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Engineering the Schottky Interface of 3.3 kV SiC JBS Diodes Using a P_2O_5 Surface Passivation Treatment

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Abstract. A systematic study is presented into the impact of a P_2O_5 surface passivation treatment, carried out prior to the deposition of a high refactory metal contact to 3.3 kV JBS diodes. Electrical results from Mo, W and Nb diodes reveal that those diodes that undergo the treatment have a major leakage current reduction, most significantly by 3.5 orders of magnitude to 1.5×10^{-6} A x cm^{-2} for treated W diodes. When applied to fully optimized 3.3 kV Mo/SiC JBS diodes, the P_2O_5 surface passivation treatment reduces the apparent barrier height, as well as the leakage current. SIMS analysis reveals that during the treatment, phosphorous diffuses into the top 50 nm of the SiC, achieving a peak density of 10^{19} cm^{-3}, while XPS results suggest some of this diffuses into the contact metal during the contact anneal, altering the Schottky barrier height. TCAD simulations help give more insight into band diagram changes at the Schottky interface, where the partial activation of the phosphorous ions is shown to alter the Schottky barrier, promoting a thermionic field emission conduction, effectively lowering the barrier height at the interface in Mo/4H-SiC diodes.

Introduction

SiC Schottky diodes have now been commonly adopted, replacing legacy Si PiN diodes in a number of applications [1]. Yet the voltage range of the commercial devices available is still narrow, 600-1700 V, and the widescale release of 3.3 kV devices would be attractive for traction, PV and industrial inverters. Just as at lower voltages, the Schottky barrier height (SBH) can be controlled by the choice of contact metal and the related processing steps. The choice of SBH is a trade-off between low forward voltage drop with a low SBH, and low leakage current with a high SBH. However, in reality, minimising on-state conduction losses is typically prioritised and a low SBH will be chosen by utilising titanium (Ti), or molybdenum nitride (MoN) contacts to create a SBH as low as 0.86 eV [2, 3]. This group recently reported on the development of a surface passivation treatment, in which a phosphorous pentoxide (P_2O_5) layer is grown on the surface, and then removed, prior to the deposition of a Mo contact metal [4]. This resulted in a reduced on-state SBH, 0.11 eV lower than the untreated version, and a lower leakage current by two to three orders of magnitude. In this paper, we use secondary ion mass spectrometry (SIMS), transmission electron microscopy (TEM) and x-ray photoelectron spectroscopy (XPS) to provide a detailed picture of the changes that occur in the SiC Schottky subsurface region. The P_2O_5 treatment is also applied to other refractory metals, tungsten (W) and niobium (Nb), as well as to fully optimised 3.3 kV junction barrier Schottky (JBS) diodes.

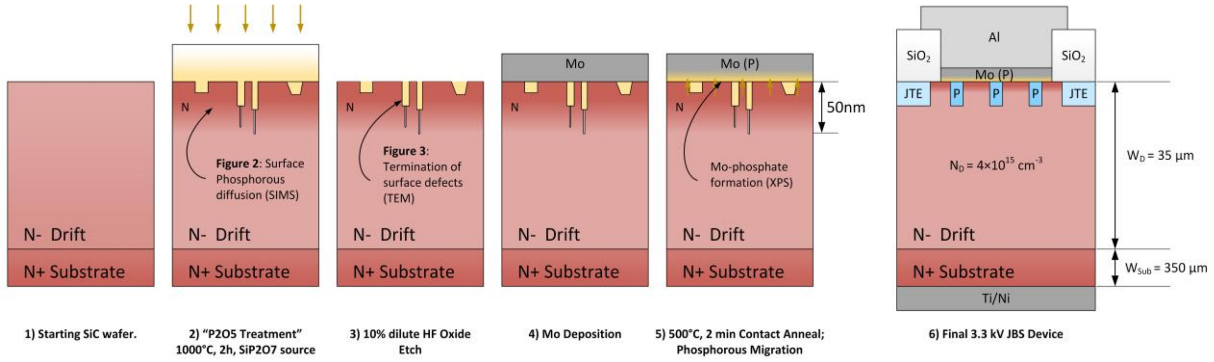


Figure 1: 1-5 show the processing steps carried out during the P_2O_5 treatment and Mo/SiC contact formation, and their effect on the Schottky interface. 6 shows the layout of the final 3.3 kV JBS diode.

