In Situ Observation of $\beta$-Ga$_2$O$_3$ Schottky Diode Failure Under Forward Biasing Condition

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Abstract—In this article, we investigate defect nucleation leading to device degradation in $\beta$-Ga$_2$O$_3$ Schottky barrier diodes by operating them inside a transmission electron microscope. Such in situ approach allows simultaneous visualization and quantitative device characterization, not possible with the current art of postmortem microscopy. High current density and associated mechanical and thermal fields are shown to induce different types of crystal defects, from vacancy cluster and stacking fault to microcrack generation prior to failure. These structural defects can act as traps for carrier and cause device failure at high biasing voltage. Fundamental insights on nucleation of these defects and their evolution are important from materials reliability and device design perspectives.

Index Terms—$\beta$-Ga$_2$O$_3$, crystal defects, in situ transmission electron microscope (TEM), Schottky barrier diodes (SBDs).

I. INTRODUCTION

HIGH breakdown field of wide bandgap materials makes them well-suited to high power electronics applications [1]–[3]. Both GaN and SiC are commercialized for power switching and control systems, while materials with even larger bandgaps, such as diamond, high-Al AlGaN, and Ga$_2$O$_3$, are attracting significant interest for achieving even higher performance levels. In particular, the beta-polytype of Ga$_2$O$_3$ is an attractive material because of its low cost, bulk growth methods, wide bandgap of 4.8–4.9 eV, and high breakdown field ($\sim$8 MV/cm) [4]–[7]. Ga$_2$O$_3$ has three times higher breakdown field strength compared to GaN and 4H-SiC [7] and possesses one order of magnitude and three times higher Baliga’s figure of merit (BFOM) compared to 4H-SiC and GaN, respectively, [4], [5]. These exceptional properties make Ga$_2$O$_3$ a suitable material for next-generation high power electronics such as Schottky barrier diodes (SBDs) and MOSFETs with low loss, high breakdown field, and high voltage switching capability [4], [5], [8]–[21].

SBDs are a particular device concept that exhibit low on-state loss, short recovery time, low on-resistance, and high switching speeds [4], [5], [8], [9], [12], [22]–[24]. A large number of studies [8], [9], [12] have shown very promising performance from $\beta$-Ga$_2$O$_3$ SBDs, with breakdown voltages over 2 kV and forward currents $>$ 30 A from large area devices. The electrical behavior of SBDs can be affected by the choice of Schottky metal contact, and the presence of interface states [25]–[31]. Crystal defects can also affect the performance of the SBDs and contribute to high leakage current [28].

Large area vertical geometry $\beta$-Ga$_2$O$_3$ SBDs are potential candidates for high power switching application [32]. Initial studies show the failure modes of $\beta$-Ga$_2$O$_3$ SBDs under forward and reverse bias conditions are different [5], [32]. The reverse bias failure mode is governed by the pit formation at the edge of the Schottky contact where the electric field strength is highest, whereas forward bias failure mode shows contact area and device layer cracking and in some cases, delamination of epitaxial layers from the underlying substrate [32]. Temperature-dependent electrical characterization of $\beta$-Ga$_2$O$_3$ SBD shows that the Schottky barrier height (SBH) can be affected by the device operating temperature [26], [27], [32]–[35], which is reflected by their current–voltage ($I$–$V$) characteristics. Relatively less is known about the fundamental mechanisms behind the evolution of damage and ultimately, failure of these devices. The majority of the studies extrapolate the failure mechanisms with either “signature” failure pattern in the device characteristics data [36]–[38] or in postfailure analysis of the device. Only
a few recent studies [39]–[41] have attempted to investigate the failure mode of electronic devices under real-time operating condition. However, such in situ or in operando experiments have not been extended to Ga2O3 SBDs yet.

In our present study, we demonstrate an in situ experimental philosophy that allows us to investigate β-Ga2O3 SBDs failure under forward biasing condition inside a transmission electron microscope (TEM). The uniqueness of the study is that it allows us for the simultaneous visualization of the microstructure and quantitative characterization during the SBD device operation. We prepared electron transparent functional specimen from a bulk β-Ga2O3 Schottky diode using a focused ion beam (FIB). The specimen was mounted and wire-bonded on customized in situ TEM chip to perform experiments. Real-time visualization at high-resolution imaging accompanied by energy-dispersive X-ray spectroscopy (EDS), high-angle annular dark-field (HAADF) imaging, and selected area electron diffraction pattern were performed to characterize the microstructure and chemistry. The assortment of device characteristics, microstructure, and elemental diffusion data is expected to provide useful insights into the failure mechanism of β-Ga2O3 SBDs and design guidelines.

