

# Empirical Model of Low-Ohmic Nickel-Based Contact Formation on N-Type 4H-SiC Depending on Thermal Budget

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**Keywords:** Laser annealing, ohmic contact, nickel, 4H-SiC, empirical model

**Abstract.** In this work, an empirical model of structural and material composition of low-ohmic nickel silicide contact formation on n-type 4H-SiC by laser annealing as well as by RTA is presented. For this purpose, systematic studies with different annealing parameters were performed. The development of the empirical model is based on results from characterization of the nickel silicide by FIB-SEM, TEM, XRD analysis as well as electrical characteristics received from 4-point-measurements.

## Introduction

The ohmic contact between metal and semiconductor is of utmost importance for low  $R_{DS, on}$  power electronic devices [1]. Therefore, the fabrication of low-ohmic contacts is one of the essential aspects in the manufacturing and development of high energy efficient SiC power semiconductor devices. For low-ohmic contact formation on n-type SiC, usually nickel or nickel compounds are deposited [1]. A following temperature treatment of the metal layer is necessary to silicide the nickel and produce low-ohmic contacts. This temperature step is usually performed by RTA (rapid thermal annealing) [1, 2]. However, nowadays SiC wafers are often back-thinned to improve the performance of vertical devices regarding the on-resistance. Thereby, the initial SiC substrate thickness of 350  $\mu\text{m}$  is reduced to 50 to 100  $\mu\text{m}$ . Due to the fragility of the thinned wafers, the thinning of the wafer takes place very late in the process, when the frontside processing is already finished. Therefore, the thermal treatment of the backside contacts has to be done by laser annealing, where the wafer backside is heated up to temperatures above 1000°C, while the thermosensitive layers on the frontside are not affected.

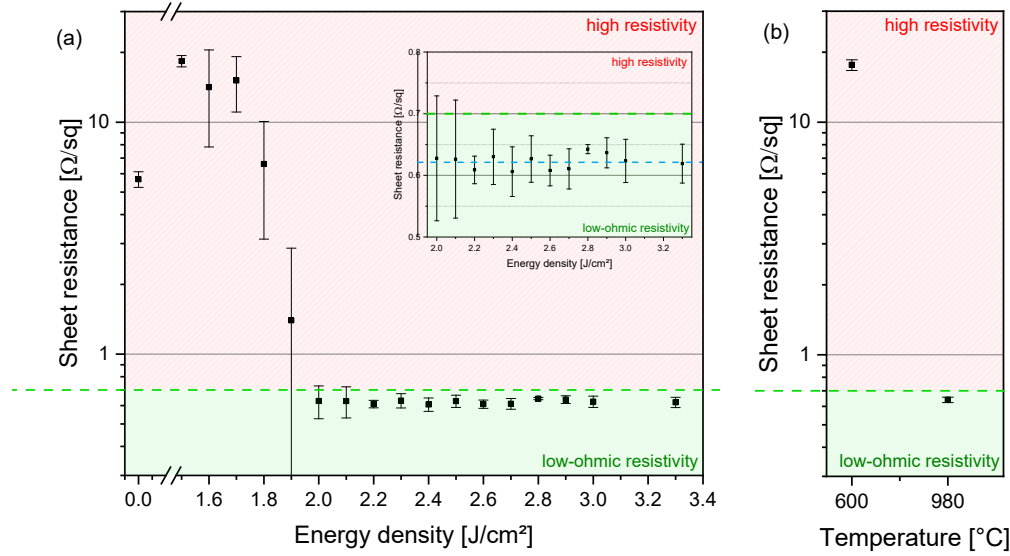
Thereby many kinds of lasers like green, infrared or UV lasers are used. A few publications can be found about parameter studies for nickel silicide processes on laser annealing systems [3, 4]. However, the usage of different types of lasers makes a direct transfer of the findings of those studies to different laser annealing systems difficult. Nevertheless, in addition to the optimized manufacturing parameters, also the understanding of the ohmic contact formation is essential.

Purpose of this work was to derive an empirical model of low-ohmic nickel silicide contact formation on n-type 4H-SiC in dependence of the thermal budget by using laser annealing compared to RTA by applying different annealing parameters.

