

# STABILITY OF SCHOTTKY CONTACTS WITH TA-SI-N AMORPHOUS DIFFUSION BARRIERS AND AU OVERLAYERS ON 6H-SiC

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## Abstract

Backscattering spectrometry and electrical measurements are used to study the thermal stability of three sputter-deposited Schottky contact metallizations. A <6H-SiC>/TaSi<sub>2</sub>/Ta<sub>20</sub>Si<sub>40</sub>N<sub>40</sub>/Au metallization changes its Schottky barrier height from 0.71eV to 0.62eV upon annealing at 600°C for 30 min., while its ideality factor changes from an initial value of 1.55 to 1.18. Both Schottky barrier height and ideality factor remain stable upon further annealing of the sample at 700°C for 30 min. and for 90 min. The observed stability is attributed to the known thermal stability of TaSi<sub>2</sub> with SiC and to the effectiveness of the Ta-Si-N diffusion barrier. A <6H-SiC>/Ta<sub>36</sub>Si<sub>14</sub>N<sub>50</sub>/Au that does not include the silicide contacting layer becomes ohmic after vacuum annealing at 600°C for 30 min., while no signs of metallurgical interaction are evidenced in its backscattering spectrum.

An initial Schottky barrier height of 0.71 and ideality factor of 1.6 was measured for a <6H-SiC>/Re sample. After 2hrs. annealing the Schottky barrier height and ideality factor have changed to 1.04 eV and 1.16, respectively and remained stable after annealing for additional 2hrs. at the same temperature.

## 1. INTRODUCTION

Today's high power and high temperature semiconductor devices are based mainly on silicon and GaAs. The temperature limit for continuous operation of silicon- and GaAs- based devices is known to be 300°C and 460°C, respectively, when special fabrication methods and precautions are applied in their production [1,2]. For applications in deep wells, avionics, space, and high density packaging, there is a need for electronic devices that could operate at 600°C. The natural choice for high-temperature applications is a wide bandgap material, as a wider bandgap provides lower intrinsic carrier concentration for a given temperature and therefore a larger temperature range over which a pn junction can exist.

Among the wide bandgap materials that are available over an adequate range of doping, silicon carbide offers the widest bandgap together with a high thermal conductivity (4.9 W/cmK) and an avalanche breakdown field ( $3 \times 10^6$  V/cm) which is an order of magnitude larger than that of silicon. Silicon carbide occurs in many polytypes differing from one another only in the stacking sequence of the double closed packed layers of Si and C atoms [3]. The two most common polytypes of silicon carbide are 3C-SiC ( $E_g=2.2\text{eV}$ ) and 6H-SiC ( $E_g=2.86\text{eV}$ ). The interest in the 6H polytype has grown

rapidly in the last few years owing to new growth techniques which made available epitaxial layers grown on bulk material [4].

In view of its high chemical stability and low intrinsic carrier concentration of 6H-SiC, its high-temperature applications will be limited by the stability and the reliability of the contact metallization. The thermal stability of several metal/SiC contacts have been studied so far, most of these metals were found to react with SiC at elevated temperatures. Schottky barrier height measurements were made mostly on as-deposited samples, but also on annealed samples [5]. All the Schottky diodes reported so far were found to change their characteristics because the metal reacted with the substrate upon annealing.

In this paper we report on the thermal stability of the barrier height of Schottky diodes utilizing complete metallization schemes with an amorphous Ta-Si-N diffusion barrier and Au overlayer. Amorphous diffusion barriers are the most promising candidates for high-temperature metallizations. They do not have extended defects of the kind that provide fast diffusion paths in polycrystalline materials. Ta-Si-N belongs to the class of amorphous barriers which effectiveness has been demonstrated in metallizations for silicon, gallium arsenide and diamond [6-8]. Crystallization temperature of Ta<sub>36</sub>Si<sub>14</sub>N<sub>50</sub> barrier is about 900°C and its resistivity is about 600 μΩcm. Backscattering spectrometry and I(V) measurement were used to study the <6H-SiC>/Ta<sub>36</sub>Si<sub>14</sub>N<sub>50</sub>/Au, and <6H-SiC>/TaSi<sub>2</sub>/Ta<sub>20</sub>Si<sub>40</sub>N<sub>40</sub>/Au systems before and after thermal annealing. The same methods were also used to study Schottky barrier height and stability of <6H-SiC>/Re.

