

## Evolution of the Electrical and Microstructural Properties of Mo/4H-SiC Contact with the Annealing Temperature

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**Abstract.** In this work, we investigated the electrical properties evolution of Mo/4H-SiC Schottky contacts following thermal annealing treatments at temperature up to 950 °C. The electrical characterization under forward and reverse bias revealed a reduction of the barrier height from 1.45 eV (as-deposited contact) to 1.30 eV (950°C-annealed contact), with the presence of inhomogeneity in the contact, while the leakage current followed a thermionic-field emission (TFE) model after annealing at 750 °C and presented a significant increase for the 950°C-annealed contact. The electrical characterization was associated with microstructural analyses, which highlighted an enlargement of the grains forming the structure of the Mo-film and the presence of voids near the Mo/4H-SiC interface. These observations can be at the base of the variation in the electrical behavior of the contact.

### Introduction

Nowadays, Schottky-barrier diode (SBD) on 4H-SiC is an established technology used in several real-world applications [1]. Although this large use, additional improvement is still possible for a fully exploitation of the 4H-SiC potentialities. Essentially, the properties of the metal/4H-SiC contact are at the base of the SBD performance and the achievement of a superior control on this interface drives an optimization of the use of the SBD. Over the last two decades, various approaches have been considered for gaining control in this system. Particular attention was paid to the choice of the metal and its evolution with thermal annealing in the Schottky contact formation [2,3]. Recently, the exploration of low-work function materials, such as W and Mo-based contacts, has demonstrated promising results for minimizing the power dissipation of Schottky diodes and offering good thermal stability [3,4]. In particular, Mo showed a large variability of the Schottky barrier height ( $\phi_B$ ) value dependent on the passivation treatment of the surface [5] or the temperature of the metal deposition [6], with the  $\phi_B$  varying between 1.0 and 1.5 eV. From a structural point of view, Mo can readily form carbides and silicides and for that reason Mo-film deposited with Si or C element can be useful in preventing the reaction with SiC surface. For example, Mo-based contacts containing C were recently investigated, either deposited in laminated layers or from Mo-C alloyed targets [7,8], demonstrated stability of the electrical characteristics even at high annealing temperature. However, the origin of this electrical behavior is not clear and additional investigation on the Mo/4H-SiC interface is necessary: on the one hand to correlate the electrical properties of the contact with the process, on the other hand to link the electrical behavior also to the microstructural properties, for better understanding the role of the Mo, Si and C in the contact formation.

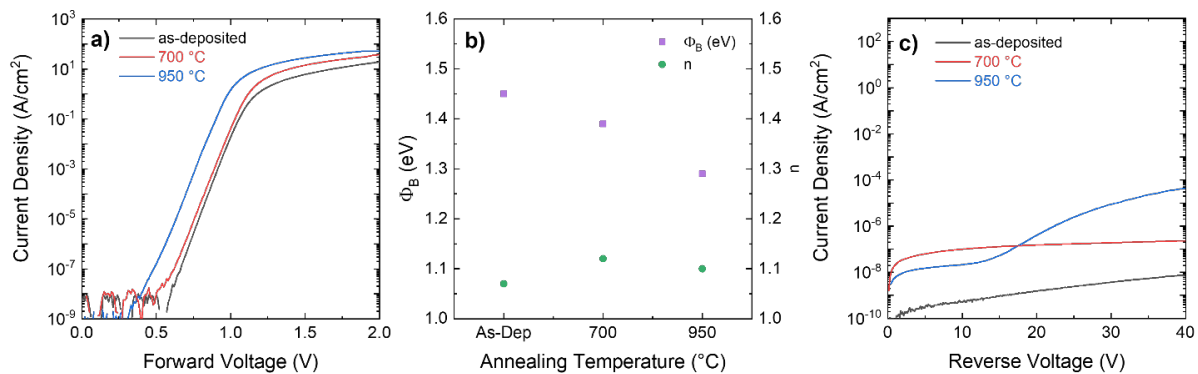
In this study, we follow the evolution of the electrical properties of Mo/4H-SiC contacts with increasing the annealing temperature up to 950 °C. The electrical characterization is combined with a microstructural analysis to shed light on the interface behavior and possible reactions to finally explain the electrical behavior.