Experimental

For the fabrication of W, Nb and Mo mesa isolated Schottky diodes on 4 x 10^{15} cm^{-3} lightly nitrogen doped epitaxial layers (starting wafer in Fig. 1, step 1), the P_2O_5 deposition was carried out at 1000°C for 2 hours in nitrogen (N_2) ambient in a tube furnace, utilising a silicon diphosphate (SiP_2O_7) source wafer. This process results in the deposition of P_2O_5 on the surface of the SiC samples (Fig. 1, step 2), with phosphorous partly diffusing into the SiC. After having removed the previously deposited oxide on top of SiC (Fig. 1, step 3), the e-beam deposition of 100 nm of W, Nb or Mo was done on the diodes, respectively. The formation of a Schottky contact was then finished after a rapid thermal anneal at 500°C for 2 minutes was carried out. The exact process conditions of the fabrication can be found in [4].

To test the P_2O_5 process on fully optimised and terminated device structures operating at high currents and reverse voltages, 3.3 kV SiC JBS diodes (active areas 1.56 mm^2 and 42.25 mm^2) were then produced. The full details of the fabrication process of these JBS devices can be found in [5].

Results and Discussion

On-state and off-state rectifying characteristics of the unterminated Mo, W, and Nb diodes were measured using a Keysight B1505A with a Semiprobe semi-automatic probe station. Ideality factors (*n*) and barrier heights in the on-state were extracted between forward current densities of 1×10^{-7} to

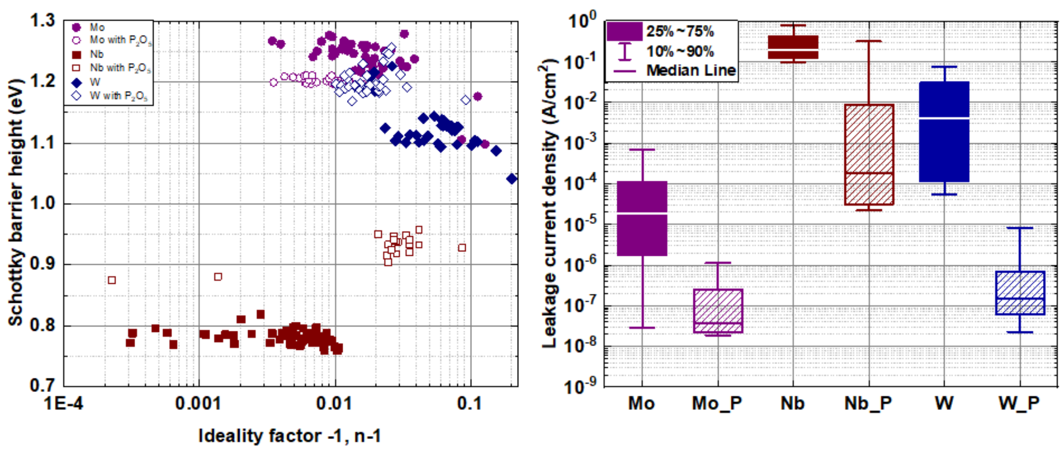


Figure 2: (left) Ideality factors and SBHs for 4.39 x 10^{-2} mm^2 refractory metal/SiC Schottky diodes. (right) Leakage current densities (at -200 V) of more than 100 devices of each small area refractory metal/SiC Schottky diodes.