## **2. EXPERIMENTAL PROCEDURES**

The 6H-SiC wafer purchased from CREE Research, Inc. was n-type, 280 μm thick, with an n-type epilayer 10 μm-thick having an open silicon face. The wafer and the epilayer were doped with nitrogen with doping levels of  $7.3 \times 10^{17}/\text{cm}^3$  and  $1 \times 10^{16}/\text{cm}^3$ , respectively. Prior to deposition the samples were degreased in organic solvents in an ultrasonic bath (trichlorethylene, acetone, and methanol, sequentially). Circular diodes of three different diameters (0.05, 0.1, 0.25 cm) were fabricated by photolithographic patterning and lift-off. Immediately before the deposition the samples were etched in a 10% HF solution for 10s to clean up the contact windows and dried in N<sub>2</sub> gas flow. All films in this study were deposited by rf-sputtering using a planar magnetron cathode of 7.5 cm in diameter. The substrate plate was placed 7 cm below the target and was neither cooled nor heated externally. The sputtering system is equipped with a cryopump and a cryogenic baffle that yields a background pressure of  $4 \times 10^{-7}$  Torr prior to the sputter deposition.

The TaSi<sub>2</sub> layers were deposited in Ar at 10 mTorr total pressure and 300W rms forward sputtering power. The Ta-Si-N films were deposited in a discharge of Ar/N<sub>2</sub> gas mixture at a N<sub>2</sub> to Ar flow ratio of 0.036 and a total gas pressure of 10 mTorr. The Au overlayers and Re films were deposited at 5 mTorr total pressure and 200W rms from elemental targets. The flow of Ar and the total gas pressure were adjusted by mass flow controllers and monitored with a capacitive manometer in a feedback loop.

Annealings after the deposition were done in an evacuated tube furnace ( $5 \times 10^{-7}$  Torr). Samples for backscattering were processed concurrently with the diode samples.

The Current-Voltage I(V) characteristics were measured using a HP-4145A parameter analyzer and were performed at room temperature. An indium-gallium alloy was used as a back

contact. The I(V) characteristics were analyzed using the thermionic emission model. Lien's method [9] was employed to calculate the series resistance, followed by a least-squares fit of the corrected I vs. V-IR to obtain the saturation current density ( $J_s$ ) and the ideality factor. With  $J_s$ , The barrier height was calculated from the equation [10]:

$$\Phi_B = \frac{kT}{q} \ln \left( \frac{A^{**} T^2}{J_s} \right)$$

where  $A^{**}=72 \text{ A/cm}^2\text{K}^2$  is the effective Richardson constant for 6H-SiC.

Before and after the thermal annealing, the diode samples were characterized by I(V) measurements to determine the Schottky barrier height and the ideality factor. The backscattering samples were characterized by 2 MeV  $^4\text{He}^{++}$  backscattering spectrometry to determine compositional profiles and monitor interdiffusion or reactions in the samples.

### 3. RESULTS AND DISCUSSION

In all cases studied in the frame of this work it was verified that the current was scaling with the area of the diodes. This proves that it is the metal/epilayer interface that determines the I(V) characteristics and not the back contact, and that the current is not due to a peripheral leakage, but flows across the area of the contact.

#### 3.1 <6H-SiC>/TaSi<sub>2</sub>(50 nm)/Ta<sub>20</sub>Si<sub>40</sub>N<sub>40</sub>(80 nm)/Au(50 nm)

The forward I(V) characteristics of <6H-SiC>/TaSi<sub>2</sub>(50 nm)/Ta<sub>20</sub>Si<sub>40</sub>N<sub>40</sub>(80 nm)/Au(50 nm) Schottky diodes change after 1h annealing in vacuum at 700°C from a barrier height of 0.70 eV to 0.61 eV and from ideality factor of 1.55 to 1.18, but show no significant changes upon further annealing at 700°C (Fig.1). As most of the silicides are known to be stable with SiC (that includes TaSi<sub>2</sub>, see the Ta-Si-C phase diagram given in ref [11]) and have a tieline with SiC, it is expected that TaSi<sub>2</sub> provides a thermally stable contacting layer. However, to avoid an interaction between a Au overlayer and the contacting layer or SiC during high temperature operation of devices, it is necessary to use diffusion barriers in the contacting scheme [6]. Our results show that the Schottky barrier height of such a contact is stable at 700°C.

