Toward a better understanding of Ni-based ohmic contacts on SiC

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\textbf{Abstract.} There is still little consensus regarding why low contact resistivity is achieved when Ni on n-type 4H- and 6H-SiC is annealed at temperatures above 950°C. The objective of this paper is to provide an answer to this question. It has been reported that even Ni-based contacts formed in the n++ region exhibited a steep reduction of contact resistivity in an annealing temperature range > 900°C. This reduction cannot be explained by the carbon vacancy induced donor model (V\textsubscript{c} model) proposed by Han and his coworkers [Appl. Phys. Lett., Vol. 79, p. 1816 (2001)]. It was observed that the surface of substrates annealed at 1000°C was not covered with Ni\textsubscript{2}Si but with a thin layer of NiSi. Finally, a plausible model is proposed that annealing at higher temperatures results in the formation of a NiSi/SiC system at the substrate interface, causing contact resistivity to be reduced significantly.

\textbf{Introduction}

Ohmic contacts in power devices play an extremely important role in the injection and ejection of high current from and to the power source and electrical load. Ni-based contacts, fabricated by thin Ni film deposition followed by rapid thermal annealing (RTA) at 950°C-1050°C, have now become the mainstream contacts to the n-type region on SiC power devices. However, as reviewed by Roccaforate [1], there is still little consensus regarding why low contact resistivity is achieved when Ni is annealed at temperatures above 950°C. The objective of this paper is to present some experimental results that provide an answer to this question.

\textbf{Experimental}

Linear transmission line model (TLM) contacts 100×200 µm\textsuperscript{2} in area and Schottky barrier diodes (SBDs) 200 µm in diameter with Ni-based electrodes were fabricated together on 8° off-cut (0001)\textsubscript{Si} face n+ 4H-SiC substrates with an epitaxially grown 10-µm-thick n–layer (Fig. 1). The electrodes were prepared by RTA of 50-nm-thick Ni at temperatures ranging from 600°C to 1000°C. The RTA time was 30 min at 600°C, 5 min at 700°C and 2 min at the other higher temperatures. The TLM contacts, having a Ta/TaN/Al-Si overlayer, were formed in phosphorus ion hot-implanted and activated n++ regions (N\textsubscript{D} = 2.5×10\textsuperscript{20} cm\textsuperscript{-3}, \textit{X}_f = 250 nm), which were electrically isolated from the substrate and the surrounding area by p-well (Al+)
implantation and mesa etching. The fabrication process is described in §13.2.3 and §13.2.4 of Ref. 2. The Al electrode was deposited at the back side of the SBDs by electron beam (EB) evaporation after removal of the back thermal-oxide preceded by top Ni-silicide formation, which showed superior ohmic contact properties. Blanket Ni-based electrode samples were also formed on epitaxial 4H-SiC substrates for physical characterization by X-ray diffraction spectroscopy (XRD) and cross-sectional transmission electron spectroscopy-energy dispersive X-ray spectroscopy (XTEM-EDS). All Ni-based electrodes (or contacts) described here were formed by high-vacuum EB deposition just after removal of the surface thermal oxide immediately followed by RTA under an Ar ambient with a very low dew point. The specific contact resistivity, $\rho_C$, of the TLM contacts was precisely measured with the transfer length method and a four-point probe remote sensing technique. XRD (0-2θ) analysis revealed that silicidation of Ni was completed for all the samples and that only the Ni$_2$Si phase was detected regardless of the annealing temperature.

Results and Discussion

The TLM contacts exhibited linear I-V characteristics independent of the RTA temperature, $T_A$, even for the as-deposited sample. Figure 2 shows the logarithmic average $\rho_C$ as a function of $T_A$, indicating a steep decline in $\rho_C$ at temperatures over 800°C. The minimum $\rho_C = 1.1 \times 10^{-6}$ $\Omega$cm$^2$ was attained at 1000°C. A similar result was previously reported for TLM contacts in an n$^+$ epilayer on p-type 4H-SiC, in which nitrogen was doped at a level of $1.5 \times 10^{19}$ cm$^{-3}$ [2]. This steep temperature dependence of $\rho_C$ for contacts in the n$^{++}$ region cannot be explained by the carbon vacancy induced donor model (Vc model) proposed by Han and his coworkers [3, 4] because heavy doping eclipses the increased donor effect. Figure 3 shows the interface between the Ni-silicide and the epilayer (n$^{++}$ region) captured by high-resolution XTEM, when the Ni (TLM) electrode was annealed at 1000°C. We can see from this image that the Ni-silicide just contacts the undeformed and ordered 4H-SiC crystal. Previously, Han and Lee used X-ray photoelectron spectroscopy (XPS) to observe the changes in the atomic ratio of Si/C at the interface for various annealing temperatures. Their results indicated that, after annealing at 950°C, the ratio abruptly increased up to Si/C > 1.2, implying that Vc was produced below the contact [4]. An unbalance in the Si/C ratio of more than 20% would naturally destroy the 4H-crystal structure. That would be inconsistent with our result in Fig. 3. We speculate that this inconsistency was caused by a misinterpretation of XPS depth profiling data. Recently, Calcagno [5] and La Via [6] used deep level transient spectroscopy (DLTS) in an effort to detect a high concentration of Vc under 950°C-annealed contacts, as predicted by Han and Lee, but a DLTS signal suggesting the presence of such Vc was not observed at all. Thus, it can be concluded that the Vc model is suspect.

