C higher than the typical growth temperatures. This makes it possible to achieve high Al content near 60% in the monoclinic phase based on the phase diagram. Tremendous research opportunities are foreseen in the development of high Al content β-(AlxGa1-x)2O3 films. Expanding the growth regime through MOCATAXY using In could help improve heterostructure growth for future devices.

Keywords—Ga2O3; heterostructure; molecular beam epitaxy; 2DEG, MOCATAXY

I. INTRODUCTION

Beta-phase gallium oxide (β-Ga2O3) was recently recognized as a promising candidate for electronic device applications because of its excellent intrinsic material properties, including the wide band gap energy (4.8 eV), the projected high breakdown field near 8 MV/cm and the feasibility for controllable n-type doping and contacts.[1] This leads to high figure of merit for power switching applications. Moreover, the availability of high quality single-crystal material using melt-based techniques[2] is beneficial for mass production of high quality bulk films with low defect density, which makes β-Ga2O3 especially attractive for power electronics applications when compared to other wide bandgap semiconductors, such as SiC and GaN. Alloying of In and Al to β-Ga2O3 enables further band gap tunability and provides flexibilities in device design using heterostructures.

First principle calculations suggested a staggered band alignment with a positive conduction band offset and small valence band offset between monoclinic phase (AlxGa1-x)2O3 (AlGO) and β-Ga2O3 (GO).[3] Carrier confinement is therefore feasible at the AlGO/GO heterointerface. When a thin layer of dopants is placed in the AlGO layer, the free carriers could be transferred to the AlGO/GO interface, and thereby forming a high density two-dimensional electron gas (2DEG) through modulation doping as shown in Fig. 1. The spatial separation between the ionized impurities and the 2DEG channel can lead to significant improvement in the transport properties.[4] At the same time, the high density 2DEG could lead to enhanced screening of the scattering centers, making it possible to achieve higher electron mobilities that exceed theoretical limits in bulk doped films. Theoretical calculations[5] indicated a 2DEG mobility exceeding 500 cm²/Vs at a charge density higher than 5×10¹² cm⁻², while the bulk mobility has been demonstrated both theoretically and experimentally to be less than 180 cm²/Vs due to strong polar optical phonon scattering[6-8]. This intrigued significant research interest on the modulation doped structures.

II. GROWTH CHALLENGES OF ALGO

The β-(AlxGa1-x)2O3/Ga2O3 (AlGO/GO) heterostructures have been mainly investigated using oxygen plasma-assisted molecular beam epitaxy (PAMBE), focusing on producing high quality, coherent β-AlGO/GO heterostructures with high Al content. The initial demonstration and analysis of coherent...
epitaxially grown (010) $\beta$(Al$_{1-x}$Ga$_x$)$_2$O$_3$ was done by Kaun et al.[9]. Further X-ray and compositional analysis was performed by Oshima et al.[10], who derived a linear dependence of the Al composition on the separation between the (020) peaks of the AlGO and GO layers[10]. This provides an essential guidance to the evaluation of the epitaxial heterostructures.

Since Al$_2$O$_3$ is most stable in corundum phase, it is challenging to alloy between Al$_2$O$_3$ and monoclinic $\beta$-Ga$_2$O$_3$ to achieve monoclinic phase AlGO. While high quality AlGO films with sharp heterointerfaces have been demonstrated following growth optimizations, significant challenges were recognized for the realization of high Al contents while sustaining single crystal monoclinic structure in the AlGO layers. The maximum Al content has been shown to depend on growth temperature with a maximum of ~16% at 600 °C and concentrations of 25% achieved at 725 °C for fully coherent, single crystalline $\beta$(Al$_{1-x}$Ga$_x$)$_2$O$_3$.[9] Attempts for higher Al compositions resulted in severe phase segregation in the AlGaO layer. As a result, the conduction band offset at the AlGO/GO interface is limited to be below 2×10$^{12}$ cm$^{-2}$ without forming a parasitic channel in the modulation doped structure.[4]

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The dependence of the maximum Al incorporation on growth temperature is consistent with the Al$_2$O$_3$-Ga$_2$O$_3$ phase diagram produced by ceramic analysis by Hill et al. in 1952 [11], shown in Fig. 3. This strong agreement with the expected thermodynamically stable phases is an interesting feature of $\beta$-(Al$_{1-x}$Ga$_x$)$_2$O$_3$ growth, but also makes it difficult to achieve high Al contents at typical (010) $\beta$-(Al$_{1-x}$Ga$_x$)$_2$O$_3$ growth temperatures of 600 – 750 °C. The phase diagram predicts a congruent point around 800 °C above which Al contents of more than 60% can be stable in the $\beta$ phase. Achieving a high Al content is essential to high conduction band offset and therefore better heterostructure devices, but the conventional $\beta$-(Al$_{1-x}$Ga$_x$)$_2$O$_3$ PAMBE growth regime is limited to temperatures of 600 – 750 °C because of the reduced growth rate at high temperatures due to suboxide formation.[12]

Recently, the use of In-catalyzed growth has demonstrated a remarkable expansion of the PAMBE growth regime available for $\beta$-Ga$_2$O$_3$. This involves an exchange mechanism between Ga and In in In$_2$O$_3$ formed at the growth surface with a supplied In flux[13, 14]. Ga favorably incorporates over In and at high Ga fluxes almost no In is incorporated into the single crystalline (010) $\beta$-Ga$_2$O$_3$. Through this mechanism, growth can be performed at higher temperatures and higher Ga fluxes while achieving higher growth rates that are less limited by Ga$_2$O suboxide desorption. This Metal Oxide Catalyzed Epitaxy (MOCATAXY) can be expanded to $\beta$-(Al$_{1-x}$Ga$_x$)$_2$O$_3$ growth as shown in Fig. 4.