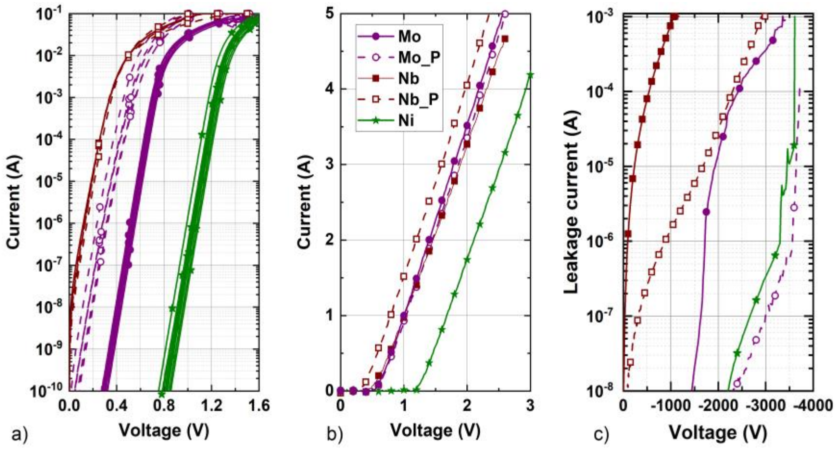
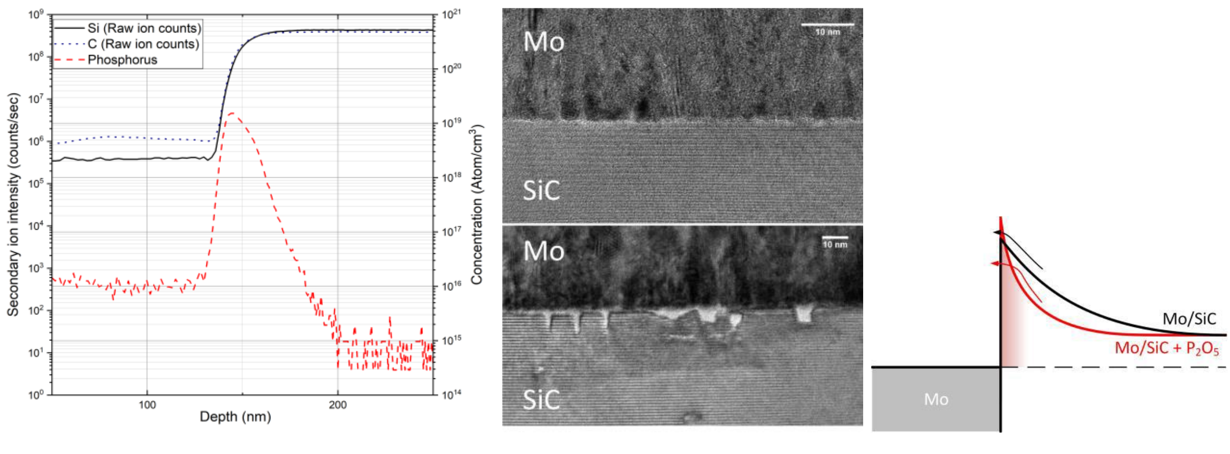


Figure 3: On state characteristics of a) the 1.56 mm^2 JBS diodes and b) the 42.25 mm2 JBS diodes; c) off state characteristics of the 1.56 mm^2 JBS diodes [5].

1×10^{-3} A x cm^{-2}. An overview of the distribution of these parameters can be seen in Fig. 2. Across the entire dataset, the P_2O_5-treatment consistently reduces leakage current densities (J_R), the largest reduction being for the W diodes, which reduces from 4.12×10^{-3} A x cm^2 for those untreated, to 1.46×10^{-6} A x cm^{-2} for those treated. A similar reduction by three orders of magnitude to 3.71×10^{-8} A x cm^{-2} takes place in the P_2O_5-treated Mo devices, and to 1.85×10^{-4} A x cm^{-2} in the Nb devices.

In the on-state, all measured devices showed ideality factors lower than 1.12 which proves the applicability of the thermionic emission model [6]. The trends of the SBH vary according to the metals: the initially low barrier height of Nb Schottky diodes of 0.78 eV is increased after the P_2O_5 treatment to 0.93 eV. This trend is repeated in the W diodes, where the average barrier height is raised from 1.13 eV to 1.20 eV post treatment. However, as previously reported [4] the P_2O_5-treatment once again lowered the SBH of the Mo/SiC contacts, the average barrier height of treated diodes having reduced from 1.26 eV to 1.21 eV.