### Experimental Details

The starting material for this study consisted in a 4H-SiC wafer with a n-type epitaxial layer (doping concentration of  $1.5 \times 10^{16} \text{ cm}^{-3}$ ) grown onto a  $n^+$ -doped substrate. Schottky diodes were fabricated starting from the deposition of a large-area back-side Ohmic contact by sputtering 100 nm-thick Ni layer, followed by a rapid thermal annealing (RTA) treatment in a furnace at 950 °C in  $N_2$  for 60 s [9]. Then, for the front-side Schottky contact, 80 nm-thick Mo film was sputtered with the contact area defined by optical photolithography, lift-off processing steps and RTA treatments for 10 min in  $N_2$  at temperatures of 700 and 950 °C. On these annealed samples, the electrical characterization under forward and reverse bias was carried out for a set of equivalent diodes by I-V measurements in a Karl-Suss MicroTec probe station equipped with a parameter analyzer. For comparison, the as-deposited Mo/4H-SiC contact was also investigated. The temperature dependence of both forward and reverse I-V characteristics (I-V-T) was studied for selected samples. A microstructural analysis was associated to the electrical characterization, with lamellae for the annealed samples prepared by a Dual Beam Thermofisher Helios 5 focused ion beam (FIB) and analyzed by probe Cs corrected JEOLARM200F Scanning Transmission Electronic Microscope (S/TEM). A Gatan GIF Quantum ER system was also used for electron energy loss spectroscopy (EELS) measurements.

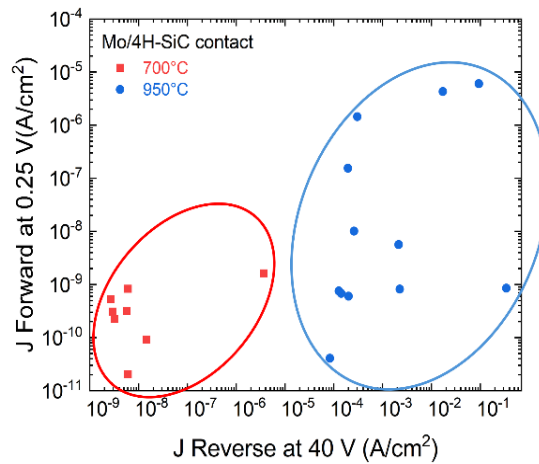
### Results and Discussion

Firstly, the investigation on the electrical behavior of the Mo/4H-SiC contacts under forward and reverse bias is reported in Fig. 1. Specifically, Fig. 1a shows the forward current density–voltage (J-V) characteristics, representative of a set of 10 diodes, for the as-deposited, 700 °C and 950 °C-annealed Mo/4H-SiC contacts, while the significant parameters of the contact (i.e. the Schottky barrier  $\Phi_B$  and ideality factor  $n$ ) extrapolated from the linear part of the J-V curves in Fig. 1a according to the thermionic emission (TE) model [10], are reported in Fig. 1b. A preliminary statistics study demonstrated the possible occurrence of double-barrier curves mostly after annealing at 950 °C. This aspect requires however further investigation and will be the object of a future focused work. The J-V characteristics under reverse bias are plotted in Fig. 1c.



**Fig. 1.** a) Forward J-V curves of the as-deposited, 700 and 950°C-annealed Mo/4H-SiC Schottky contacts. b) Ideality factor  $n$  and Schottky barrier height  $\Phi_B$  for the as-deposited and annealed Mo/4H-SiC contacts. c) Reverse J-V characteristics of the as-deposited, 700 °C and 950°C-annealed Mo/4H-SiC Schottky contacts.