With the Al-O bond being even stronger than Ga-O and In-O bonds, Al can favorably incorporate over the other group III metals allowing for the growth of $\beta$-(Al$_{1-x}$Ga$_x$)$_2$O$_3$ with very
limited In incorporation as demonstrated by Vogt et al.[13, 14] Despite supplying an In flux that was higher than the Al flux in III-rich conditions, β-(Al,Ga)O found to be uniform in the films. This expands the range of growth temperatures at which coherent β-(Al,Ga)O was still formed. APT confirmed random distribution of Al with only about 1% In incorporation despite similar Ga and In fluxes during growth. The compositions of constituents on the group III sites was found to be 15%, 18% and 22%.

The heterostructure was coherent and of high quality, but the formation of β-(Al,Ga)O requires atomic oxygen to form, however further studies of In catalyzed growth are needed. β-GaO has been shown to not form without striking the plasma, suggesting that it requires atomic oxygen to grow.

Controllable doping of the epitaxial films is necessary for device applications. For n-type doping in PAMBE of β-GaO, the dopant should ideally be robust to various growth conditions, easily controllable, and be easy to use in the high vacuum chamber without oxidizing in the growth environment. Sn, Si, and Ge have all been shown to be shallow donors in β-GaO and potential options for doping of PAMBE grown films. As a source, Si shows the most difficulty due to oxidation of the solid Si in the high background oxygen environments in PAMBE growth (i.e., the chamber pressure during growth is ~10^3 torr – nearly all due to molecular oxygen). However, successful pulsed delta doping has been used to realize high n-type doping concentrations and employed in various devices.[15] This scheme involves only opening the Si shutter for about a few seconds over the span of a minute and continuing this throughout the growth of a doped layer. This limits the Si source’s exposure to oxygen while obtaining large fluxes of Si over a short time to achieve a target average doping concentration. Modulation doped channels with carrier density less than 2x10^{12} cm^{-2} and improved transport properties have been realized using Si delta-doping.[4]

Because of the poor doping uniformity and the ability to realize low doping concentrations using Si as dopant in oxide MBE systems, significant challenges arise for a range of device applications. Sn and Ge have demonstrated a wider range of doping achievable with Ge being the most investigated in (010) β-GaO PAMBE.[16] Initial attempts to dope β-(Al,Ga)O with Sn have been able to produce doping concentrations on the order of 3 x 10^{18} cm^{-3}, which is desirable for MODFET structures and further suggests Sn’s capability as a shallow donor for PAMBE growth.
rich growth yielding much higher Ge doping levels of greater than $10^{20}$ cm$^{-3}$ for conditions that would achieve $10^{18}$ cm$^{-3}$ in metal rich growth regime. In comparison, Sn doping was also shown to achieve a wide range of doping concentrations from $5 \times 10^{17}$ cm$^{-3}$ to $10^{20}$ cm$^{-3}$ achieving a mobility of 120 cm$^2$V$^{-1}$s$^{-1}$ for the lowest doping conditions. Sn doping showed robustness to growth temperature and group III flux in the typical growth regimes of (010) $\beta$-Ga$_2$O$_3$ as shown in Fig. 6. This makes it appealing for its application to growth at varying growth conditions. For MOCATAXY growth, effective doping concentrations above $10^{18}$ cm$^{-3}$ was realized regardless of the significantly higher growth temperatures, making it feasible to achieve modulation doped structures using Sn as n-type dopant.

V. FUTURE CHALLENGES AND OPPORTUNITIES

Even though the studies on $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/Ga$_2$O$_3$ heterostructures are still in the early stages, tremendous progress has been made, including the optimized growth conditions for sharp interfaces and the demonstrations of modulation doping. However, several challenges remain to be explored for future studies:

1. While $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ is expected to be stable in monoclinic phase up to Al composition of ~60% based on the phase diagrams, successful growth of $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ films with high Al content has not been realized. The MOCATAXY growths provide a tremendous growth space to explore. At the same time, the mechanism behind the catalytic growth mode is not fully understood. Better growth control of the $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ films is expected base on further understanding of the growth kinetics. This provides great research opportunities in both materials science and device development for $\beta$-Ga$_2$O$_3$.

2. Understanding of the band structures of $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ is essential for the heterostructure device applications. However, the fundamental properties, including the conduction band offset, band gap energy, and impurity states, have not been investigated systematically. Evaluation of those properties relies on the growth of high crystalline films.

3. Theoretical calculations predicted high electron mobility in a high density 2DEG channel because of the screen of the scattering centers. Improved mobility above 500 cm$^2$/Vs would enable both high power and high frequency device applications. Realization of the high 2DEG charge density and experimental exploration of the transport properties could be another challenge for the heterostructures.

To summarize, the modulation doped structures could be promising for electronic device applications. The MODFETs are currently limited by the low conduction band offset due to low Al incorporation in the $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ films. There is great potential for improvement of $\beta$-Ga$_2$O$_3$ and $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ growth by MBE. The MOCATAXY growth condition provides a broad window for future investigation of $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ films with high Al content. At the same time, the possible n-type dopants will remain to be evaluated based on different device applications. The development of novel growth conditions and the exploration of n-type doping are expected to enable heterostructures that are suitable for high performance electronic device applications.

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