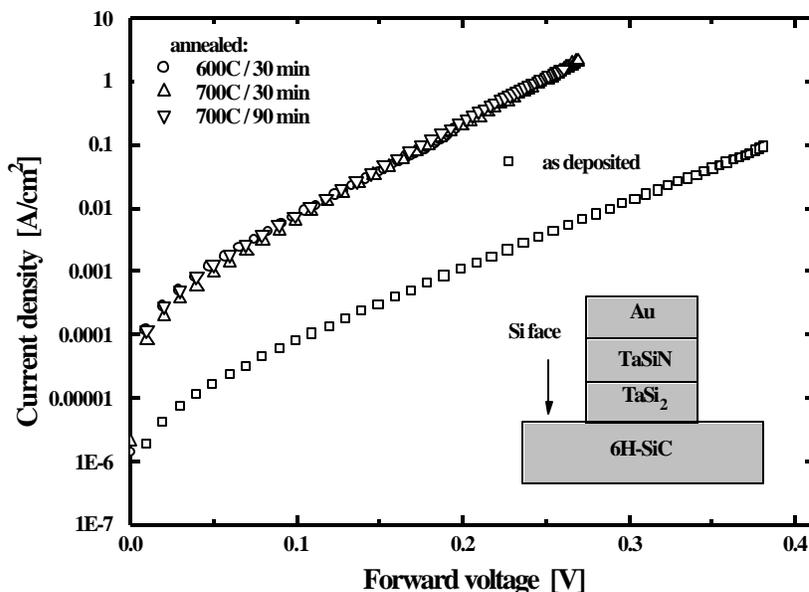


Fig.1 A semilogarithmic I(V) plot <6H-SiC>/TaSi<sub>2</sub>/Ta<sub>20</sub>Si<sub>40</sub>N<sub>40</sub>/Au diode before and after in-vacuo annealing at 700°C.

### 3.2 <6H-SiC>/Ta<sub>36</sub>Si<sub>14</sub>N<sub>50</sub> (80 nm)/Au(45 nm)

Omitting the TaSi<sub>2</sub> contacting layer results in a contact that seems metallurgically stable as the backscattering spectra obtained from a <3C-SiC>/Ta<sub>36</sub>Si<sub>14</sub>N<sub>50</sub>(80 nm)/Au(45nm) after thermal annealing at 600°C for 1 h perfectly overlaps with that of the as-deposited sample (fig.2). However, diodes of the same metallization change to "soft" I(V) characteristics following the same annealing procedure(fig.3). The effects causing the change in the I(V) characteristics have yet to be investigated as they may provide means for making ohmic contacts to SiC. In any case, this observation shows that the omission of the TaSi<sub>2</sub> reduces the stability, while the incorporation of this layer favors the stability of the Schottky contact.

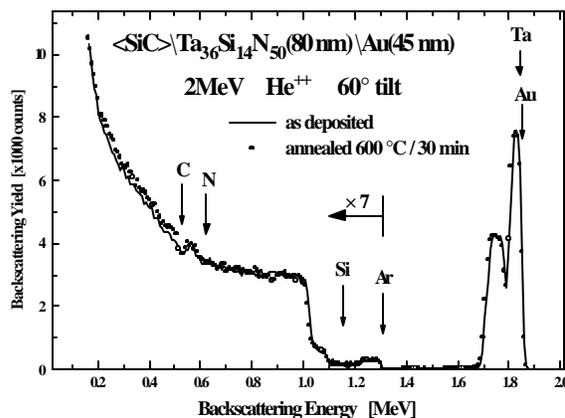


Fig.2 2 MeV <sup>4</sup>He<sup>++</sup> backscattering spectra of <SiC>/TaSi<sub>2</sub>/Ta<sub>36</sub>Si<sub>14</sub>N<sub>50</sub>/Au before and after in-vacuo annealing at 600 °C for 30 min.

