Materials Science Forum Vols. 615-617 (2009) pp 573-576
online at http://www.scientific.net

On the Formation of Ni-based Ohmic Contacts to n-type 4H-SiC

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Keywords: metal contacts, nickel, nickel silicides, contact resistance

Abstract. In this study, the formation of Ni, Ni-rich Ni_2Si and Si-rich $NiSi_2$ ohmic contacts to n-type 4H-SiC are investigated. The Ni/n-SiC ohmic contact with resistance $r_c \sim 4.2\times10^{-4}$ Ω cm^2 is formed after annealing at 1050°C. For Ni_2Si/n-SiC, the contact resistances were $r_c \sim 4\times10^{-4}$ Ωcm^2 and $r_c \sim 3.5\times10^{-4}$ Ωcm^2 after annealing at 1000 and 1050°C, respectively. The non-ohmic *I-V* characteristics are observed for $NiSi_2$/n-SiC contact even after annealing at 1050°C. The features of ohmic contact formation for Ni-based metallization to 4H n-SiC are discussed.

Introduction

Realization of great application potential of SiC in various new devices requires developing of low resistance ohmic contacts. Ni-based metallization are one of the most investigated contacts to n-SiC, but a question about the mechanism of the ohmic contact formation is still open. The Ni-based ohmic contacts are usually formed during high temperature annealing (> 1000°C), when nickel silicides and free carbon atoms are created. Some works conclude that silicides [1,2] and carbon precipitates [3,4] are responsible for ohmic contact formation. There are and other versions of the ohmic contact formation mechanism: (i) inhomogeneity of metal-SiC Schottky barrier [5]; (ii) creation of carbon vacancies [6,7] or defect states [8] near the interface region; (iii) snowplow effect of dopants in the SiC substrate [9]. Despite these open questions, the non controlled high temperature reaction between Ni and SiC limit the reliability of the Ni-based ohmic contacts. For fabrication of reliable Ni-based contacts to SiC, and to attain a clear consensus on the ohmic contact formation mechanism further investigations are desired.

In this study, we focus on the comparative investigation of the metallurgy and formation mechanism of the Ni, Ni-rich Ni_2Si and Si-rich $NiSi_2$ contacts to n-type 4H-SiC.

Experimental

In experiments, the Si-faced (0001) n-type 4H-SiC substrates with a doping concentration ~ 2×10^{17} cm^{-3} from Cree Research Inc. were used. Before deposition of contacts the substrates surface was cleaned according to the procedure described previously in details [10]. The Ni and Si thin films were deposited by magnetron sputtering of Ni and Si targets in Ar plasma, respectively. One series of structures were Ni(90nm)/n-SiC, the second one were Ni/Si/Ni/Si(32/29/32/29nm)/n-SiC and the third were Ni/Si/Ni/Si(14/50/14/50nm)/n-SiC structures. The multilayer structures were first annealed at 600°C (N_2, 15 min.) to form stoichiometric Ni_2Si and $NiSi_2$ [10], and next subsequently at 950, 1000 and 1050°C. The Ni/n-SiC contact was annealed at the same temperature regimes.

Current-voltage (*I-V*) characteristics of the c-TLM structures were measured and contacts resistance (r_c) were estimated. The phase composition of the contacts was investigated by X-ray diffraction (XRD). The interaction at the metal/SiC interface was examined by Rutherford backscattering spectrometry (RBS) and by secondary ion mass spectrometry (SIMS). The optical microscope with Nomarski contrast was used to study the surface morphology of the contacts.

Results

First, to evaluate electrical properties of the Ni/n-SiC, Ni_2Si/n-SiC and $NiSi_2$/n-SiC contacts the current-voltage (*I-V*) characteristics were measured. As shown in Fig. 1, rectifying *I-V* characteristics were observed for all as-deposited and annealed up to 950°C contacts. The transition to quasi-linear *I-V* characteristic after annealing at 1000°C and ohmic contact formation with contact resistance $r_c \sim 4.2\times10^{-4}$ Ω cm^2 at 1050°C were observed for Ni/n-SiC contact (Fig. 1a). For Ni_2Si/n-SiC contact, the ohmic *I-V* characteristics were revealed after annealing at 1000 and 1050°C (Fig. 1b). The contact resistances were $r_c \sim 4\times10^{-4}$ Ωcm^2 and $r_c \sim 3.5\times10^{-4}$ Ωcm^2 for Ni_2Si/n-SiC ohmic contacts annealed at 1000 and 1050°C, respectively. Annealing up to 1050°C of $NiSi_2$/n-SiC contacts does not enhance significantly the conduction current through the contact, and *I-V* characteristics are still nonlinear (Fig. 1c).