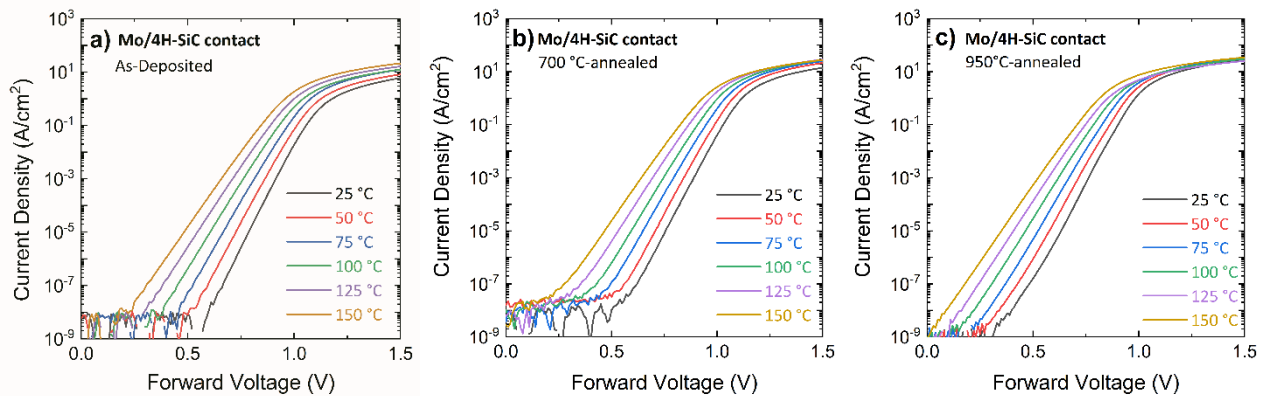
We observed that the as-deposited and 700 °C-annealed Mo/4H-SiC contacts have similar electrical characteristics, whereas a slight shift towards lower voltage appeared for the J-V curves of the 950 °C-annealed contact. As shown in Fig.1b, up to annealing at 700 °C only a slight variation of the  $\phi_B$ , from 1.45 eV to 1.40 eV occurred while  $\phi_B$  is 1.30 eV for the 950 °C-annealed contact. The ideality factor  $n$  is low, including for the 950 °C-annealed sample. Regarding the reverse characteristics reported in Fig.1c, the 700 °C-annealed contact featured an increase of the leakage current from the as-deposited, suggesting the predominance of a thermionic field emission mechanism (TFE) [11] for the current transport. Instead, a different electrical behavior under reverse bias was observed for the 950 °C-annealed sample, with an increase of the leakage current mainly over 15 V. More quantitative analyses are ongoing to better understand the physical mechanisms ruling the transport under reverse bias. In order to highlight the variation of the forward and reverse characteristics for the set of measured diodes in the two cases (700 °C and 950 °C-annealed contacts), Fig.2 reports the forward J value at 0.25 V against the reverse J value at 40 V.



**Fig. 2.** Forward current density at 0.25 V versus reverse current density at 40 V for a set of Mo/4H-SiC diodes annealed at 700 °C and 950 °C.

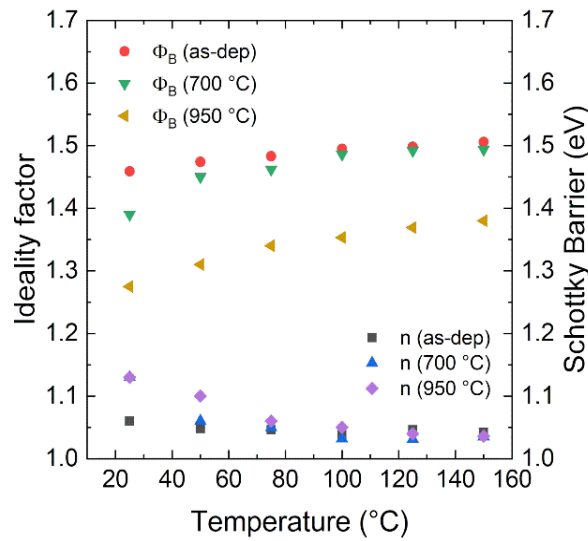
Clearly, the 950 °C -annealed Mo/4H-SiC contact presented a larger statistical distribution than that related to the 700 °C-annealed contact, supposed related to a certain level of inhomogeneity of the metal/semiconductor interface.

