Temperature Dependent Performance of ITO Schottky Contacts on β- Ga₂O₃

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Abstract

Sputtered ITO was used as a rectifying contact on lightly n-type ($n\sim10^{16}$ cm⁻³) β - Ga₂O₃ and found to exhibit excellent Schottky characteristics up to 500K, with no thermally-driven degradation to this temperature. The barrier height extracted from current-voltage characteristics was 1.15 ± 0.04 eV at 300K and 0.78 ± 0.03 eV at 500K, with thermionic behavior of charge carriers over the image force lowered Schottky barriers dominating the carrier transport at low temperatures. The breakdown voltages were 246, 185 and 144 V at 300, 400 and 500K, respectively. At 600K, the diodes suffered irreversible thermal damage. The diode on/off ratio was $>10^5$ for reverse biases up to 100V. At higher reverse voltage, the current shows an I \propto Vⁿ relationship with voltage, indicating a trap-assisted space-charge-limited conduction (SCLC) mechanism. We observed this SCLC relation when the reverse voltage was larger than 100 V for 300 K and 400 K and at <100V at 500K. The ITO can also be used to make Ohmic contacts on heavily doped Ga₂O₃ suggesting the possibility of completely optically transparent power devices.

Introduction

There are two particular polytypes of Ga₂O₃ that are attracting interest for high power transistors and rectifiers and solar-blind UV photodetectors $^{(1-6)}$. The α -polytype has a larger bandgap and a hexagonal crystalline structure (in contrast to the low-symmetry monoclinic structure of the β -phase) the same as of sapphire (α -Al₂O₃) and so it has a better lattice matching to α -Al₂O₃ substrates. This facilitates improvement of the epilayers structural quality. The β polytype is available in melt-grown bulk form, with controllable n-type doping, and is the most stable form ⁽¹⁻³⁾. The high breakdown field of this wide bandgap semiconductor has enabled many demonstrations of vertical and lateral rectifiers with reverse breakdown voltages in the kV range of interest for electric vehicle (EV) charging stations, power management in residential solar systems and battery energy storage systems ⁽⁷⁻²⁹⁾. In particular, the transition to fast EV charging stations equipped with advanced DC chargers is accelerating -the state of the art is that currently a DC charger with 150 kW can put a 200 km charge on an EV in ~15 minutes ^(30,31). For most low-voltage urban applications, breakdown voltages of 1.2 kV suffices. The high breakdown field of Ga₂O₃ enables greater voltage blocking capability and lower conduction losses due to a lower on-resistance reduction in comparison with Si-based devices ^(3,4,9,30).

A crucial aspect of these high-power rectifiers are the Schottky contacts. These contacts need to be thermally stable, the interface between the metal and the Ga₂O₃ needs to be of high quality so that any defect-related leakage current is insignificant and finally, the largest barrier height is needed if the maximum electric field is to be reached $^{(32-42)}$. Li et al.⁽²⁹⁾ calculated that to reach the intrinsic breakdown electric field in Ga₂O₃, the barrier height of the Schottky contact would \need to be of the order of 2.2 -3 eV. These values have not been reached with any of the metals examined to date, with the highest values of ~2.1 eV reported for oxidized metal contacts

of PtO_x and IrO_x deposited by reactive sputtering on (-201) Ga₂O₃ substrates ^(37,41). In highpower Schottky rectifiers, the largest barrier is needed to reach the maximum electric field (2.2-3eV in the case of Ga₂O₃). However, in power-rectifiers if the barrier height is too high, the forward voltage drop at the targeted current will be also high, thus leading to a high power dissipation, so that striving for the highest barrier height is not always desirable. Previous work has shown that the orientation of the Ga₂O₃ has a strong influence on whether there is a correlation of barrier height with metal work function ^(32,33). Lyle et al.⁽³²⁾ showed that (100) surfaces showed the strongest correlation, while (-201) and (101) had stronger Fermi level pinning effects, due to the differences in dangling bond densities ⁽³²⁾.

In this work, we describe the performance of sputtered ITO contacts on (100) Ga₂O₃, as a function of temperature up to 500K. Transparent gates would also facilitate probing of single event radiation upsets using x-ray excitation sources ⁽⁴⁴⁾. They may also be useful in limited types of optically-triggered Ga₂O₃ power devices if a gap state is employed, since the bandgap of ITO is around 4 eV and that of Ga₂O₃ is larger. Optically-triggered power management devices use optical control to avoid the thermal degradation of the gate electrode when used at high temperature and there is complete electrical isolation between the low-voltage controller and HV power stages ⁽⁴³⁾. An all optically-controlled gate would add flexibility to thyristor designs, allowing them to be used to their full potential.

