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The Formation Mechanism of Ni-based Ohmic Contacts to 4H-n-SiC

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Abstract. In this work the electrical properties of Ni and Ni_2Si contacts on n-type 4H-SiC were correlated to the strong structural changes at the contact/SiC interface upon annealing. We can conclude that only δ-Ni_2Si grains play a main role in determining electrical transport properties of the Ni-based ohmic contacts to n-SiC. It is presumed that a recrystallization and [013] texturization of δ-Ni_2Si phase on (0001)SiC-surface during high temperature annealing (> 900^{o}C) contributes to the change of barrier heights, as well as specific contact resistance of contacts.

Introduction

Commonly recognized difficulties in the fabrication of reliable and low-resistance ohmic contacts to SiC impede to take full advantage of excellent SiC properties with regard to high power high temperature electronic devices [1]. To solve this problem, deeper understanding of the mechanism of formation of ohmic contact is required; specifically more information on interfacial reactions at metal/SiC interface governing the transition from rectifying to ohmic contact is needed.

For n-type SiC, Ni-based contacts are the most commonly used ones and there are different explanations in the literature concerning their formation mechanisms [1]. The most controversial is the formation of nickel silicides [2] or graphitized carbon [3] at the contact/SiC interface. As the silicide formation occurs at much lower temperature (~ 600^{o}C) than the transition to ohmic behaviour (~ 950^{o}C) [4] it has been suggested that a formation of an interfacial graphite is responsible for the ohmic contact formation. This hypothesis was supported by the Raman spectroscopy analysis of annealed Ni, Ni_2Si and Pd contacts to 4H-n-SiC before and after acid etching [5]. On the other hand, by using the Photoelectron spectroscopy and electrical measurements to study the graphite/4H-n-SiC(0001) interface it has been shown that the Schottky barrier (φ_B) is 0.6 eV [6]. Thus, the formation of a carbon/graphite layer at the interface between metal and n-type 4H-SiC does not ensure ohmic behavior.

In order to better understand the formation mechanism and to correlate the microstructure of Ni-based contacts to n-SiC with the change of electrical properties during high-temperature annealing, a comparative study of Ni vs. Ni_2Si contacts on the same n-type 4H-SiC epitaxial wafers annealed at similar temperatures was carried out.

Experimental

In this work n-type (~ 1×10^{19} m^{-3}) Si-face 4H-SiC(0001) epitaxial wafers (~ 2.97 μm thick) from Cree Research Inc. were used. Before the deposition of the contacts the surface was chemically cleaned according to the procedure described previously [7]. The Ni (100 nm) and Ni/Si (66/60 nm) with Si first-layer contacts were sputter-deposited on unheated substrates. The samples were annealed at 600^{o}C (N_2, 15 min.) and subsequently at temperatures rising from 950 to 1100°C (N_2, 3 min.). Annealing of the Ni/Si multilayers at 600^{o}C led to the formation of stoichiometric silicide δ-Ni_2Si [4,7] and for convenience, the Ni/Si metallisations are denoted as Ni_2Si below in the text.

The electrical characterization of the contacts involved measurements of current-voltage (I-V) characteristics and of the specific contact resistance (r_c) using circular transmission line model (c-TLM). The c-TLM pattern prepared by lift-off photolithography consists of inner contact pads with a diameter of 100 μm and a metallized area separated by rings with a space of 10, 20, 30, 45 and 60 μm. The phase composition of the contacts was investigated by X-ray diffraction (XRD) using Philips X'Pert-MPD diffractometer with a Cu K_α radiation source. The contact/SiC interface was observed by transmission electron microscope (TEM) JEOL JEM-2100.

Results and discussion

The electrical properties of Ni and Ni_2Si contacts to 4H-n-SiC epi-wafers after annealing are shown in Fig. 1a. Non-ohmic I-V characteristics were observed for all as-deposited and annealed at 600°C contacts. The changes of the specific contact resistances with annealing temperature (≥ 950°C) for both ohmic contacts correlate well and annealing at 1000°C gives the minimal $r_c \sim 6\times10^{-5}$ Ω cm^2.