## Experimental

In this work, experiments were performed on the C-side of 4H-SiC wafers. The C-side was thinned back by 10  $\mu\text{m}$  using a Disco DAG810 grinder with a fine grinding wheel resulting in a surface roughness of 3 to 4 nm. A 60 nm thick NiAl 2.6 wt% layer was sputtered as contact metal after an argon sputter clean. The nickel layer was silicided by a Sumitomo SWA20US-M laser annealing tool with a frequency-tripled Nd:YVO<sub>4</sub> laser with 355 nm wavelength, a beam diameter of 80  $\mu\text{m}$  and a pulse duration of 50 ns. The energy density was varied from 1.5 to 3.3 J/cm<sup>2</sup>. The single pulses had

an overlap of 67 % in scan direction and 50 % in step direction. Sheet resistance measurements of the resulting layers are presented in fig. 1a.

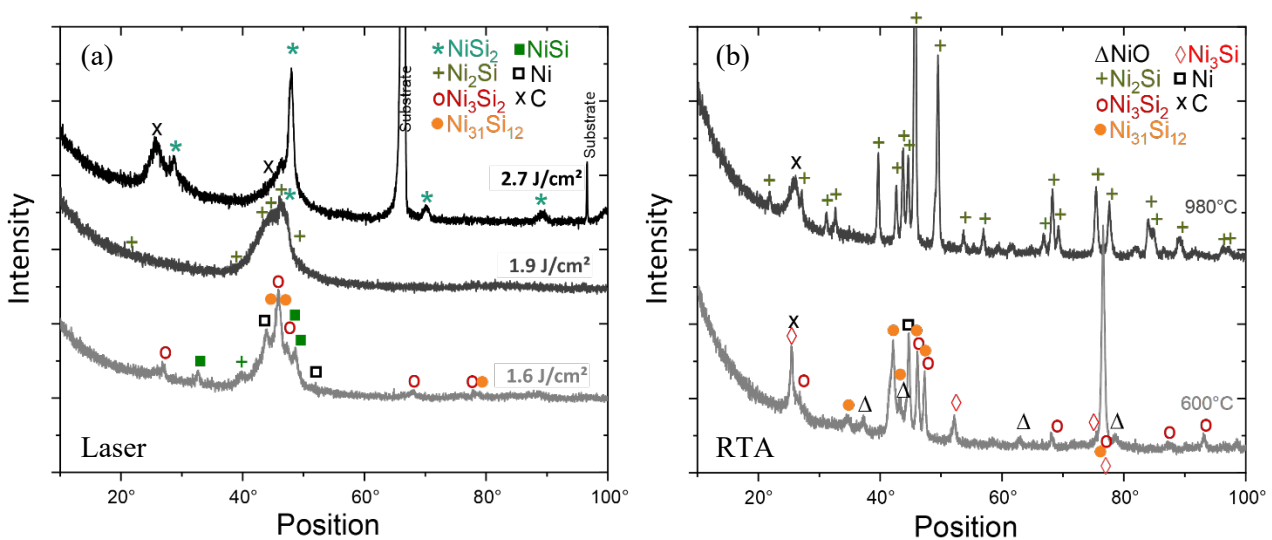


**Fig. 1.** Sheet resistance measurement results of 60 nm NiAl (2.6 wt%) layer (a) processed by laser annealing as a function of energy density and (b) processed for 120 s at RTA as a function of temperature

As reference RTA samples were processed analogously, but the nickel layer was silicided by RTA instead of the laser annealing. Hereby, the wafers were processed in graphite boxes. One sample was annealed at 600°C for 2 minutes and one at 980°C for 2 minutes. The according sheet resistance measurements are presented in fig. 1b. The development of the empirical model is based on results from both electrical characteristics by 4-point-measurements and characterization of the nickel silicide by FIB-SEM, TEM and XRD analysis.

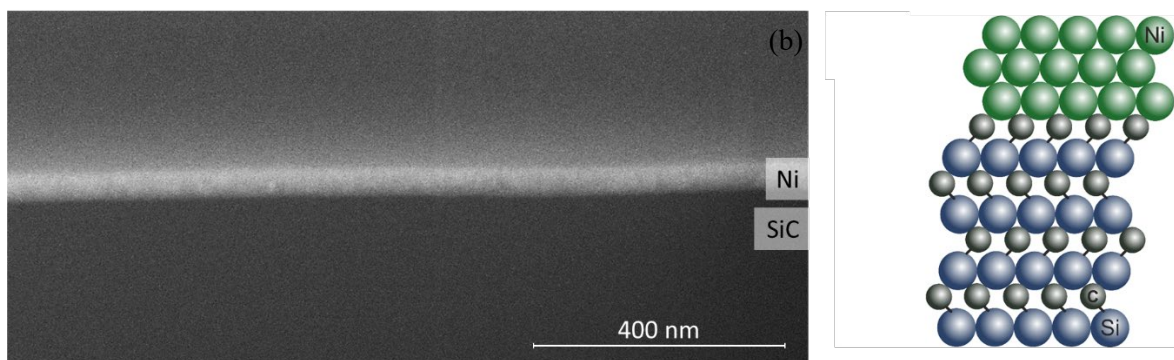
## Results and Discussion

The present work focused on nickel layers sputtered on the C-side of fine grinded 4H-SiC wafers (cf. fig. 3a and b). During the thermal treatment in the RTA, first chemical reactions between the nickel layer and SiC substrate already take place at temperatures starting from 550°C [5].