The on-state of the optimised device structures shows the reduction of barrier height for the Mo devices on smaller die size (Fig. 3 a)) as well as for the 42.25 mm^2 JBS diodes (Fig. 3 b)), a trend that follows the description presented in the previous paragraph.



(a) (b) (c)

Figure 4: a) SIMS analysis showing the build-up of P at the P2O5 treated Mo/SiC interface, b) HR-TEM images of the untreated (top) and P2O5 treated (bottom) Mo/SiC interface [5], and c) Mo/SiC band diagrams, pre-and post-treatment, based on TCAD simulations.

In the off-state of the 3.3 kV JBS diodes (Fig. 3 c)), a higher proportion of the treated devices reached the rated voltage without suffering soft breakdown. This effect is thought to be attributable to the passivation of leakage current paths beneath the Schottky interface, as XPS, SIMS and TEM results show [4]. Little difference was witnessed between treated and untreated devices, in either the resistance of large area devices (Fig. 3b)), or the switching performance of the devices. These results suggest that P_2O_5-treated Mo/SiC devices could be utilised to reduce leakage current in a 3.3 kV JBS diode, so maximising the size (the current rating) that these chips could be scaled up to.

A number of characterisation techniques offer up an insight into the effect of each step of the P_2O_5 treatment and subsequent metallization, and this is summarized in Fig. 1. First, SIMS analysis (Fig. 4a), shows that the treatment results in the diffusion of P into the subsurface, to a depth of 50 nm, and a peak concentration of 10^{19} atoms/cm^{-3}. However, with a processing temperature of just 1000°C, only a small fraction of these are expected to be electrically active. Second, TEM micrographs (Fig. 4b) taken before and after the P_2O_5 treatment suggest that surface imperfections form, and are subsequently filled, during the P_2O_5 deposition. EDX analysis on these confirmed that the oxide remains in place after HF etching and metallization. Third, XPS analysis (not shown) of thin Mo layers formed on untreated and treated surfaces shows that the work function of the interfacial metal increases by around 0.1-0.2 eV, likely the result of P diffusion from the subsurface during the contact anneal, forming a Mo phosphate at the interface.

The combined effect of these three observed changes brings about a complex change to the band structure at the Schottky interface, as modelled in TCAD (Fig. 4c). The increase in metal work function is counteracted by a reduction in Fermi level position relative to the conduction band edge (E_C-E_F). If 1% of the subsurface P is electrically active (peak concentration of 10^{17} cm^{-3}), then E_C-E_F is reduced by 80 meV. The increase in interfacial doping also encourages thermionic-field emission through the barrier at lower energy levels. These competing effects heavily influence the on-state, and an overall reduction in the Mo/SiC SBH (from forward I-V measurements) is consistently recorded in both the small area diodes (Fig. 2) and the JBS diodes (Fig. 3). However, the SBH of treated Nb and W contacts is consistently higher than that of their untreated counterparts, likely due to a larger metal work function increase.

Conclusion

Electrical results of refractory metal (W, Nb and Mo) Schottky diodes that had undergone a P_2O_5 treatment demonstrated a consistent reduction of leakage current across the entire dataset, when they were compared to their untreated counterparts. For Mo SBDs, this occurred in parallel to a reduction in barrier height. Whilst the application of the same treatment on fully optimised 3.3 kV Mo JBS diodes repeated the observed improvement, surface investigations using SIMS, XPS and EDX showed that this was likely due to the diffusion of phosphorous into the SiC top surface, and later into the contact metal. TCAD simulations suggested that the changes in the on-state were caused by an increase in subsurface doping due to the presence of partially-activated phosphorous ions after the treatment. These causes a reduction of E_C-E_F by approximately 80 meV, whilst the increased doping enhances thermionic field emission conduction through the barrier.

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