To form the ohmic contacts, the main transport mechanism through the interface of metal/semiconductor is considered as the thermionic emission (TE), field emission (FE) or thermionic field emission (TFE). The ratio E_{00}/kT gives an indication of the relative importance of TE ($E_{oo}/kT \ll 1$), FE ($E_{oo}/kT \gg 1$) or TFE ($E_{oo}/kT \sim 1$) [8]. In our case, (n-type 4H-SiC), the Padovani-Stratton parameter $E_{oo} = qh/4\pi\sqrt{N_d / m^*\varepsilon} = 31.5\ \text{meV}$, where q is the electronic charge, h is the Planck's constant, m^* is the effective mass of the electron in the semiconductor, ε is semiconductor dielectric constant and N_d is the donor concentration. A comparison of E_{oo} to the thermal energy kT shows thermionic field emission to dominate ($E_{oo}/kT = 1.25$). Thus, the φ_B of the contacts after annealing were estimated by comparing the measured and calculated r_c using Yu's thermionic field emission theory [8]. The calculated barrier heights are well correlated for both Ni_2Si(Ni)/n-SiC contacts with the minimal values of $\varphi_B \sim 0.43$ eV after annealing at 1000°C (Fig. 1b). These data quantitative correlate with previously reported for Ni-contacts to n-type 4H-SiC annealed at 1100°C ($\varphi_B = 0.44$ eV for $N_d = 7.7\times10^{15}$ m^{-3}) [6]. Thus, the similar changes of r_c and φ_B with high-temperature annealing for both contacts indicate on the same interaction processes at the contact/SiC interface region.

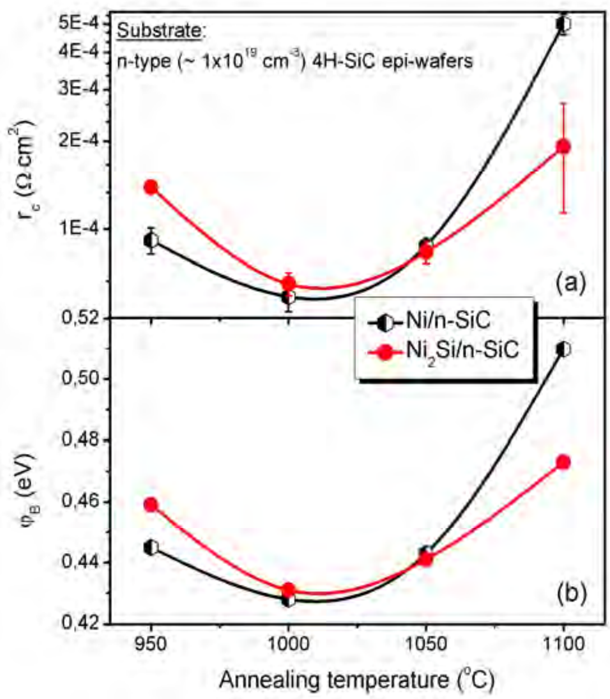

Fig. 1. Specific contact resistance (a) and effective barrier height (b) of Ni and Ni_2Si ohmic contacts to 4H-n-SiC vs. annealing temperature.

In order to investigate the reaction at the metallization/SiC interface leading to the formation of ohmic contacts, XRD and TEM techniques were applied to study the microstructure and interfacial properties of Ni_2Si/n-SiC contacts.

The results of XRD measurements performed in a Bragg-Brentano geometry, which probes through the depth of metallization, are shown in Fig. 2a. For the as-deposited Ni_2Si/n-SiC contact, only the (111) diffraction peak from textured polycrystalline Ni was detected. For the contact annealed at 600°C, the (013) and (020) peaks corresponding to the δ-Ni_2Si orthorhombic phase and the (300) peak corresponding to the $Ni_{31}Si_{12}$ hexagonal phase are observed. Taking into account that no trace of the Ni or Si peaks appears in the XRD pattern we conclude that a full thermally activated interaction between Ni and Si single layers took place. For the contact annealed at 950°C, only the (013) and (020) peaks of the δ-Ni_2Si phase were detected. The disappearance of the peak corresponding to the $Ni_{31}Si_{12}$ phase indicates a full transformation of other Ni-silicides into the δ-Ni_2Si orthorhombic phase. Moreover, as the intensity of the (013) peak is the highest, we can deduce a strong [013] texturization of the δ-Ni_2Si grains. For the contact annealed at 1050°C the