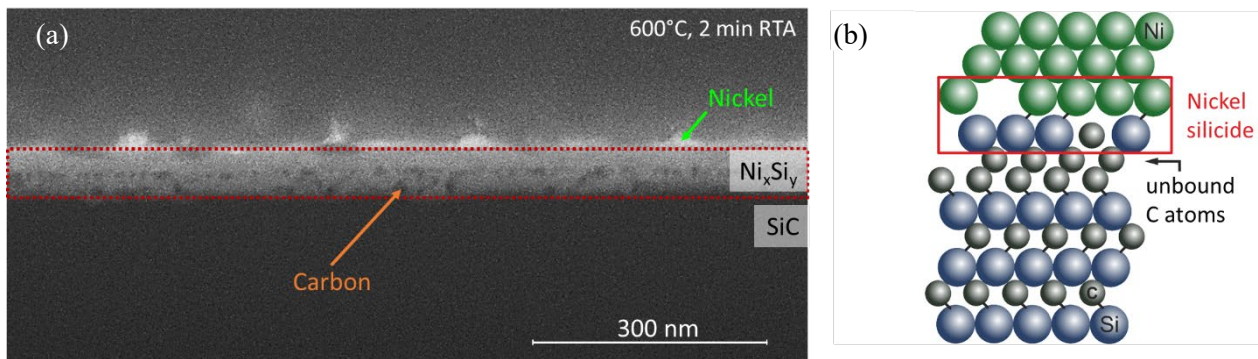


**Fig. 2.** XRD analysis of (a) laser treated nickel-based ohmic contacts depending on the energy density and (b) RTA treated nickel based contacts depending on the temperature

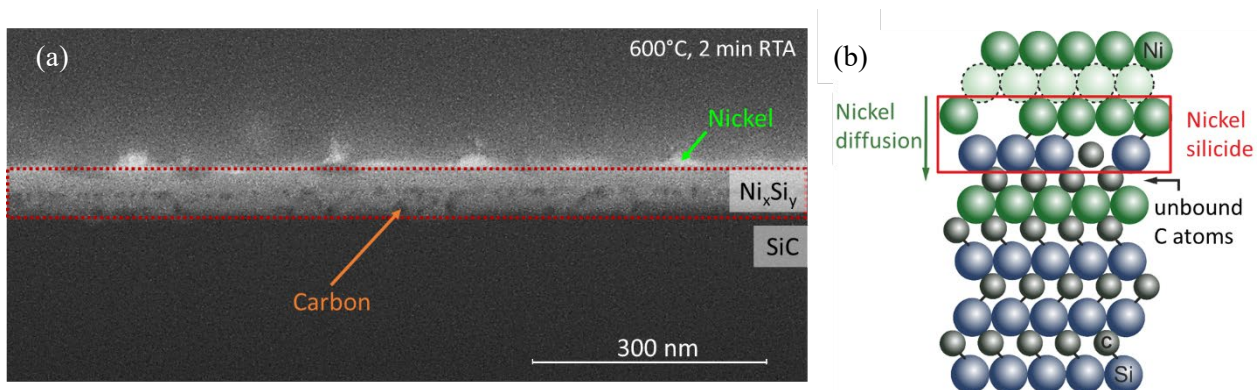
As shown in fig. 4a, an increase in the layer thickness and a structural change of the nickel silicide layer could be detected by FIB cross sections after a 600°C RTA step for 120 seconds. During the temperature step, nickel atoms at the direct interface with the SiC substrate first react with the silicon contained therein (see fig. 4a and b). In this process, crystal damages in the surface of the SiC substrate serves as condensation nuclei, where the chemical reaction occurs more easily [6]. This deep damage can be enhanced, especially by a previous grinding step, which makes the surface more reactive [7]. As XRD analysis shows, for temperatures up to about 700°C mainly nickel-rich silicides such as  $\text{Ni}_{31}\text{Si}_{12}$  and  $\text{Ni}_3\text{Si}$  [8] are formed during chemical reaction (see fig. 2b), releasing unbound carbon. As the process continues, nickel atoms diffuse through the newly formed nickel silicide layer to the interface with the SiC substrate (cf. fig. 5b). These nickel atoms now react again with the silicon atoms of the adjacent silicon carbide, leaving carbon atoms behind (cf. 6a and b). Thus, the nickel silicide layer continues to grow until either the temperature is too low for a further chemical reaction or the nickel atoms are completely consumed.



