

Doping and minority carrier lifetime uniformity of 4H-SiC homoepitaxial layers: role of C/Si ratio distribution

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Received 20 August 2024/Revised 17 October 2024/Accepted 15 April 2025/Published online 11 September 2025

Citation Liu W J, Tong Z Y, Zhang C, et al. Doping and minority carrier lifetime uniformity of 4H-SiC homoepitaxial layers: role of C/Si ratio distribution. *Sci China Inf Sci*, 2025, 68(10): 209401, <https://doi.org/10.1007/s11432-024-4385-5>

4H silicon carbide (4H-SiC) is the material of choice for high power, high frequency and high temperature electronics due to its outstanding properties such as wide bandgap, high breakdown electric field strength, high carrier mobility, high thermal conductivity, and high stability [1]. The thickness and doping concentration of the homoepitaxial layer, as well as their wafer-scale uniformities, determine the breakdown voltage and specific on-resistance of power devices [2]. However, as the thickness of 4H-SiC epitaxial layer increases, both the nonuniformity of thickness and doping concentration, as well as the morphological defect density of thick 4H-SiC epitaxial layers severely increase [3]. For ultra-high voltage 4H-SiC devices, improving the minority carrier lifetime and optimizing the wafer-scale doping uniformity are critical to the design of the depth profile of injected carrier density during their on-state operation. The conventional hot-wall chemical vapor deposition (CVD) is maturely developed for the epitaxy of 4H-SiC thin films with the thickness below 12 μm . However, as the thickness of 4H-SiC epitaxial films exceeds 50 μm and even 100 μm , the thermal field and the gas flow changes, and the step-flow growth becomes perturbed. This disturbance severely degrades the uniformity and increases the defect density of ultra-thick 4H-SiC epitaxial layers. Therefore, it is crucial to understand the origin of the nonuniformity of ultra-thick 4H-SiC epitaxial layers, which in turn provides solutions for the optimization of the CVD equipment and processing parameters.

In this study, the dependence of the distribution of doping concentration and minority carrier lifetime under different inlet C/Si ratios is investigated by combining trichlorosilane (TCS)-ethylene (C_2H_4)-hydrogen (H_2) CVD and numerical simulations. By increasing the inlet C/Si ratio from 1.32 to 1.52 and fixing the inlet nitrogen (N_2) flow rate, we find that the net doping concentration decreases and the dis-

tribution of net-doping concentration changes from “M” to “ \cap ” shape. Numerical simulations indicate that the wafer-scale distribution of N dopants exhibit the invariable “ \cap ” shape. Since the net carrier concentration is realized by N substituting N_C , we then evaluate the effect of the distribution of V_C on the net carrier concentration by minority carrier lifetime distribution. The results show that the non-uniform distribution of C/Si ratio contributes to a non-uniform distribution of net carriers.

A schematic diagram of the reactor is depicted in Figure 1(a). C_2H_4 and TCS are introduced from the inlet by the dilution of a flow rate of 100 standard liters per minute (slm) H_2 gas. The N_2 gas flow ratios between the center and edge are set as 0.27 and 0.16 sccm, respectively. The TCS is diluted by the H_2 carrier gas with the flow of 365.00 sccm and pressure of 1.5×10^5 Pa. Upon heating at 1620°C , the decomposition of gas components, reaction and adsorption of Si- and C-components happened during the CVD of 4H-SiC. Exhaust gases are removed by a vacuum pump, maintaining a pressure of 1×10^4 Pa. The substrates used in this study are *n*-type 4H-SiC with a diameter of 150 mm, having Si-terminated (0001) faces with 4° off-axis oriented toward the [11 $\bar{2}$ 0] orientation. Numerical simulations are performed using the commercial software COMSOL Multiphysics, which couples the electromagnetic heating, non-isothermal flow, and reaction kinetics. The main coupled equations and the numerical simulation details can be found in Appendix A. The three-dimensional (3D) heat and mass transfer are solved simultaneously together with the reaction kinetics, which gives the temperature distribution and reactant distribution in solid parts and in the gas. In our study, C_2H_4 and TCS are used both in experiments and simulations. The C/Si ratio is defined by the molar ratio of C and Si in the inlet of the reactor. The reaction kinetics with the reaction rate constants are described in

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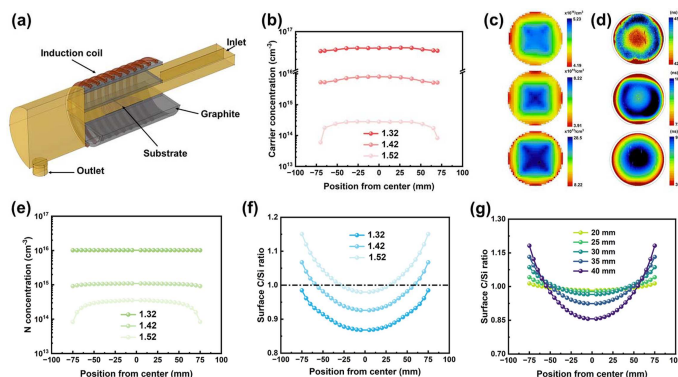


Figure 1 (Color online) (a) Schematic diagram of the horizontal hot-wall CVD reactor; (b) the radial distribution of net carrier concentration under different inlet C/Si ratios; (c) wafer-scale distribution of net carrier concentration and (d) the minority carrier lifetime under the inlet C/Si ratios of (top) 1.32, (medium) 1.42, and (bottom) 1.52; (e) simulated radial distribution of N concentration under different inlet C/Si ratios; (f) simulated surface C/Si ratio distribution under the inlet C/Si ratios; (g) surface C/Si ratio at different hot wall heights with the inlet C/Si ratio of 1.52.