Then, a current-voltage-temperature (I-V-T) study was performed on the as-deposited, 700 °C and 950 °C-annealed contacts with measurements temperature varying between 25 °C and 150 °C. The J-V curves acquired at varying temperature for the three cases are reported in Fig.3, respectively.



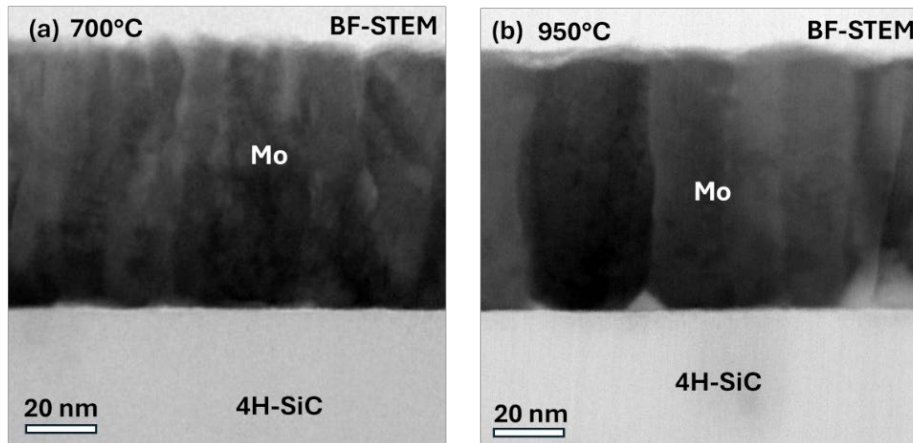
**Fig. 3.** a) Forward J-V characteristics acquired in a range of temperature varying between 25 °C and 150 °C (step of 25 °C) for a) as-deposited Mo/4H-SiC contact annealed, b) 700 °C and c) 950 °C annealed Mo/4H-SiC contacts.

The temperature-dependence of the ideality factor  $n$  and Schottky barrier  $\Phi_B$ , derived from the analysis of the forward characteristics, is plotted in Fig.4. A similar behavior is observed by the  $n$ - and  $\Phi_B$  temperature-dependence for the three cases.



**Fig. 4.** a) Forward J-V characteristics acquired in a range of temperature varying between 25 °C and 150 °C (step of 25 °C) for a) as-deposited Mo/4H-SiC contact annealed, b) 700 °C and c) 950 °C annealed Mo/4H-SiC contacts.

Finally, we combined the electrical characterization of the 700 °C and 950 °C-annealed contacts to a microstructural investigation by bright-field S/TEM analysis. The micrographs of the two annealed contacts are shown in Figs. 5a and 5b.



**Fig. 5.** Bright-field S/TEM of a) 700 °C and b) 950 °C thermal annealed Mo/4H-SiC Schottky contacts.

This analysis demonstrated a different situation occurred after 700 °C and 950 °C annealing: in the first case, an unreacted 4H-SiC surface is still present, keeping the Mo layer in the metallic form with grain sizes in the range of few tens of nanometers and providing continuous and homogeneous interface. Instead, at 950 °C we observed the presence of columnar grain in the Mo-film, therefore with a vertical size of about 75 nm. Noteworthy, even upon treatment at high temperature (950 °C), it was not observed a reaction between the Mo-film and the semiconductor interface. In addition to the variation of the grain size, the Mo-films in the contact annealed at highest temperature revealed the presence of less dense (brighter) areas near the interface, as consequence of the re-organization of this film, as confirmed by the associated High-Angle annular Dark-Field (HADF) imaging (not shown here). Chemical analyses performed by EELS in the interfacial region demonstrated that no reaction occurred between the Mo and 4H-SiC, while the brighter regions observed at 950°C can be

associated to voids formed as a consequence of the grains' enlargement. The different structure of the Mo film and interface morphology can explain the evolution of the electrical characteristics of the Mo/4H-SiC contacts annealed at 950°C.