**Fig. 3.** (a) FIB cross-section of a sputtered nickel layer on SiC substrate, (b) schematic drawing illustrating the initial situation before thermal treatment



**Fig. 4.** (a) FIB cross-section of a sample treated at 600°C for 120 s in the RTA, (b) schematic drawing illustrating the interfacial reaction between nickel and SiC during silicidation

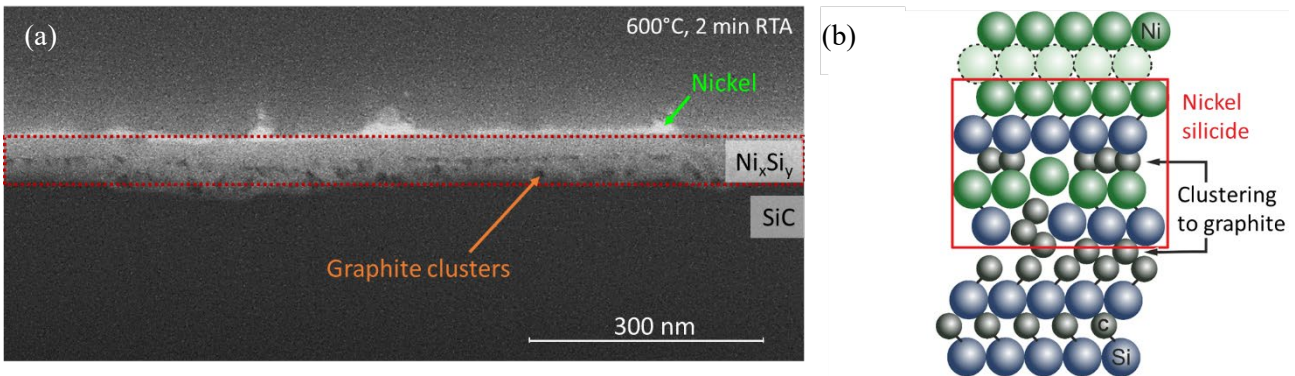


**Fig. 5.** (a) FIB cross-section of a sample treated at 600°C for 120 s in the RTA, (b) schematic drawing illustrating the nickel diffusion through the formed silicide

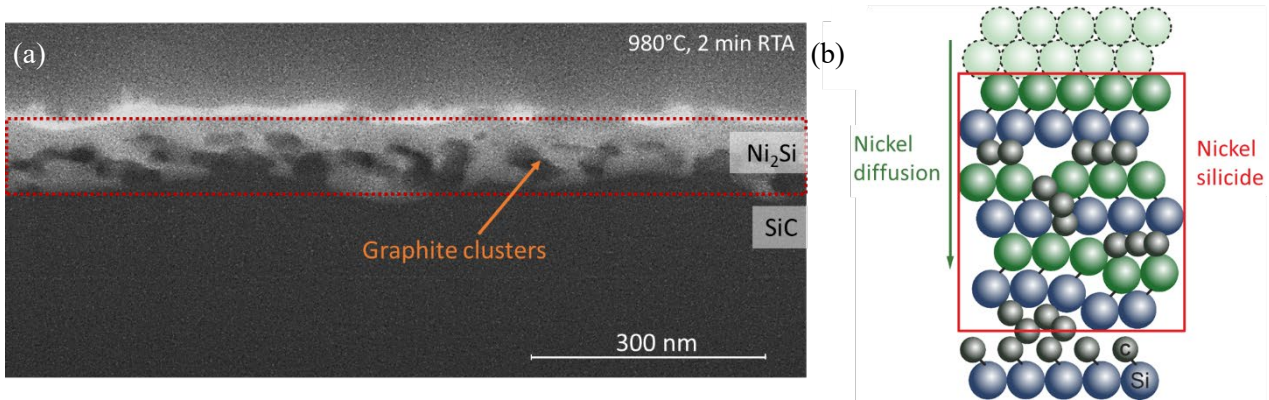


Since the diffusion coefficients exponentially depend on temperature [9], the sputtered nickel atoms diffuse only slowly through the formed nickel silicide layer due to the low temperature. Thus, after RTA at 600°C for 120 seconds, unreacted nickel as well as the nickel-rich and high-resistance silicides  $\text{Ni}_3\text{Si}_2$ ,  $\text{Ni}_{31}\text{Si}_{12}$  and  $\text{Ni}_3\text{Si}$  can still be detected by XRD analysis (see fig. 2b). The resulting resistance values also indicate a Schottky contact (see fig. 1b).