II. EXPERIMENTAL SECTION

The device structure and fabrication have been described in detail previously [14]. Briefly, the field-plated, edge-terminated vertical Schottky diodes were fabricated on a 20-μm-thick Si-doped n-type Ga2O3 drift layer grown on 650-μm thick β-Ga2O3 substrate using halide vapor phase epitaxy (HVPE). The β-Ga2O3 substrate was an Sn-doped β-Ga2O3 single crystal wafer with (001) surface orientation grown by the edge-defined film-fed method with a carrier concentration of 3.6 × 10^{18} cm^{-3}. A backside Ohmic contact was formed with electron-beam-deposited Ti/Au followed by rapid thermal annealing at 550 °C for 30 s in N2. Next, 40 nm of SiO2 and 360 nm of SiNx were deposited as dielectric layers. Dielectric contact windows were opened with buffered oxide etchant (BOE). E-beam-evaporated Ni/Au (80 nm/420 nm) metallization was used for the Schottky contacts, which overlapped the dielectric windows by 10 μm.

Electron transparent (nominally 100-nm thick) β-Ga2O3 coupons were prepared and lifted out from the SBD [Fig. 1(a)] using a Ga+ FIB [Fig. 1(b)] in a Helios Nanolab DualBeam scanning electron microscope (SEM). This involved three important steps: 1) 100-nm thin sample preparation, 2) transfer of 100-nm thin sample on microelectromechanical system (MEMS) device [Fig. 1(e)] [39], [40], and 3) wire bonding of MEMS device [42] on a TEM chip carrier [Fig. 1(d)]. At first, a coupon was lifted out from the bulk β-Ga2O3 SBDs and attached on a copper TEM grid [Fig. 1(c)] using Ga+ FIB. Thinning down of the coupon involves a series of ion beam accelerating voltages and a wide range of current steps 21 nA–72 pA. The thickness of the sample was monitored at regular intervals during the thinning down process, and both accelerating voltage and currents were adjusted depending on the sample thickness. The second-step sample preparation uses low accelerating voltage to transfer the sample from TEM copper grid to the MEMS device. Low, i.e., 5-kV accelerating voltage-transfer steps were chosen to avoid any beam damage and redeposition. Electrical connections [Fig. 1(e)] were made using FIB-deposited platinum. Fig. 1(e) shows the transferred sample on the MEMS device, which is further mounted on an in situ TEM holder [Fig. 1(d)]. Electrical characterization was performed inside a field emission 200-kV FEI Talos F200X TEM equipped with energy dispersive spectroscopy (EDS) with 1.2-Å resolution.
Fig. 2. (a) I–V characteristics under forward biasing condition. TEM BF images during failure at time (b) \( t = 0 \) s and (c) \( t = 15 \) s. Structural transformation in the \( \beta \)-Ga\(_2\)O\(_3\) layer after failure. (d) TEM BF image of vacancy clusters. (e) HRTEM images of SFT [corresponds to the pink color region in (c)]. (f) Defects near the cathode area.

### III. RESULTS AND DISCUSSION

The 11 \( \mu \)m \( \times \) 7 \( \mu \)m \( \times \) 100-nm electron transparent \( \beta \)-Ga\(_2\)O\(_3\)SBDs [Fig. 1(f)] were tested under accelerated forward biasing conditions. During the experiment, we gradually increased the forward bias at an interval of 20 mV until the device fails. Each biasing step was followed by a 1-min delay for relaxation, at which point the system was stable both mechanically and electrically. Fig. 2(a) shows the SBD current–voltage (I–V) characteristics under forward biasing condition. Low magnification TEM bright field (BF) images [Figs. 1(f) and 2(b) and (c)] show bend contours which arise from elastic bending during specimen preparation. Fig. 2(b) and (c) shows the TEM BF images to capture microstructural changes during operation. The calculated current density prior to the failure is \( 3.2 \times 10^2 \) A/cm\(^2\), which is well agreement with the reported [5], [30] value. This high current density is enough to introduce thermal stress in the device which could further initiate microstructural changes at the anode and cathode areas, as shown in Fig. 2(b) and (c). High-resolution TEM (HRTEM) images [Fig. 2(d)–(f)] indicate generation of severe crystal defects, such as vacancy clusters, [Fig. 2(d)] amorphization, stacking fault tetrahedron (SFT), and crack [Fig. 2(f)] formation in the device layers.

As shown in Fig. 2(e) SFT is a pyramidal shape vacancy defect, and it may appear as a triangular shape in the TEM BF image [43]. SFT defects are an obvious indication of vacancy generation in the device layer under high current density as shown in Fig. 2(e). These vacancies further accumulate to form SFT defects [44]. Similar types of stacking fault defects in Ga\(_2\)O\(_3\) have been reported recently [45]. During the failure both metal pool (green color dotted lines) and discernable cracks (cyan color dotted lines) formed in the device layer near the cathode as shown in Fig. 2(f). High current density accompanied by the thermal field could induce a sufficient amount of thermal stress in the device layer and initiate this mechanical cracking [9]. These structural defects might act as carrier traps and further accelerates device degradation.

