Mechanism of Si Doping in O_2 Plasma-Assisted MBE Growth of β-Ga_2O_3

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Si has been shown to be a shallow donor in β-Ga_2O_3 and the MBE growth of Si-doped β-Ga_2O_3 thin films is of extensive importance for realization of electronic and optoelectronic devices based on this promising ultra-wide bandgap material. The dependence of Si flux on effusion cell temperatures have been found to be significantly higher in oxygen environments when compared to non-oxide growth chambers, suggesting that the mechanism of Si flux generation is different from sublimation [1]. *In this work, we report on understanding the mechanism of Si doping during oxygen plasma-assisted MBE (PAMBE) growth of* β-Ga_2O_3.

We studied the dependence of Si deposition as a function of oxygen chamber pressure, Si cell temperature, plasma power and shutter time using Secondary Ion Mass Spectroscopy analysis. Our studies show that (a) Si flux is not limited by Si vapor pressure but by the formation of SiO species on the Si surface, (b) the low sublimation energy of SiO leads to weak dependence of the SiO flux on Si cell temperature and strong dependence on the background oxygen pressure and (c) extended exposure to activated oxygen can lead to passive oxidation of Si surface to SiO_2 leading to reduction in SiO flux.

The work reported provides key understanding for incorporating Si into future oxide-based semiconductor heterostructure and device MBE growth. This work was funded by AFOSR GAME MURI (Grant FA9550-18-1-0479, Program Manager Dr. Ali Sayir).

[1] Xia, Zhanbo, et al." *IEEE Electron Device Letters* 39.4 (2018): 568-571.

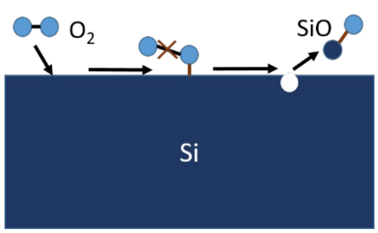

Fig.1 Formation of SiO on Si

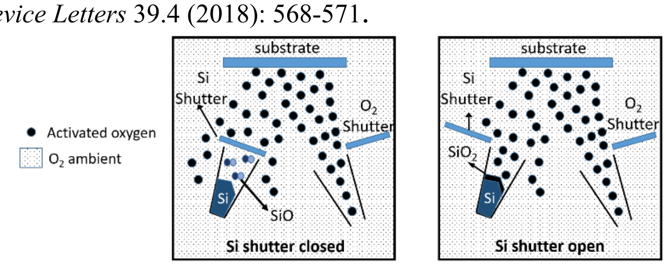

Fig.2 SiO and SiO_2 formation inside MBE chmaber

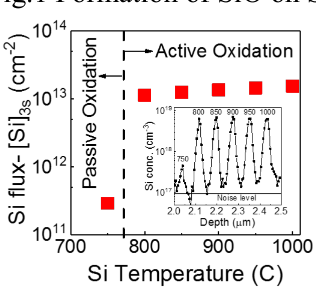

Fig.3 Si flux vs Temperature

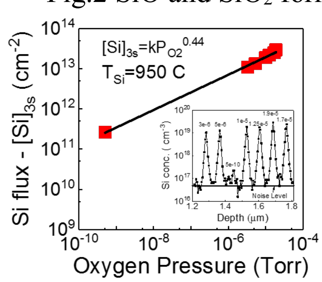

Fig.4 Si flux vs O_2 pressure

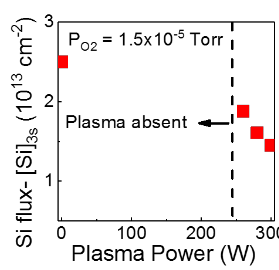

Fig.5 Si flux vs plasma power

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Supplementary Pages

Fig.6 shows the large, nearly three orders of magnitude, disparity between theoretically calculated Si flux based on vapor pressure and experimentally reported values for PAMBE grown β-Ga_2O_3. Sublimation of solid Si cannot therefore account for the observed Si flux. Fig.8 shows the epitaxial structure of β-Ga_2O_3 used for the SIMS analysis where the Si cell temperature, oxygen pressure, oxygen plasma power, and shutter time were varied. Each black line represents the Si delta doping where the Si shutter was kept open for 3 s (or as labeled). The epitaxial growth was carried out on Tamura (010) substrate with Ga BEP of 8×10^{-8} Torr and substrate temperature of 630 °C in a Riber MBE solutions M7 system. Since the Si dopant source is in an oxidizing environment we consider the Si-O pressure-temperature (P-T) diagram as shown in Fig.7. In the temperature region of interest, Si has two oxidation regimes separated by a broad transition region given by the following chemical reactions.

$$Si\ (s) + 0.5\ O_2(g) \rightarrow SiO\ (g) \qquad (1)$$
$$Si\ (s) + O_2(g) \rightarrow SiO_2\ (s) \qquad (2)$$

Where (1) represents active oxidation of Si and (2) represents passive oxidation of Si.