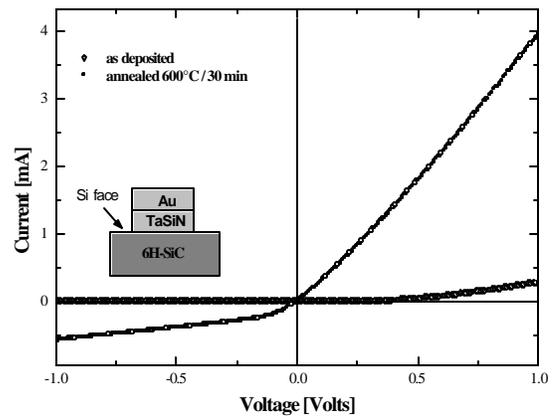


Fig.3 A linear I(V) characteristics of <SiC>/TaSi<sub>2</sub>/Ta<sub>36</sub>Si<sub>14</sub>N<sub>50</sub>/Au before and after in-vacuo annealing at 600 °C for 30 min.

### 3.3 <6H-SiC>/Re(100 nm)

Rhenium is the only known metal that has a tieline to SiC in a ternary Si-C-Re phase diagram [12]. The stability of Re thin films on SiC was confirmed in a study by Chen et al. [12]. They used backscattering spectrometry, x-ray diffractometry and cross-sectional transmission electron microscopy to confirm that Re is thermally stable on Beta-SiC up to 1100°C. This property makes Re an excellent candidate for a stable

Schottky contact. Figure 4 shows the backscattering spectra of a 100 nm thick Re film on 6H-SiC before and after annealing in vacuum at

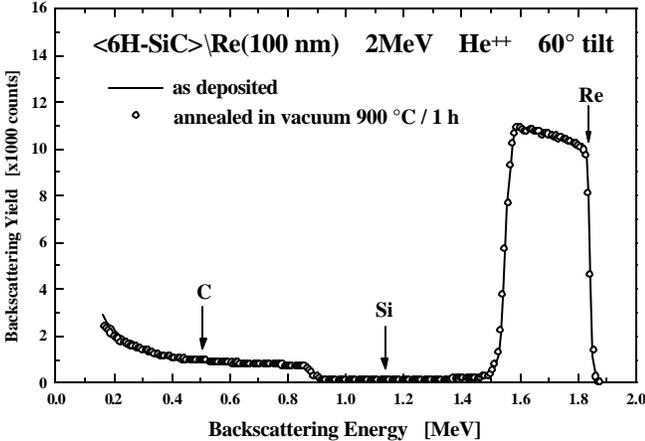


Fig.4 2 MeV 4He++ backscattering spectra of <6H-SiC>/Re before and after in-vacuo annealing at 900°C for 1 h.

900°C for 1h. The spectra overlap entirely within experimental accuracy, which confirms the thermal stability of Re with 6H-SiC. Fig.5 depicts the forward I(V) characteristics of a 100 nm-thick Re film sputtered on the n-type 6H- SiC epilayer before and after vacuum heat treatment for 2 and 4 hours at 700°C.

An exponential behavior is observed in all cases with ideality factor of 1.6 for as-deposited Re and of 1.16 for both 2 and 4 h annealing steps. The barrier height increases from a value of 0.71eV for the as-deposited sample to a value of 1.04 eV after the 700°C annealing. A comparable behavior was reported for sputter deposited TiN [13] and for W-Si-N and Ta-Si-N [14] Schottky diodes on n-type silicon. Both papers describe an observed increase in barrier height upon annealing. In both cases, an explanation is suggested, which connects a possible annealing out of donor-like traps formed by sputter-induced damage with the barrier height rise.

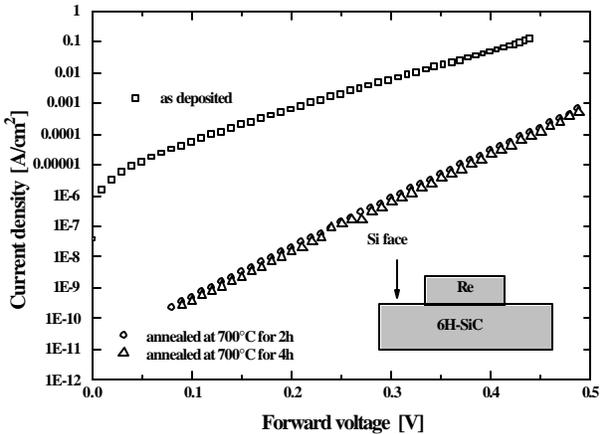


Fig.5 A semilogarithmic I(V) plot <6H-SiC>/Re before and after in-vacuo annealing for 2 and 4h at 700°C.