## Summary

In this paper, we performed an electrical characterization on Mo/4H-SiC Schottky diodes. In particular, the electrical properties of the contacts following thermal annealing treatments at temperature up to 950 °C were studied under forward and reverse bias. Under forward bias, a reduction of the barrier height from 1.45 eV (as-deposited contact) to 1.30 eV (950°C-annealed contact) was observed, with the presence of a certain level of inhomogeneity for all the contacts. Under reverse bias, leakage current followed a thermionic-field emission (TFE) model after annealing at 750 °C, whereas it presented a significant increase after 15 V for the 950°C-annealed contact. Microstructural analyses were carried out by S/TEM analyses, highlighted an enlargement of the grains forming the structure of the Mo-film and the presence of voids near the Mo/4H-SiC interface. These observations occurring at the Mo/4H-SiC interface can explain the variation in the electrical behavior of the contact.

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## References

- [1] F. Roccaforte, P. Fiorenza, G. Greco, R. Lo Nigro, F. Giannazzo, F. Iucolano, M. Saggio, Emerging trends in wide band gap semiconductors (SiC and GaN) technology for power devices, *Microelectron. Eng.* 187–188 (2018) 66-77.
- [2] R. Yakimova, C. Hemmingsson, M.F. MacMillan, T. Yakimov, E. Janzén, Barrier Height Determination for n-Type 4H-SiC Schottky Contacts Made Using Various Metals, *J. Electron. Mater.* 27 (1998) 871-875.
- [3] M. Vivona, G. Bellocchi, R. Lo Nigro, S. Rascunà, F. Roccaforte, Electrical evolution of W and WC Schottky contacts on 4H-SiC at different annealing temperatures, *Semicond. Sci. Technol.* 37 (2022) 015012 1-8.
- [4] R. Rupp, R. Elpelt, R. Gerlach, R. Schomer, M.; Draghici, A new SiC diode with significantly reduced threshold voltage. In *Proceedings of the 2017 29th International Symposium on Power Semiconductor Devices and IC's (ISPSD)*, Sapporo, Japan, 28 May–1 June 2017; pp. 355–358.
- [5] A. B. Renz, V. A. Shah, O. J. Vavasour, Y. Bonyadi, F. Li, T. Dai, G. W. C. Baker, S. Hindmarsh, Y. Han, M. Walker, Y. Sharma, Y. Liu, B. Raghothamachar, M. Dudley, P. A. Mawby, P. M. Gammon, The improvement of Mo/4H-SiC Schottky diodes via a P2O5 surface passivation treatment, *J. Appl. Phys.* 127 (2020) 025704 1-9.
- [6] T. N. Oder and S. B. Nardella, Effects of deposition temperature on Mo/SiC Schottky contacts, *AIP Advances* 12 (2022) 025117 1-6.
- [7] T. Suzuki, H. Wakabayashi, K. Tsutsui, H. Iwai, K. Kakushima, Laminated Mo/C Electrodes for 4H-SiC Schottky Barrier Diodes with Ideal Interface Characteristics, *IEEE Electron. Dev. Lett.* 37 (2016) 618-620.

- [8] Z.-Y Yang, Y. Wang, X. Li, J. Yang, D. Shi, F. Cao, Thermal stability of Mo–C alloy Schottky contacts on n-type 4H-SiC, *Microelectron. Eng.* 239 (2021) 111531 1-5.
- [9] M Vivona, G Greco, F Giannazzo, R Lo Nigro, S Rascunà, M Saggio and F Roccaforte, Thermal stability of the current transport mechanisms in Ni-based Ohmic contacts on n- and p-implanted 4H-SiC, *Semicond. Sci. Technol.* 29 (2014) 075018 1-7.
- [10] S. M. Sze, and K. N. Kwok, *Physics of Semiconductor Devices*; John Wiley & Sons: Hoboken, NJ, USA, 2007.
- [11] F. A. Padovani and R. Stratton, Field and thermionic-field emission in Schottky barriers. *Solid-State Electron.* 9 (1966) 695–707.