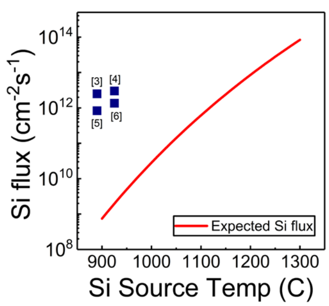

Fig.6 Theoretical Si flux vs temperature, blue boxes represent experimentally reported values

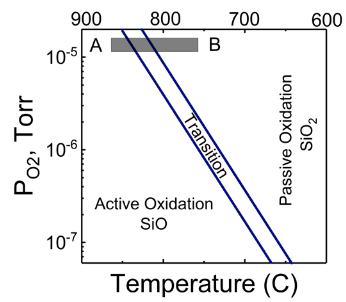

Fig.7 Si-O P-T diagram [2]

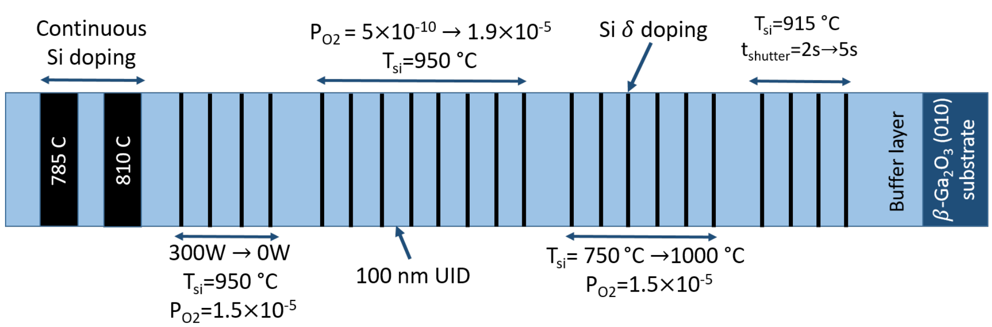

Fig.8 Epitaxial structure used for SIMS analysis (All pressures are in units of Torr)

The variation of Si flux as a function of temperature (Fig.3) shows a lack of exponential behavior and a large drop in flux at 750 °C. This behavior of the Si cell can be understood based on the Si-O P-T diagram (Fig.7). As the Si temperature is varied from 1000 °C to 750 °C we are essentially traversing the P-T diagram from A-B (Fig.3). This shifts the oxidation characteristics from active to passive, explaining the sudden drop in Si flux. Fitting the variation of Si flux and oxygen pressure (Fig.4) shows a power law relation of order 0.44. The fitted value of exponent in this experiment matches very closely with the theoretical rate equation of SiO formation given by

$$[Si] = kP_{O2}^{0.5}$$

Where P_{O2} is the oxygen pressure. To understand the effect of activated oxygen on the Si flux, the plasma power was varied from 300 W to 0 W (Fig. 5). Reduction in oxygen plasma power results in an increase in Si flux suggesting that activated oxygen suppresses the formation of SiO. Since active oxygen (O_2^*) has a much higher oxidation efficiency compared to molecular oxygen, the former can promote the complete oxidation of Si to SiO_2 which reduces the flux of SiO. Additionally, the effect of shutter time was studied by two experiments, one where the shutter time was limited to few seconds while the other was used to study extended shutter open time. Short pulses were found to provide a constant flux of SiO (Fig.8) while extended shutter open time results in diminishing flux (Fig.9)

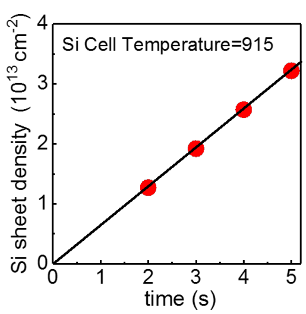

Fig.9 Si sheet density vs shutter time (s)

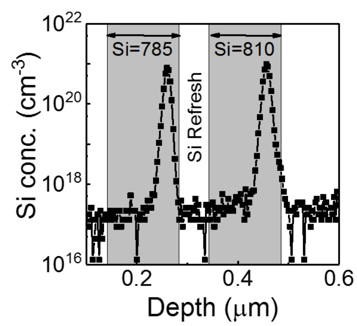

Fig.10 Si sheet density for extended shutter time

In conclusion we have shown that the anomalous Si flux observed in the plasma assisted MBE growth of β-Ga_2O_3 arises from the formation of volatile SiO. The flux of SiO has a weak temperature dependence above 800 °C and shows a power law relation of order 0.44 with oxygen pressure. Activated oxygen was found to suppress the formation of SiO and promotes the growth of a thin layer of SiO_2 on the Si surface. A constant flux vs. time relation was confirmed for short shutter pulses of few seconds while extended exposures diminish the flux of SiO.

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