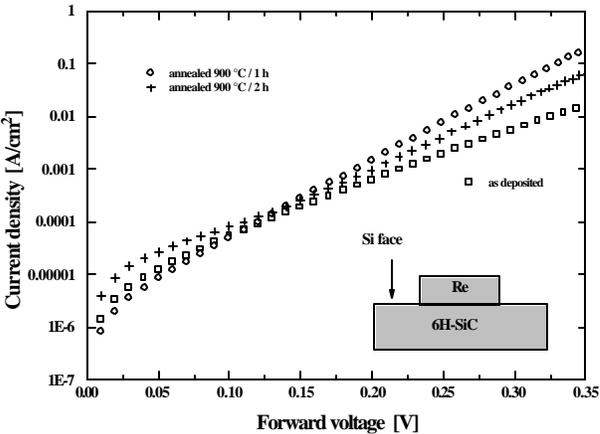


Fig.6 A semilogarithmic I(V) plot <6H-SiC>/Re before and after in-vacuo annealing 1 and 2 h at 900°C.

Further annealing at 900°C for 1 h of the sample previously annealed at 700°C results in a lowering of the Schottky barrier height from 1.04eV to 0.76eV and a slight increase in the ideality factor from 1.16 to 1.25 (Fig.6). The same results were obtained for a sample directly annealed at 900°C (not shown in Fig.6). Annealing for additional hour at 900°C results in a further increase of the ideality factor from 1.25 to 1.36 and occurrence of a "leaky" current component. This type of increase of the current in the low values of the applied voltage is usually attributed to recombination in the depletion region. Small local atomic displacements that are likely to take place upon annealing at 900°C, and are small enough not to be detected in transmission electron microscopy can still significantly alter the electronic transfer across the interface. Similar observation was described by Tung [15] and was attributed to an inhomogeneity of the Schottky barrier height. Our measurements, however, cannot provide this type of microscopic information.

#### **4. SUMMARY AND CONCLUSION**

Backscattering spectrometry and forward IV measurements were used to study the thermal stability of three rf-sputtered metallizations for 6H-SiC. Table 1 summarizes I(V) measurements results:

contacting layer	as-deposited		600 °C		700 °C		900 °C	
	$\phi$ [eV] ( $\pm 0.01$ )	n ( $\pm 0.02$ )	$\phi$ [eV] ( $\pm 0.01$ )	n ( $\pm 0.02$ )	$\phi$ [eV] ( $\pm 0.01$ )	n ( $\pm 0.02$ )	$\phi$ [eV] ( $\pm 0.01$ )	n ( $\pm 0.02$ )
TaSi <sub>2</sub>	0.70	1.55	0.62	1.18	0.61	1.18	-	-
TaSiN	0.76	1.27						
Re	0.71	1.60			1.04	1.16	0.76	1.36

Table 1: Summary of I(V) measurements results

I(V) measurement done at different stages of heat treatment show that thermal stability of the contacting layer/SiC couple is an advantage for the stability of the resulting I(V) characteristic. Both TaSi<sub>2</sub> and Re are thermally stable in contact with SiC, and in both cases, stable I(V) characteristics have been demonstrated for hours of annealing at temperatures as high as 700°C. Yet the thermal stability of the contacting layer by itself is insufficient to prevent changes in the characteristics upon initial annealing. Minor thermally-induced interfacial atomic rearrangements, too small to be detected even by transmission electron microscopy (see [12]), can evidently alter the electronic transport across the SiC/metal interface in major ways. Some of these changes are attributable to the removal of sputtering-induced defects that act as electron traps and are introduced in the SiC near its surface during the deposition of the film. A thermal annealing of these traps raises the barrier height, such as is observed with Re. But other interfacial processes that appear to be element-specific evidently also exist and they can reduce the barrier height upon initial annealing, as is exemplified by the case of TaSi<sub>2</sub> contacting layer. At temperatures near 1000 °C, diffusional interactions, possibly involving impurities, also begin to play a role.

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