Next, reaction at metallization/SiC interface induced by thermal annealing was investigated by complementary methods: RBS, XRD and SIMS. From analysis of RBS spectra of Ni/n-SiC contact (Fig. 2a), we can deduce that annealing at 1050°C enforces diffusion of Ni atoms towards the SiC substrate and migration of Si and C atoms towards the surface. Several well distinguished plateaus in the RBS signals for Ni and Si indicate the formation a few intermetallic compounds. Simulation of RBS spectra by SIMNRA code shows that near the top surface a part of the 25 nm-thick layer at the atomic ratio of Ni:Si ~ 2 contains ~ 12 at.% of C, next a 60 nm-thick Ni_2Si sublayer encloses ~ 26 at.% of C, subsequently a 35 nm-thick mixture of ~ 32 at.% of Ni, ~ 19 at.% of Si and ~ 49 at.% of C, and finally - near interface a 16 nm-thick film of NiSi silicide with smaller content of ~ 33 at.% of C could be distinguished. Significant diffusion of Ni is observed into SiC, where ~ 17 at. % of Ni was estimated at the depth of about 40 nm. The XRD spectra of Ni/n-SiC structure (Fig. 2b) show: (i) 111 Bragg reflection from polycrystalline Ni layers for as-deposited contact, and (ii) 121 and 002 peaks of the δ-Ni_2Si orthorhombic phase for annealed at 1050°C contact, which testifying on the thermally activated interaction between Ni films and SiC substrate. The chemical composition Ni:Si ~ 2 at the 85 nm-thick top layer correlate well with δ-Ni_2Si phase identified by XRD in the Ni/n-SiC contact annealed at 1050°C. The SIMS elements depth profiles of Ni_2Si/n-SiC contact shown that when Ni reacts with Si at 600°C to form Ni_2Si, no reactions at the contact/SiC interface takes place (Fig. 3a). Thus, the Si layer initially placed between the Ni and SiC prevents reaction between the Ni and SiC. However, when the Ni_2Si/n-SiC contacts are annealed at 1000 and 1050°C, the out-diffusion of C atoms to surface and in-diffusion of Ni atoms at about 30 nm into SiC substrate are observed. From the XRD spectra of Ni/Si/Ni/Si(32/29/32/29nm)/n-SiC structures annealed at 600°C (Fig. 3b) only 121 and 002 peaks corresponding to the δ-Ni_2Si phase are visible.

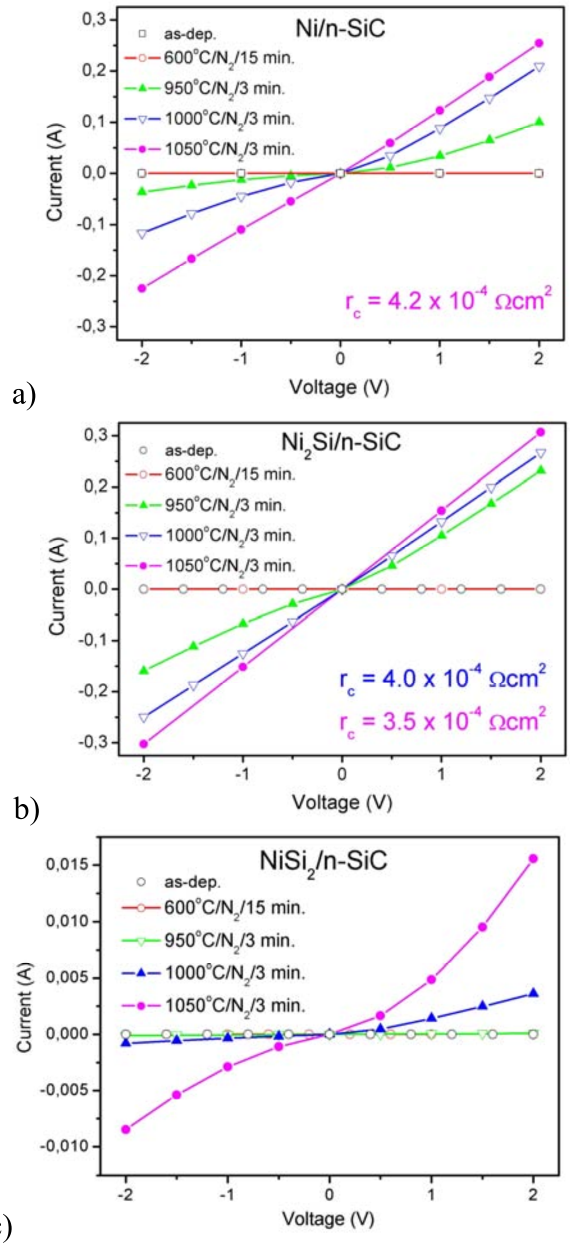

Fig. 1. *I-V* characteristics for as-deposited and annealed up to 1050°C contacts: (a) Ni/n-SiC; (b) Ni_2Si/n-SiC; (c) $NiSi_2$/n-SiC.