Likewise, due to the low process temperature, the unbound carbon can only diffuse very slowly through the nickel silicide layer to the surface and therefore remains at the point of origin. Due to the long process time and the subsequent slow passive cooling, the carbon atoms accumulate to form larger carbon clusters with a size of up to 20 nm and in some cases already form longer linked chains (see fig. 7a and b). Due to the processing at atmospheric pressure and the resulting temperatures in the substrate, it can be assumed that the carbon forms graphite clusters, since this is the thermodynamically most stable form for the prevailing conditions [10, 11].



**Fig. 6.** (a) FIB cross-section of a sample treated at 600°C for 120 s in the RTA, (b) schematic drawing illustrating graphite clustering of the unbound carbon atoms

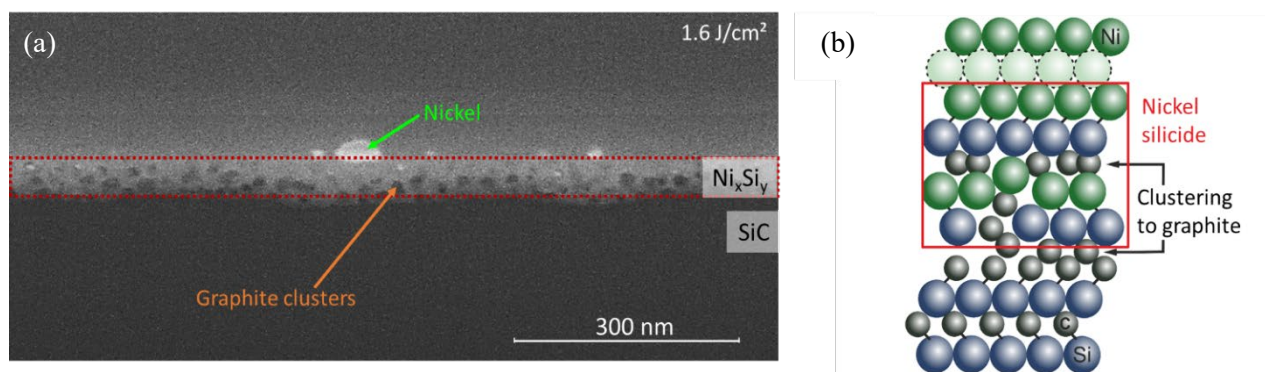


**Fig. 7.** (a) FIB cross-section of a sample treated at 980°C for 120 s in the RTA, (b) schematic drawing illustrating the reaction products after RTA treatment at 980°C for 120 s

Comparing the reaction products after the RTA treatment in the range of 550 – 700°C with those after laser processing similar results are obtained for energy densities of 1.4 to 1.8 J/cm<sup>2</sup>. After laser processing, FIB cross-sections show structural changes in the metallization and an increase in layer thickness (see fig. 8a). Also the results of XRD analysis of the laser processed sample at 1.6 J/cm<sup>2</sup> show the existence of mainly nickel-rich high-resistance silicides, such as  $\text{Ni}_3\text{Si}_2$  and  $\text{Ni}_{31}\text{Si}_{12}$ , and carbon (see fig. 2a). In addition, first low-ohmic silicides such as NiSi and  $\text{Ni}_2\text{Si}$  can be detected [8], which would be expected due to high peak temperatures during laser processing and corresponds to the reaction path expected in a ternary phase diagram of Ni-Si-C [11]. However, due to the predominantly high-ohmic nickel silicides, the resulting contact has a Schottky behavior.

In contrast to the RTA, in laser treatment the maximum temperature prevails only for a very short period (< 100 ns). During this short process duration, chemical equilibrium cannot occur in this transit process compared to RTA. In addition, due to the very local temperature, the sample also cools back to room temperature very quickly (in the range of 10 μs). As a result, the diffusion of the nickel atoms

through the formed nickel silicide layer is strongly time-limited by the time, so the time span is not sufficient for the entire sputtered nickel layer to react completely (see fig. 8a). Since predominantly nickel-rich silicides are formed at the prevailing process temperatures less carbon is formed during the reaction in relation to nickel-poor silicides. In this process, the carbon concentration decreases with increasing distance from the nickel silicide-SiC interface (see fig. 8a). The carbon atoms probably accumulate into clusters according to Ostwald ripening [13]. However, they can only unite into small clusters during the process (see fig. 8a and b), since the substrate cools down in a few microseconds after laser treatment. It can be assumed that the crystal structure of the carbon changes and graphite is formed [10, 11].