![Fig. 2](image1.png)

Fig. 2 The average specific contact resistivity, $\rho_C$, of the TLM contacts as a function of RTA temperature, $T_A$.

![Fig. 3](image2.png)

Fig. 3 High resolution XTEM photograph showing the interface between Ni-silicide and the epilayer (n$^{++}$ region). Ni was annealed at 1000°C.
Figure 4 displays the $T_A$ dependence of the Schottky barrier height, $\phi_B$, of the SBDs where the $\phi_B$ values were evaluated from their forward IV characteristics. The results indicate that $\phi_B$ also rapidly dropped with increasing $T_A$ at temperatures above 800°C. It is interesting that the plotted profile closely resembles that in Fig. 2. Figure 5 plots the correlation between log($\rho_C$) for TLM contacts and $\phi_B$ for the SBDs using $T_A$ as the parameter. A significant linear relationship was found between these variables, which strongly suggests that the steep decrease in $\rho_C$ of the TLM contacts shown in Fig. 2 resulted from the marked drop in the $\phi_B$ of the contacts themselves. This conclusion is based on the fact that the SBDs were probably identical in interface properties to the TLM contacts since they were structurally the same and simultaneously fabricated, the repudiation of the $V_c$ model and the results of the DLTS validations [5, 6].

Figure 6 shows (a) an XTEM photograph and (b) an EDS elemental analysis along the yellow line in (a) for the cross section of a blanket contact sample on 4H-SiC annealed at 1000°C where Ni was exceptionally 100 nm in thickness. Note that the EDS signal ratio of Ni to Si was adjusted so as to be 2 in the major part of the Ni-silicide electrode, based on the results of the XRD analysis mentioned earlier. It can be seen from this figure that: (1) the Ni-silicide electrode includes three discrete carbon

![Fig. 4 The Schottky barrier height, $\phi_B$, of the SBDs as a function of RTA temperature, $T_A$.](image)

![Fig. 5 Correlation between specific contact resistivity and Shottky barrier height](image)

![Fig. 6 XTEM-EDS analysis for a cross section of a blanket Ni contact sample on 4H-SiC annealed at 1000°C: (a) XTEM photograph and (b) EDS elemental profile along the yellow line in (a).](image)
bands, C1, C2 and C3; (2) there is a pure Ni-silicide layer about 20 nm in thickness between the C1 band and the SiC substrate [2, 5]; (3) this thin silicide layer corresponds in composition to NiSi rather than to Ni2Si. The formation of NiSi is thermodynamically feasible at higher temperatures > 900°C since the Gibbs free energy, ΔG, is negative in the reaction [7],

\[ \text{Ni} + \text{SiC} \rightarrow \text{NiSi} + \text{C}, \quad \Delta G_{950^\circ C} = -34.4 \text{ kJ/mol}. \]

Actually, Han et al. [3,4,8] and Kuchuk et al. [9] indicated the presence of NiSi right above the C1 band for 950°C annealing and at the substrate interface for 1050°C annealing, respectively. Probably, the NiSi/4H-SiC system might be lower in φB than the Ni2Si/4H-SiC system. Thus, the following plausible model is proposed which may explain why low contact resistivity is achieved with annealing of Ni on SiC at temperatures higher than 950°C: when the RTA temperature exceeds ~900°C, NiSi (inducing lower φB) starts to form or gather at the SiC substrate interface; as a result, the contact resistivity steeply declines and finally reaches its minimum when the interface is completely covered with NiSi.

Summary

Ni-based (TLM) contacts formed in the n++ region exhibited a steep reduction in contact resistivity with annealing at TA > 900°C. The carbon vacancy induced donor model cannot well explain this reduction. A linear relationship was clearly observed between log(ρC) for TLM contacts and φB for SBDs when plotted using TA as a parameter. This fine correlation strongly suggests that the steep reduction in ρC of the TLM contacts does not result from an increase in carrier concentration under the contacts but from a decrease in their φB. XTEM-EDS analysis revealed that the substrate surface annealed at 1000°C was covered with a very thin Si-rich silicide, most probably, NiSi. It is presumed that the formation of the NiSi/SiC system contributes to the significant reduction in contact resistivity observed with contact annealing at temperatures above 900°C.

Acknowledgments

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