The SIMS and XRD results indicate that reaction, if present, between the Ni_2Si and the SiC layers is limited to a very small scale at the interface. The exceptionally strong diffraction 121 peak of δ-Ni_2Si phase observed after annealing at 1050°C indicates only the change of degree of preferential orientation of grains in the Ni_2Si film.

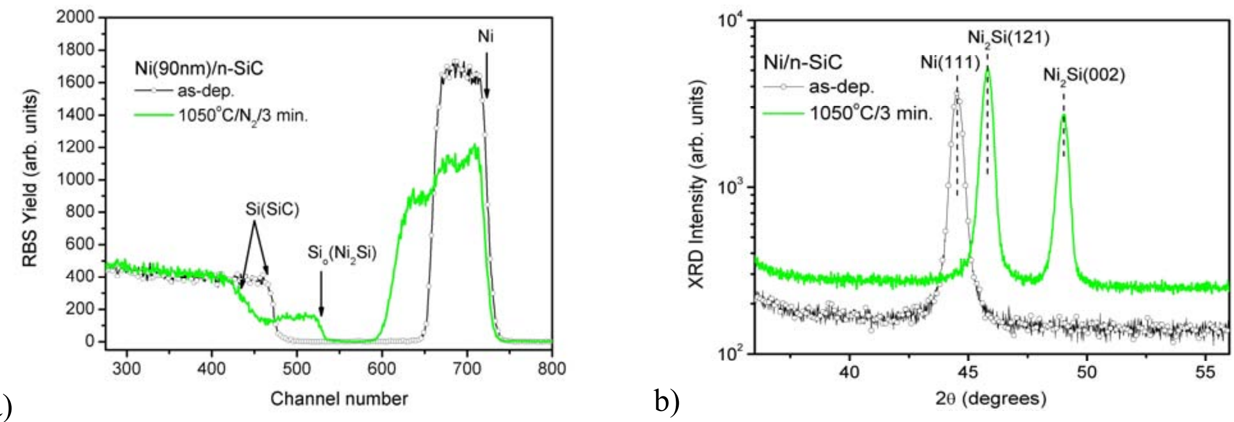

Fig. 2. RBS (a) and XRD (b) spectra of Ni/n-SiC contact: as-deposited and annealed at 1050°C.

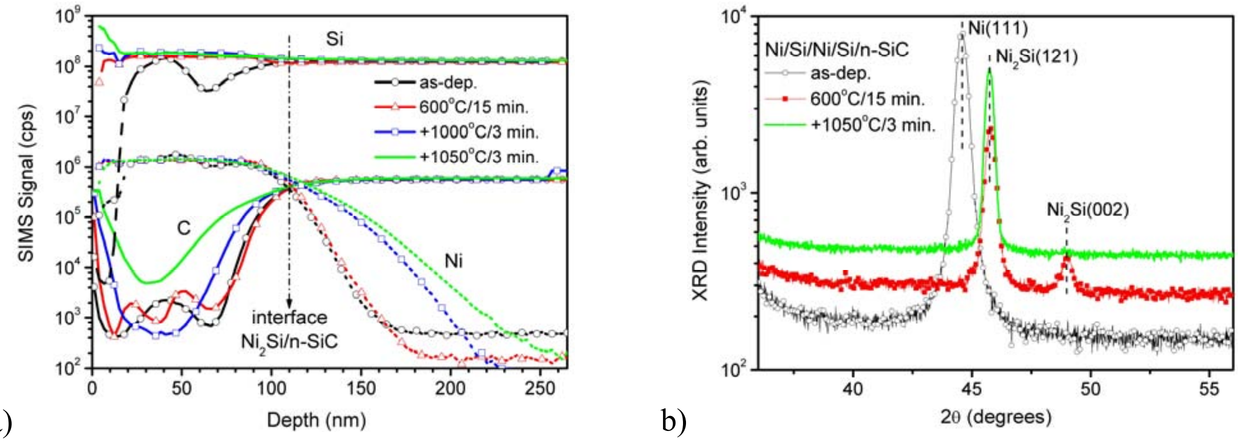

Fig. 3. SIMS (a) and XRD (b) spectra of Ni_2Si/n-SiC: as-deposited and annealed up to 1050°C.