Thin (10nm) sputtered indium tin oxide (ITO) has been employed previously as an intermediate layer between Ti/Au and heavily doped (-201) β -Ga₂O₃ to enhance formation of an Ohmic contact upon annealing at 400-600°C ^(45,46). The band alignment of ITO on Ga₂O₃ under those conditions is favorable for electron injection, with a conduction band offset of -0.32 eV

 $^{(45,46)}$. However, in the as-deposited state on lightly doped Ga₂O₃ and for anneal temperatures up to 500K, we find the ITO to provide a rectifying contact.

Experimental

The drift region of the material consisted of a 10 μ m thick, lightly Si doped epitaxial layer grown by halide vapor phase epitaxy (HVPE) with carrier concentration of 3 × 10¹⁶ cm⁻³, and this epitaxial layer was grown on a (001) surface orientation, 2-inch diameter Sn-doped (n=10¹⁹ cm⁻³) β -Ga₂O₃ single crystal (Novel Crystal Technology, Japan). The HVPE layer was actually grown initially to a thickness of ~ 20 μ m, but then chemically mechanically polished to planarize the surface by removing ~10 μ m of material. The wafer surfaces were ultrasonically cleaned in acetone, methanol, and isopropyl alcohol.

A full area Ti/Au backside Ohmic contact was formed by e-beam evaporation and was annealed at 550 °C for 30s under N₂ ambient. After backside Ohmic formation, the front of the sample was cleaned using HCl and then treated with ozone for 20 minutes to remove residual hydrocarbons. Next, the sample was patterned for Schottky contact formation. A 100 nm ITO layer was deposited by dc sputtering at room temperature using a 3-in. target of ITO. The dc power was 125 W and the process pressure was 5 mTorr in pure Argon ambient. Edge termination was not used, in order to focus on the ITO contact characteristics free of any edge effects. Figure 1 shows a schematic of the competed devices, with circular contact diameters of 50-200 μ m and square contacts of length 400 μ m. There was no clear dependence of forward and reverse current densities over the range of contact sizes investigated. Figure 2 shows an optical microscope image and contact geometry of the fabricated diodes.

The current-voltage (I-V) characteristics were recorded over the temperature range 300-500K on a temperature-controlled stage. Forward current measurements were recorded with a HP 4156 parameter analyzer. No hysteresis was observed in any of the rectifier characteristics. Reverse currents were measured with a Tektronix 370-A curve tracer. We measured 4-5 different diodes for each condition, with the results being within 5% within this distribution. The forward direction was dominated by the thermionic emission (TE) current over most of the temperature range, while in the reverse direction, the thermionic field emission (TFE) and tunneling currents played an important role at high reverse bias. To extract the zero-bias equivalent barrier height (Φ_b) and ideality factor (n), we used the relationship for current density in TE theory, given by (32,46,47)

$$J = J_0 \exp (eV_A/nkT) [1-exp (-eV_A/kT)]$$

where $J_0 = A^* m_{eff}/m_0 T^2 \exp(\Phi_B / kT)$, e is electronic charge and A^* is the Richardson constant (33.7 A.cm⁻²K⁻²) and V_A is the bias voltage applied. The values of barrier height were corrected for the image force (IF) lowering, as described elsewhere and also represent the average of 4-5 different diodes at each condition. ⁽⁴¹⁾. Capacitance-Voltage (C-V) characteristics were recorded with an Agilent 4284A Precision LCR Meter to conform the carrier concentration in the epi layer. The diode on/off ratio is another figure-of-merit was measured when switching from 3V forward to reverse biases up to 100V. The reverse breakdown voltage was defined as the bias for a reverse current reached before 3mA.

Results and Discussion

Figure 3 shows the forward current density for the 100 μ m diameter circular diodes as a function of temperature. The devices were sequentially measured at increasing temperatures up to 500K, then returned to 300K and re-measured. For these temperature cycled diodes, the junction diameter is 500 micrometer, which converts to an increase in junction current of about 2 nA (2x10⁻⁹ A) after the heating cycle to 500 K. However, a change of nA in current densities

many orders higher is not sufficient to draw the conclusion the samples are not thermally stable after that cycling. Small shifts in forward turn-on voltage can result from changes in onresistance or barrier height. As stated earlier, there was no difference in current density as a function of contact size or geometry. The carrier concentration in the epi layer did not change as a result of the thermal cycling as determined by C-V measurements, indicating that compensating Ga vacancies or other defects were not created at these temperatures. The on-state resistance of the rectifiers, R_{ON} , was 12 m Ω .cm² at 300K and 29 m Ω .cm² at 500K. At 600K, the diodes suffered irreversible thermal damage.