**Fig. 8.** (a) FIB cross-section of a sample laser treated with 1.6 J/cm<sup>2</sup>, (b) schematic drawing illustrating carbon clustering during progressive silicidation at laser treatment

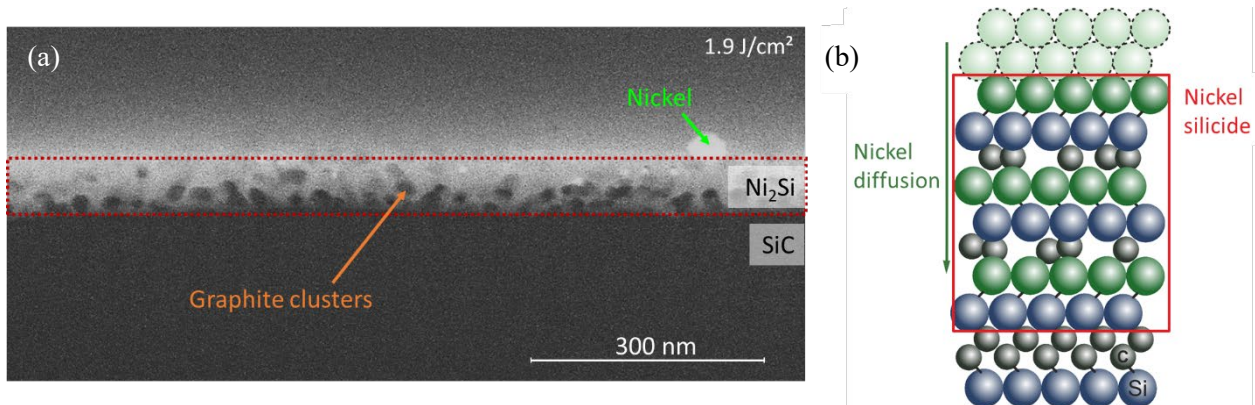
For higher RTA temperatures of 800°C to 900°C, XRD analyses show the absence of nickel-rich silicides such as Ni<sub>31</sub>Si<sub>12</sub> [5, 8]. Instead, mainly low-resistance NiSi and Ni<sub>2</sub>Si are detected [8]. It can be assumed that due to the low heating rate in the RTP of maximum 25 K/s, nickel-rich silicides are initially formed at the interface of SiC and nickel. In the further process, NiSi or Ni<sub>2</sub>Si can also form directly at higher temperatures. In addition, it is possible that nickel-rich silicides can also transform to low-resistance silicides after further thermal treatment at higher process temperature, as shown in the so-called silicide process [5]. However, electrical measurements show that low-resistance contacts cannot yet be formed below 900°C [8].

If the RTA temperature is increased further, optimized low-resistance nickel silicide contacts are formed above about 950°C and higher [8]. During a 980°C RTA step for 120 seconds, a low-resistance nickel silicide layer could be produced (see fig. 1b). This is due to the formation of low-resistance Ni<sub>2</sub>Si, which is the only silicide detected in the XRD analysis (see fig. 2b). Due to the higher process temperature and the lower melting temperature of nickel silicide compared to nickel, the nickel atoms diffuse faster through the formed nickel silicide layer, which is why almost the whole nickel layer has reacted after the 980°C temperature step. This is also consistent with the FIB cross-sections of the nickel silicide layer (see fig. 7a). Assuming an initial 50 nm thick nickel layer, which reacts completely with SiC to form Ni<sub>2</sub>Si in a ratio of 2:1, an average layer thickness of 100 nm can be expected. Compared to the high-resistance nickel silicides discussed so far, more unbound carbon is formed during the reaction, which mostly remains in the original place, where it got unbound during reaction. Caused by the progressive nickel diffusion and thus progressive movement of the interface at which the silicidation takes place, carbon can be detected in the entire nickel silicide layer (see fig. 7a). The carbon atoms gather into clusters according to Ostwald ripening [13], the size of which decreases as a function of the distance from the SiC interface. Since the substrate only slowly cools down after thermal treatment, the carbon atoms can accumulate into much larger clusters with a size of up to 70 nm during the process, which can be assumed to be graphite clusters [10, 11]. Even if the sheet resistance indicates a low-resistance contact, large carbon clusters can cause problems by leading to delamination [4].