Appendix B.

Figure 1(b) shows the radial distribution of net carrier concentration under different inlet C/Si ratios. When the inlet C/Si ratio increases from 1.32 to 1.52 by enlarging the C_2H_4 flux, the average carrier concentration decreases from 4.8×10^{16} to $2.2 \times 10^{14} \text{ cm}^{-3}$, which changes from “M” shapes, as a result of the site compensation effect [4]. Meanwhile, the nonuniformity (σ/mean) of doping concentration increases from 5.4% to 34.4% as the C/Si ratio at the inlet increases, as shown in Figure 1(c). 3D simulations of the 4H-SiC CVD reactor, including inductive heating and fluid dynamics as well as gas phase and surface chemistry, are then performed to explain the deteriorative doping uniformity with different inlet C/Si ratios. We find that the N concentration gradually increases along the direction of gas flow as described in Appendix C, numerical simulations indicate that the wafer-scale distribution of N exhibits the invariable “ \cap ” shape as shown in Figure 1(e).

In order to explain the deteriorative doping uniformity with higher inlet C/Si ratios, we investigate the effect of wafer-scale C/Si ratio on the doping uniformity. Because the minority carrier lifetime is closely related to the concentration of V_C , and thus related to the C/Si ratio, we then investigate the wafer-scale distribution of minority carrier lifetime of 4H-SiC under different inlet C/Si ratios. As shown in Figure 1(d), the minority carrier lifetime maximum increases from 450 to 1080 ns as the inlet C/Si ratio increases from 1.32 to 1.52. And the wafer-scale distribution of minority carrier lifetime exhibits the “M” and “ \cap ” shape under the inlet C/Si ratio of 1.32 (or 1.42) and 1.52, respectively. The radial distribution of minority carrier lifetime under different inlet C/Si ratios can be found in Appendix D.

The surface C/Si ratio is then simulated to explain the variations in wafer-scale distribution of doping concentration and minority carrier lifetime. We found that the surface C/Si ratio gradually decreases along the direction of gas flow as described in Appendix E, which results in a radial nonuniformity of the surface C/Si ratio during the epitaxy process (Figure 1(f)). Since N atoms replace the C atoms in 4H-SiC crystal, the increase of surface C/Si ratio decreases the N concentration and thus the net carrier concentration. When the inlet C/Si ratio is 1.42, the surface C/Si ratio is lower than the stoichiometric ratio at the wafer center and higher at the wafer edge, showing a “U” shape. Over high surface C/Si ratio can lead to interstitial carbon atoms and

increased surface recombination velocity due to the formation of morphological defects. Hence, in regions with excessively high surface C/Si ratios near the edge, the minority carrier lifetime decreases and exhibits the “M” shape. As described in Appendix F, simulations of the thermal field indicate a temperature gradient of approximately 30 K/mm within the reaction chamber. This temperature gradient is a key factor influencing the uniformity of the surface C/Si ratio [5]. The calculations suggest that reducing the distance between the upper and lower horizontal hot walls can effectively decrease the gas temperature gradient, which in turn helps to improve both the uniformity of the surface C/Si ratio and the doping uniformity simultaneously, as shown in Figure 1(g).

In conclusion, we have found that the deteriorative doping uniformity under high inlet C/Si ratios, which exhibits the “ \cap ” shape, is contributed by the “U” shape surface C/Si ratio distribution. Our simulations suggest that lowering the hot wall height and reducing the edge C/Si ratio improve the uniformity of net carrier distribution in ultra-thick 4H-SiC layers.

Acknowledgements This work was supported by National Key Research and Development Program of China (Grant No. 2024YFB3814001), Zhejiang Provincial Natural Science Foundation of China (Grant Nos. LD24F040004, LD25F040002), National Natural Science Foundation of China (Grant Nos. U23A20569, U23B20136, 6227414), Entrepreneur Team Introduction Program of Hangzhou (Grant No. TD2022012), Fundamental Research Funds for the Central Universities (Grant No. 226202200200), and Qianjiang Distinguished Experts of Hangzhou.

Supporting information Appendixes A–F. The supporting information is available online at info.scichina.com and link.springer.com. The supporting materials are published as submitted, without typesetting or editing. The responsibility for scientific accuracy and content remains entirely with the authors.

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