The zero bias effective barrier height and ideality factors were extracted from the linear portion of the forward bias characteristics through the correction factor $[eE/4\pi\epsilon]^{0.5}$, where E is the electric field at the ITO/Ga₂O₃ interface and ϵ is the dielectric constant of the semiconductor ⁽⁴¹⁾. The results are shown as a function of temperature in Figure 4. The barrier height decreases monotonically with increasing temperature, while the ideality factor increases. This is commonly observed for contacts on Ga₂O₃ ^(32, 33,37,39). However, in many cases ^(34-36,38,40,41) the behavior of n and barrier height is exactly opposite, i.e. n decreases with temperature (tending to one) and barrier height increases with temperature. This can be due to the presence of other conduction mechanisms and also contact inhomogeneity. Another notable exception is the large thermally activated increase in the barrier height for Pd Schottky contacts occurring between 250-450 °C when heated in air ⁽⁴¹⁾. This change was ascribed to the oxidation of the Pd metal layers, creating higher barrier height PdO_x regions. The high ideality factor above ~400 K indicate other current transport mechanisms are present as the barrier is lowered.

If the Mott-Schottky relationship holds for ITO on (100) Ga₂O₃, the expected barrier height would be 0.75 eV from the difference in energy between the metal work function of 4.8

eV ⁽⁴⁷⁾ and the electron affinity of Ga₂O₃ of 4.05 eV. This is not an unreasonable assumption given the high degree of ionicity of the bonds in Ga₂O₃ ⁽³²⁾. However, the experimental value of 1.15 eV at room temperature is larger than this prediction, suggesting that additional factors are determining the effective barrier height and is certainly larger than expected from contact inhomogeneity considerations. The SBH can be dependent on the surface orientation of Ga₂O₃, Lyle et al.⁽³²⁾ have made investigations of different metals on different orientations of Ga₂O₃ found that the change of barrier height with metal work function can be used as a useful measure of the applicability of the Mott-Schottky relationship. In Figure 5, we plot previously reported values ⁽³²⁾ for Ti, Mo, Co and Ni on (100) Ga₂O₃ with the experimental value for ITO determined in this work for (001) orientation, which are the two surfaces with highest stability ⁽⁴⁸⁾. Thus we feel a comparison is more likely to be valid relative to results on the other orientations. There is an extensive discussion of this by Lyle et al. ⁽³²⁾. The straight line is to guide the eye and not to explicitly evaluate the presence of Fermi level pinning.

Overall, there is a positive correlation between Schottky barrier heights and the work function of the metal contacts for these orientations and the experimental value for ITO on the (001) orientation fits well with previous results for the other metals on the (100) orientation, the other stable surface ⁽³²⁾. This is in contrast to contacts on (-201) and (010) β -Ga₂O, which exhibited little or mixed correlation between these parameters ^(32,49). In the case of (-201) surfaces, the higher density of O dangling bonds was proposed to explain the strong Fermi level pinning on this surface ⁽³²⁾. Harada et al. ⁽⁴⁸⁾ employed a novel layered PdCoO₂ contact on Ga₂O₃ to achieve a barrier height of 1.8eV, well above that expected from the Mott-Schottky relation. This significantly expands the temperature range for achieving good rectification ratios ⁽⁴⁸⁾. It is clear in the case of ITO on (001) Ga₂O₃ that Fermi level pinning is present. Figure 6 shows the reverse current density characteristic as a function of temperature. The breakdown voltages were 246, 185 and 144 V at 300, 400 and 500K, respectively, showing that impact ionization is not the breakdown mechanism, since that should exhibit positive temperature coefficient. It is common for new technologies like Ga_2O_3 to exhibit defect-dominated behavior in the early stages of development, as was observed with both SiC and GaN ^(1,9). There was also no significant change in current density at room temperature as a result of the thermal cycling to 500K. The variation in reverse current densities as a function of temperature were within the experimental variation from diode-to-diode of ~10%.

The on-off ratio is another figure of merit is the figure of merit in that having high oncurrent and low leakage current in reverse bias is desirable. This was $>10^5$ for all temperatures measured, as shown in Figure 7.