Analogous to the RTA, low-resistance nickel silicide contacts are formed after laser treatment from 1.9 J/cm<sup>2</sup>, which is confirmed by sheet resistance measurements (see fig. 1a). For energy

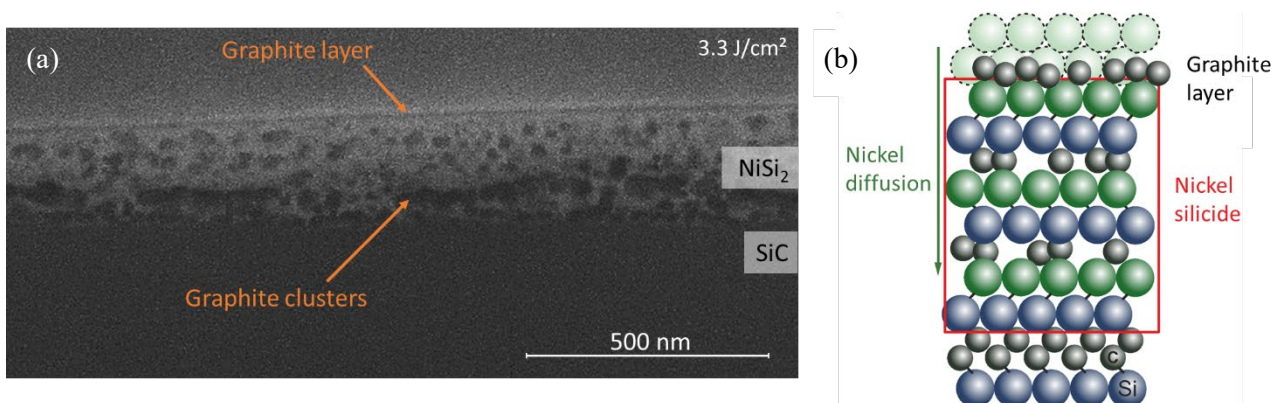


densities up to  $2.3 \text{ J/cm}^2$ , the reason, analogously to the RTA, is the exclusive formation of the low-resistance  $\text{Ni}_2\text{Si}$ , which is indicated by film thickness analysis after laser treatment using FIB cross-sections (see fig. 9a) and confirmed by XRD analysis (see fig. 2a). However, according to temperature simulations [14], the prevailing process temperature, is much higher than during the  $980^\circ\text{C}$  RTA step and is close to or even above nickel's ( $1455^\circ\text{C}$ ) or dinickel silicide's melting point ( $1309^\circ\text{C}$ ) [15]. Since the diffusion coefficient in liquids is usually several thousand times larger than that in solids [16], the nickel atoms can diffuse more rapidly through the molten nickel silicide and react at the interface with the SiC substrate. Thus, even during this short process time, it is possible to react completely with the SiC substrate. The unbound carbon formed during the reaction to  $\text{Ni}_2\text{Si}$  can be detected in the entire nickel silicide layer, forming clusters with a size up to  $30 \text{ nm}$  (see fig. 9a).



**Fig. 9.** (a) FIB cross-section of a sample laser treated with  $1.9 \text{ J/cm}^2$ , (b) schematic drawing illustrating nickel diffusion during silicidation