The optical surface images of annealed Ni/n-SiC, Ni_2Si/n-SiC and $NiSi_2$/n-SiC contacts are shown in Fig. 4. Annealing at temperature below of ohmic contact formation (950°C) of the Ni/n-SiC induces spots and roughening on the surface (Fig. 4a). In contrast, the homogeneous and smooth surface is visible after annealing even at 1050°C for Ni_2Si/n-SiC contact (Fig. 4b). Thermally induced heterogeneity and roughening are observed after annealing at 950°C for $NiSi_2$/n-SiC contact, indicating on strong interaction between $NiSi_2$ and SiC substrate at this temperature (Fig. 4c).

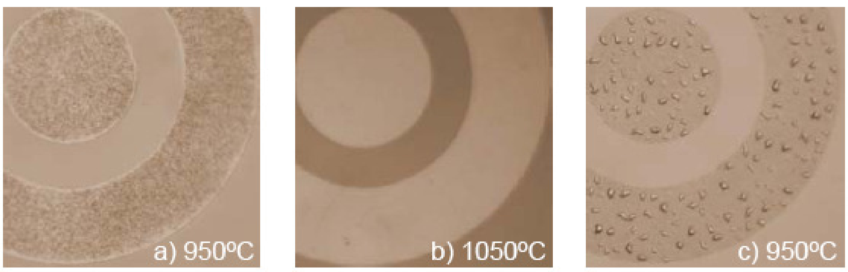

Fig. 4. Optical micrographs of annealed contacts: (a) Ni/n-SiC; (b) Ni_2Si/n-SiC; (c) $NiSi_2$/n-SiC.

Discussion and conclusion

This work demonstrates that to obtain ohmic contacts to n-type SiC, high temperature is necessary for change SiC surface at metal/SiC interface. This can be concluded from a dramatic difference between interaction of pure Ni, Ni-rich Ni_2Si and Si-rich $NiSi_2$ contacts with 4H n-SiC.

The formation of Ni/n-SiC ohmic contact at 1050°C correlates with reaction between Ni and SiC and creation of δ-Ni_2Si phase and free carbon. The reaction of Ni with SiC just at 500°C [11] temperature below ohmic contact formation, indicate that δ-Ni_2Si phase or free C are responsible for ohmic contact formation. These results correlate well with previously reported works [1-4]. However, the high value of Schottky barrier between graphite (C) and n-SiC [12], indicate that graphite is not responsible for ohmic contact behavior. Moreover, our electrical measurements show that the formation of stoichiometric δ-Ni_2Si by annealing at 600°C of separately deposited Ni and Si films is not sufficient to obtain ohmic characteristics. The Schottky-ohmic transition for Ni_2Si/n-SiC contact was observed only after annealing at 1000°C, when Ni_2Si reacted with SiC at very small scale of the interface. Thus, for ohmic contact formation to n-SiC a reaction between metal and SiC are needed, most likely for change the properties of SiC surface. It is not yet clear why the Ni_2Si/n-SiC contact become ohmic at 1000°C, but $NiSi_2$/n-SiC contact is not ohmic even after annealing at 1050°C. There are two approaches to explain that: difference between (i) work functions, and (ii) melting temperature of Ni-rich Ni_2Si and Si-rich $NiSi_2$. However, the formation of $NiSi_2$ ohmic contact to n-SiC with high doping concentration (1×10^{20} cm^{-3}) is previously reported [13], in spite of the high work function of nickel silicides (> 4.3 eV) [14]. Thus, not ohmic behavior of $NiSi_2$/n-SiC contact in our case can be explained by low melting temperature of about 980°C for the $NiSi_2$ bulk material (1200°C for the Ni_2Si) [10]. When $NiSi_2$ reacted with SiC excess Si from Si-rich $NiSi_2$ lead to a dopand deactivation, probably by the "passivation" of nitrogen dopand by Si atoms.

The *I-V-T* characteristics (not shown here) of Ni_2Si/n-SiC ohmic contacts in temperature range of 25-200°C show anomalous increase of contact resistance (r_c). This is in contrast to the theories of thermionic field emission (decrease of r_c with increase of T) and tunnelling (r_c constant irrespective of T). We proposed the creation of inclusions at the metal-SiC interface after annealing at high temperature, as possible mechanism of ohmic contact formation.

Acknowledgements

The authors are grateful for financial support from the INTAS (Grant No. 06-1000014-5957), from the President of Ukraine (Grant No. GP/F26/0095) and from the Ministry of Science and Higher Education of Poland (Grant No. 3T11B 042 30).

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Silicon Carbide and Related Materials 2008
doi:10.4028/3-908454-16-6
On the Formation of Ni-Based Ohmic Contacts to n-Type 4H-SiC
doi:10.4028/3-908454-16-6.573