During forward biasing, defects could generate near the anode area due to high current density in the SBD device (Fig. 3). Fig. 3 shows such defects evolution during forward biasing. The pink color arrowhead indicates the direction of the anode location. Before forward biasing, there was no obvious indication of crystal defects, as shown in Fig. 3(a). However, at 4.8 V, crystal defects start to appear as indicated by green circular regions in Fig. 3(b). These defects near the anode could affect SBH at the interface [22], which could affect forward output current. At this point calculated current density is \( 2.9 \times 10^3 \) A/cm\(^2\), which can facilitate the development of thermal stress due to the Joule heating, and further contributes to the crystal defects evolution. The electrical field required to initiate crystal defects is approximately 0.5 MV/cm, this
value is close to the experimental breakdown field strength approximately 0.54 MV/cm [46]. However, as we continue to increase forward biasing, the device fails by forming a vacancy-enriched area, as indicated by cyan color dotted arrowhead in Fig. 3(c). We also notice disruption in crystal structure and formation of small crystallites, as shown by green color dotted circles. This observation indicates that single-crystal Ga$_2$O$_3$ disintegrates into a polycrystalline structure due to the thermo-mechanical field, which can significantly affect the device performance. In our present study, we notice that after failure the device behaves as an open circuit, and no significant current flow was measured through the device after this failure.

We have also compared forward output current obtained from as-fabricated bulk Ga$_2$O$_3$ and electron transparent thin film device as shown in Fig. 4(a). Output current follows the similar $I$–$V$ characteristics; however, the magnitude of current density is slightly different which could be attributed to the thin film device geometry. Rigorous experimentation and modeling are required to mitigate this discrepancy and we left this issue for future study. Scanning transmission electron microscope (STEM) equipped with EDS allows us to identify individual elements in the device layer during the experiment. The chemical mapping provides insights into the diffusion of elements toward degradation of the SBD device during forward biasing. In our present study, we scan two EDS maps before and after the failure of the device, as shown in Fig. 5(a)–(d). On the EDS map, cyan and red colors represent gallium (Ga) and oxygen (O) atoms, respectively.
No discernable defects/abrupt changes in the elemental map are observed in the sample before biasing [Fig. 5(a) and (b)]. However, after failure, we observe the accumulation of Ga and O near the left side of the anode [Fig. 5(c) and (d)]. At the same time, we also identify the loss of Ga and O atoms from the cathode area of the device, which could be attributed to the Ga pool formation near the cathode area [Fig. 5(c)]. We also notice both Ga and O atoms migrate toward the anode area, which could be attributed to the thermo-migration of these atoms under the combined thermo-mechanical field at high current density. The unique geometry of the thin film SBD could introduce a nonuniform temperature profile along the thin film SBD due to the Joule heating. Thus, this thermal gradient in the sample might generate a nonuniform Ga profile in the thin film SBD device. Under high current density, the anode metal could degrade (as shown by the green dotted arrow in Fig. 4(b) and (c)). BF TEM image, EDS map [inset in Fig. 4(b)], and STEM images [Fig. 4(c)] show electrode metals diffusion in the channel layer at higher current density due to the high thermal field. This electrode degradation might significantly damage the interface layer and introduce the Schottky barrier inhomogeneity at the interface [23]. Hence, the device deviates from the ideal behavior.

STEM image and EDS mapping allow us to probe both structural and chemical transformation. For example, metal pool formation is confirmed by Fig. 5(c). However, without EDS mapping no elemental information could be extracted. The presence of a metallic pool of Ga near the cathode indicates a sufficiently high thermal field that may arise during the device operation and could transform Ga2O3 to Ga atoms. Fig. 5(e) represents the relative weight percentage of Ga and O atoms after failure. Weight percentage loss of Ga and O atoms is approximately 6% and 4%, respectively, [Fig. 5(e)], which supports the device layer degradation and decomposition of β-Ga2O3 at high current density.

Our present study reveals that high current density accompanied by the thermal field could induce a significant number of structural defects such as vacancy clusters, stacking faults, and cracking in the devices. These structural defects further act as carrier traps and might increase resistance to the current flow during the operation [24]. Observation indicates that failure mode could be attributed to the high thermo-mechanical field that may arise during the operation of the SBDs device. In situ TEM techniques have been already implemented to investigate both “on-” [47] and “off-” [39] state failure study of high electron mobility transistor. Though our present study investigates forward biasing condition, however, a similar technique could be extended to study the reverse biasing failure mode. Further work is needed to correlate the scaling physics of the electron transparent device and the effects of specimen preparation before the findings can be applied to bulk SBDs.

IV. CONCLUSION

We demonstrated a new experimental direction in electron device reliability by operating an electron transparent β-Ga2O3 SBD inside a TEM. The electrical measurements and microscopy indicate that high current density could induce a significant concentration of crystal defects both in the electrode and device layer, which in turn increase series resistance. At high current density, the electrode metal can degrade, thus introducing inhomogeneous Schottky contact at the metal–semiconductor interface. Additionally, high current density-induced point defects can act as carrier traps, which significantly affect the electrical performance of the device. Metallic pool formation during the failure of the device indicates temperature plays a dominant role in the device failure. Furthermore, EDS mapping indicates the reduction of Ga and O atoms near the cathode area could be attributed to the migration of atoms under high current density. We conclude that the existing literature considers only postfailure analysis to predict the failure modes, whereas this article probed defects evolution and failure modes during real-time operation. Continuation of this article will provide invaluable insights on SBD device design and failure mechanism in the future.

REFERENCES