(020) peak disappears leaving only the (013) peak indicating a full [013] texturization of the grains. However, after strong interaction at the metallization/SiC interface at 1100°C, a degradation of the (013) structure is visible through a significant lowering of the intensity of the (013) line and a reappearance of the (020) peak as well as the appearance of a new peak ($2\theta \approx 47.74^o$) close to the (022) reflection of the Si-rich $NiSi_2$ phase. The structural changes in Ni_2Si/n-SiC contact with increasing of annealing temperature correlate well with RBS [7] and TEM [10] results.

Fig. 2b shows the intensity ratio of the (013) to (020) peaks (I_{013}/I_{020}) and FWHM (full width half maximum) for the δ-Ni_2Si(013) diffraction peak in the function of annealing temperature. A dashed horizontal line on the chart corresponds to $I_{013}/I_{020} \sim 2.5$ which is a theoretical value for a fully polycrystalline, non-textured film. The evolution of the texture can be traced from this figure as follows: after annealing at 600°C the film is (013) textured and the preferred orientation is getting stronger with each subsequent annealing at temperatures up to 1050°C. However, after annealing at 1100°C, the ratio I_{013}/I_{020} falls below 2.5 suggesting a destruction of δ-Ni_2Si(013) texture. Moreover, localized reactions and elongated island growth were observed across the surface for this contact [10]. It is clearly seen, that the change of [013] texturization with annealing temperature correlate well with change of FWHM for δ-Ni_2Si(013), which is justified since the latter is sensitive to the perfection and size of crystallites. It should be mentioned, that the [013] texturing of the Ni_2Si phase was also observed previously and for Ni/n-SiC contact [4,9].

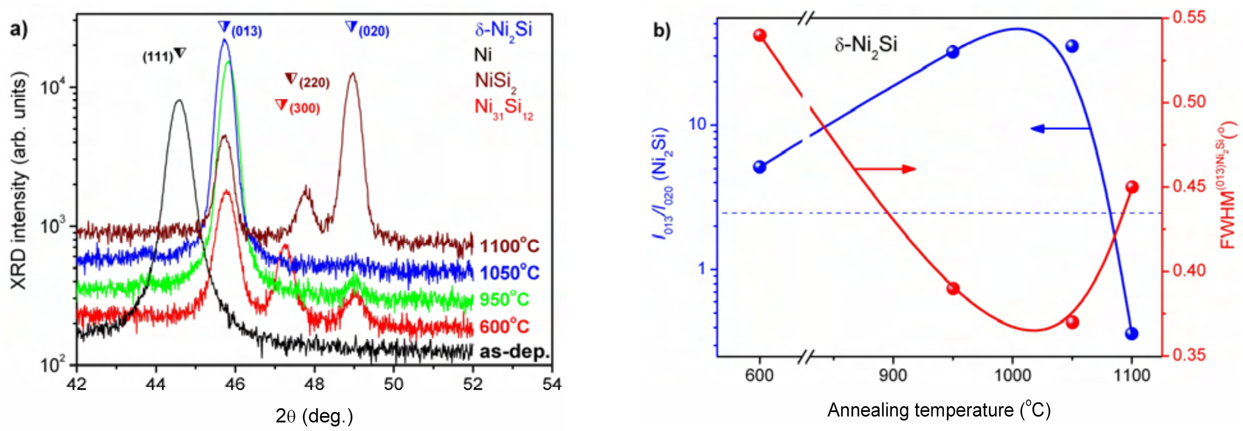

Fig. 2. (a) XRD patterns of Ni_2Si/n-SiC contacts before and after annealing at 600, 950, 1050 and 1100°C. (b) Ni_2Si texture (I_{013}/I_{020}) and FWHM of the (013) Ni_2Si peak vs. annealing temperature (horizontal dashed line shows the theoretical value for I_{013}/I_{020} in the absence of texture).