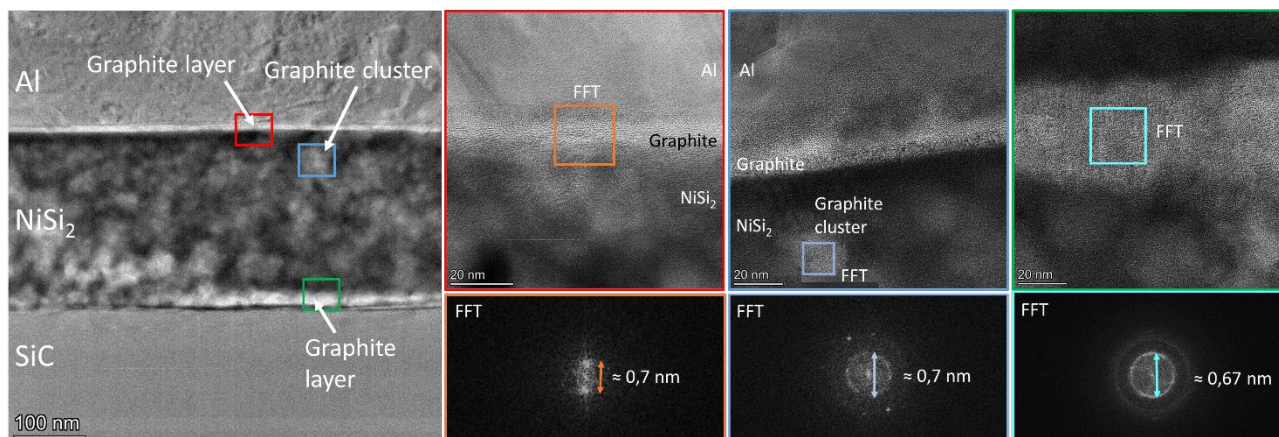
If the RTA temperature is increased further from about  $1100^\circ\text{C}$ , the thickness of the nickel silicide layer increases significantly, as shown in literature by FIB cross-sections [17]. In this context, XRD analyses show that  $\text{NiSi}_2$  is mainly formed and no longer  $\text{Ni}_2\text{Si}$  [17]. Also during laser treatment with energy densities of at least  $2.4 \text{ J/cm}^2$ , mainly nickel disilicide can be detected (see fig. 2a). For thin nickel layers it represents the thermodynamically stable phase [18]. At such high temperatures, the nickel layer locally melts completely and reacts with the underlying SiC substrate. However, the resulting nickel silicide layer of  $180 - 300 \text{ nm}$  is much thicker than the silicide layers formed so far, since for the reaction of  $\text{NiSi}_2$  nickel reacts with silicon in a ratio of 1:2. However, this produces unbound carbon in the same ratio (see fig. 10a and b). The carbon can be detected in the entire nickel silicide layer, forming larger clusters near the interface, whereas the silicide layer is interspersed throughout with smaller clusters. In addition, an almost continuous carbon layer is already visible at the surface of the nickel silicide layer (see fig. 10a and fig. 11).



**Fig. 10.** (a) FIB cross-section of a sample laser treated with  $3.3 \text{ J/cm}^2$ , (b) schematic drawing illustrating graphite formation on the surface

Using TEM analysis and FFT, it was demonstrated that the carbon layer at the surface, the small carbon clusters within the silicide layer, and the larger clusters near the interface all have a graphite

structure (see fig. 11). In this case, a 5 – 6 nm thick continuous graphite layer can be observed at the surface. Due to its layer structure, this graphite layer can lead to adhesion problems and delamination of the subsequent layers [19], which was observed in experiments [14].



**Fig. 11.** TEM analysis of laser treated sample including HRTEM image and FFT at three different positions

If the peak temperature is further increased, no further transformation of the  $\text{NiSi}_2$  takes place according to XRD analyses, so that low-resistance layers continue to form. This is also consistent with the phase diagram [18]. However, the thickness variation of the silicide layer continues to increase, so that in some cases there is no longer any continuous layer coverage. Voids can also be observed in the silicide layer, which are a hindrance to homogeneous ohmic contact formation and layer adhesion. The carbon concentration no longer increases significantly for these temperatures since the same chemical reactions take place. However, the graphite molecules in the silicide layer increasingly gather together to form larger clusters. Also the thickness of the graphite layer at the surface doesn't increase.

## Summary

Purpose of this work was to derive an empirical model of low-ohmic nickel silicide contact formation on n-type 4H-SiC by laser annealing compared to RTA based on systematic studies with different annealing parameters. In summary, the following three cases can occur during the thermal treatment of nickel layers:

- 1) For laser treatment with energy densities between  $1.4 - 1.8 \text{ J/cm}^2$  or RTA temperatures between  $550^\circ\text{C}$  and  $700^\circ\text{C}$ , mainly high-resistance nickel-rich silicides are formed, where the initial nickel layer does not fully react. The unbound carbon remains in the nickel silicide layer at the point of formation, forming graphite clusters especially near the interface with the SiC substrate.

- 2) For laser treatment with energy densities between  $1.9$  to  $2.3 \text{ J/cm}^2$  or RTA temperatures between  $950^\circ\text{C}$  and  $1050^\circ\text{C}$ , the nickel layer reacts completely with the underlying SiC substrate to form the low-resistance  $\text{Ni}_2\text{Si}$ . The unbound carbon remains in the nickel silicide layer and can be occasionally found on the surface. Graphite clusters are formed in the nickel silicide layer, the size of which decreases with increasing distance from the SiC surface.

- 3) From energy densities above  $2.4 \text{ J/cm}^2$  or RTA temperatures above  $1100^\circ\text{C}$ , the nickel layer reacts completely with the silicon atoms from the SiC substrate to form the low-resistance  $\text{NiSi}_2$ . Compared to the previous temperature ranges, more unbound carbon is formed, which can be found in the silicide layer and on the surface. After laser processing, a continuous 5 nm thick graphite layer can be detected on the surface.

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