As shown in Figure 8, at lower voltages, reverse bias leakage current density was dominated by thermionic field emission (TFE), which is strongly dependent on ambient temperature. We have reported similar data previously for Ni/Au contacts on these types of rectifiers ⁽⁴⁷⁾. When higher reverse voltages are applied, electrons are injected into the drift region, and the current shows an $I \propto V^n$ relationship with the voltage, indicating a trap-assisted space-charge-limited conduction (SCLC) mechanism ⁽⁴⁹⁻⁵³⁾. Under this mechanism, a current hump should be observed before the trap-filled limited voltage, and with electrons continue to be injected into the drift region, it will lead to a breakdown. The reverse current characteristics at different temperatures all show a I \propto Vⁿ relationship. The data fits a relationship I \propto Vⁿ, where n is ~2-6.8, dependent on temperature. Trap-mediated SCLC should have n>2 ⁽⁵²⁾. In this higher field region, the space charge limited current is proportional to the product of electron saturation velocity times voltage divided by the electrode spacing. The value of n varies with the injection

level and is also related to the distribution of trapping centers. Values as high as 22 have been reported in GaN Schottky diodes with low densities of traps $(10^{15} \text{ cm}^{-3})^{(53)}$.

As mentioned earlier, the ITO can be used to enhance Ohmic contact formation on doped Ga_2O_3 . Oshima et al.⁽⁵⁴⁾ found that sputter-deposited ITO electrodes became Ohmic contacts on n-type β -Ga₂O₃(010) substrates after rapid thermal annealing at 900–1150 °C. This raises the possibility of using ITO on both sides of vertical rectifier structures to make fully transparent power devices. An optical image of such a device is shown in Figure 9. The structure in this case is ITO top Schottky contact, epi Ga₂O₃, Ga₂O₃ substrate and ITO rear Ohmic contact. The optical transmittance was 83% at 360 nm and > 90% for 400-800nm without annealing, consistent with past reports ⁽⁵⁵⁾. We will conduct a more thorough study of the effect of annealing in future.

Summary and Conclusions.

ITO is shown to provide a rectifying contact to lightly doped (100) Ga_2O_3 up to temperatures of 500K. The barrier height at room temperature is 1.15 eV and fits a trend observed for metal contacts on the (100) orientation that correlated metal work function with the electron affinity of the semiconductor. The rectification ratio was >10⁵ up to 500 K and the contacts appear useful for applications requiring optically transparent contacts. If more heavily doped substrates are used, the ITO can be made to behave as an Ohmic contact, perhaps assisted by an annealing step, and thus to the possibility of using transparent contacts on both sides of vertical rectifier structures arises. This allows realization of a fully transparent power device.

Data Availability Statement

All data that support the findings of this study are included within the article.

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Figure Captions

Figure 1. Schematic of layer structure of vertical rectifier used in this work.

Figure 2. Optical microscope image of Schottky contact layout.

Figure 3. Forward J-V characteristics as a function of temperature for ITO Schottky contacts on

(100) β -Ga₂O₃. The diameter of each diode is 500 μ m.

Figure 4. Extracted zero-bias barrier heights and ideality factors for ITO contacts, assuming thermionic emission dominates, as a function of temperature.

Figure 5. Comparison of experimental and theoretical values for barrier height of ITO with those of Ti, Mo, Co and Ni, on (100) β -Ga₂O₃ reported by Lyle et al,⁽⁴²⁾ plotted vs metal work function. The theoretical value from the Mott-Schottky equation is also given, assuming an electron affinity of 4.05 eV.

Figure 6. Reverse J-V characteristics as a function of temperature for ITO Schottky contacts on (100) β -Ga₂O₃. The diameter of each diode is 500 μ m.

Figure 7. On/off ratio of or ITO Schottky contacts on (100) β -Ga₂O₃. The devices were measured at -1V forward basis and then the reverse bias shown on the x-axis.

Figure 8. Experimental data for reverse current density characteristics at 400-600K and fit to an I $\propto V^n$ relationship.

Figure 9. Optical microscope image of fully transparent, vertical geometry Ga₂O₃ rectifier employing ITO contacts on both sides. The structure is ITO top Schottky contact, epi Ga₂O₃, Ga₂O₃ substrate and ITO rear Ohmic contact. On the top lightly doped drift layer, the ITO is rectifying, while on the bottom surface of the heavily doped substrate, it is Ohmic after an anneal. The contact pattern is the same as in Figure 2.

