It becomes evident, that the formation of the Ni_2Si phase either by an interaction between Ni and SiC or by a solid state reaction between Ni and Si single layers on n-SiC is not sufficient for the formation of an ohmic contact to n-SiC. The recrystallization of Ni_2Si phase after annealing at high temperature (> 900°C) leads to the transition from rectifying to ohmic contact by lowering their barier height (Fig. 1b); this correlates well with the strong oriented growth of δ-Ni_2Si grains (Fig. 2b). Recently a steep reduction of r_c and decrease in φ_B at temperatures over 900°C for Ni-based ohmic contact to n-SiC was observed [11]. Using cross-sectional TEM-EDS (energy dispersive X-ray spectroscopy) analysis were made such conclusions: (i) the surface of substrates annealed at 1000°C was not covered with Ni_2Si but with a thin layer of NiSi; (ii) the formation of the NiSi/SiC system contributes to the significant reduction in contact resistance. Based on our reported results, we may conclude that only δ-Ni_2Si grains play a key role in determining electrical transport properties at the contact/SiC interface. Moreover, from Ni-silicides only the Ni_2Si is thermodynamically stable with SiC, which agrees well with the Ni-Si-C ternary phase diagram (tie lines connect Ni_2Si with SiC and C) [12].

In order to confirm this hypothesis, the interface between the 4H-SiC and the Ni-silicide was investigated using cross-sectional high-resolution TEM. For the Ni_2Si/n-SiC contact annealed at 600°C (Fig. 3a), amorphous layer, defects and grain boundary of Ni-silicides near the interface region are visible. The high-temperature annealed (1050°C) contact has a more ordered interface

(Fig. 3b), that is atomically abrupt and coherent without reaction layers, contaminants, or transition regions. Moreover, the absence of graphitic carbon at the interface, and the orientated silicide is evident. Indeed, silicide lattice fringes with distance of ~ 1.99 Å corresponding to the (013)-planes of δ-Ni_2Si (~ 1.982 Å) are perpendicular to the (0001) orientation of the 4H-SiC, indicating a texturization of the δ-Ni_2Si. The [013]-oriented δ-Ni_2Si corresponds to the highest (013) peak in the XRD patterns (Fig. 2a), which means that we have hetero-epitaxial orientation relationships: (0001)SiC//(013)δ-Ni_2Si. Similar [013] orientation of δ-Ni_2Si(Al) grain on the (0001) plane of the SiC substrate was also observed previously for Ni/Al contacts after annealing at 1000°C [13].

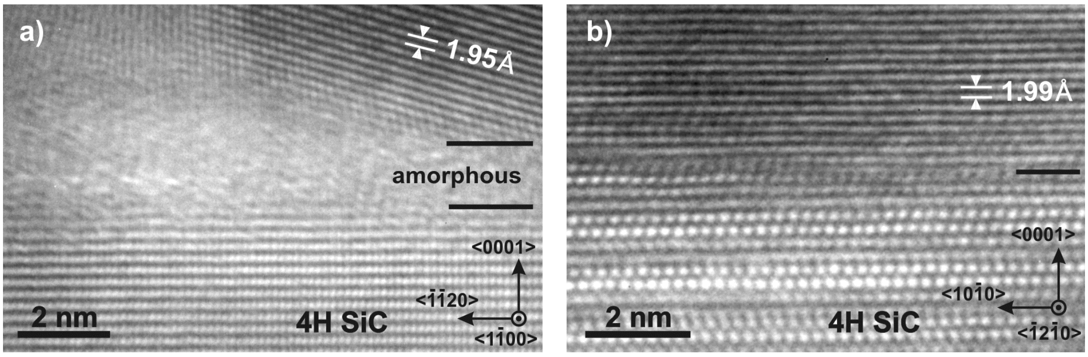

Fig. 3. Cross-sectional high-resolution TEM images of the interfacial region between the 4H-SiC and the Ni_2Si as-formed i.e. Ni/Si after annealing at 600°C (a) and 1050°C (b).

Summary

Thus, the similar trends of r_c, φ_B and δ-Ni_2Si(013) texture changes with annealing temperature for Ni_2Si(Ni)/n-SiC ohmic contacts were related with recrystallization of Ni_2Si phase and the growth of δ-Ni_2Si grains in an orientation-relationship with respect to the silicon carbide (0001) surface. This is the reason why, the Ni_2Si/n-SiC and Ni/n-SiC ohmic contacts have a similar electrical properties.

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