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# Modeling of Al Doping During 4H-SiC Chemical-Vapor-Deposition Trench Filling

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**ABSTRACT** Aluminum doping during 4H-SiC chemical-vapor-deposition (CVD) trench filling was numerically modeled toward precise design of high-voltage superjunction devices. As a first-order approximation, growth-rate- and surface-normal-scaling functions were determined based on the reported experimental results. Simulated isoconcentration contours of aluminum were confirmed to qualitatively agree with the reported imaging of doping in SiC by scanning spreading resistance microscopy. Improvement of the proposed models based on additional experiments should contribute to reducing the development time for 4H-SiC superjunction devices fabricated using CVD trench filling.

**INDEX TERMS** Aluminum, power semiconductor devices, silicon compounds, simulation.

## I. INTRODUCTION

Superjunction (SJ) devices, in which alternating p- and n-type columns are located in a drift layer [1], [2], have been developed to improve the tradeoff relationship between breakdown voltage ( $BV$ ) and specific on-resistance in unipolar devices. In the case of 4H-SiC SJ devices, ion implantation has been used to demonstrate  $BV$  of 0.8 to 2.4 kV [3]–[9]; however, chemical-vapor-deposition (CVD) trench filling, whose growth window was empirically obtained [10], should become the key technique for higher- $BV$  4H-SiC SJ devices. Although development time for such trench-filling SJ devices is expected to be reduced by using technology computer-aided design (TCAD), topography simulation [11], [12], a part of TCAD, has not been widely used due to its inability to simulate a distribution of acceptor concentration ( $N_A$ ) in filled trenches. Instead, only device simulation was carried out by assuming a fixed  $N_A$  in the filled trenches [13]–[19] or two different values of  $N_A$  in the regions close to the trench sidewalls and in the rest of the filled trenches [20].

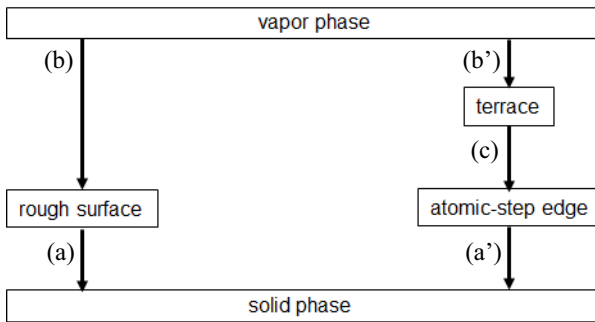
In-situ p-type doping in 4H-SiC CVD is usually carried out by the addition of trimethylaluminum. The efficiency of aluminum incorporation into solid SiC needs to be represented

in topography simulation by a scaling function  $k$ , which is, in general, influenced by the strain [21] and surface orientation effects [22]. The radius of an aluminum ion having the coordination number of four (i.e., 0.039 nm [23]) is about twice as large as the average of the radii of silicon and carbon ions having the coordination number of four {i.e.,  $(0.026 + 0.015)/2 = 0.021$  nm [23]}. An aluminum atom once incorporated into the solid thus tends to be pushed out into vapor; however, when the growth rate normal to the growing surface ( $R_g$ ) is too high, it does not have enough time to escape from the solid (i.e.,  $k = 1$ ). In contrast,  $N_A$  decreases to its equilibrium value when  $R_g$  is close to zero [24]. Such  $R_g$ -dependent  $N_A$  was experimentally observed by Forsberg *et al.* with respect to growth on 4H-SiC (0001) substrates [25]. Negoro *et al.*, on the other hand, reported an influence of  $\{1\bar{1}00\}$  faces (whose normal vector has an angle  $\theta$  of  $90^\circ$  from the  $[0001]$  direction) on  $N_A$  [26]. Although the trenches were filled with Al-doped SiC, the regions close to  $\{1\bar{1}00\}$  trench sidewalls became n-type when the carbon-to-silicon ratio in the input gas ( $C/Si$ ) was unity. Since the regions became p-type in the case  $C/Si \geq 2$  [26], the surface orientation dependence of  $k$  is considered to be a function of  $\theta$  and  $C/Si$ .

Judging from these reports [25], [26], we must set our final goal to determine  $k(R_g, \theta, C/Si)$  contours for practical topography simulation. Because of the limited experimental results, however, only a growth-rate-scaling function  $k(R_g)$  or a surface-normal-scaling function  $k(\theta)$  was used in this paper as a first order approximation.

## II. SIMULATION MODELS

The surface reactions during 4H-SiC CVD based on  $\text{SiH}_4$  and  $\text{C}_3\text{H}_8$  [(a) and (a') in Fig. 1] are known to be so fast [27] that trench filling is limited by either vapor-phase diffusion (in the case of growth on a rough surface) [(b) in Fig. 1] or surface diffusion (in the case of growth on a step-and-terrace surface) [(c) in Fig. 1] of growing species. As an example of the former case, a scanning spreading resistance microscopy (SSRM) image of doping in a 7- $\mu\text{m}$ -deep trench [20] is shown in Fig. 2. There seem to be no facets appeared on the grown surface, indicating the trench was filled in the growth mode on a rough surface. High resistivity (namely, low  $N_A$ ) regions exist along the trench sidewalls, and the resultant boundaries between the low  $N_A$  regions and the center region with high  $N_A$  are almost vertical.

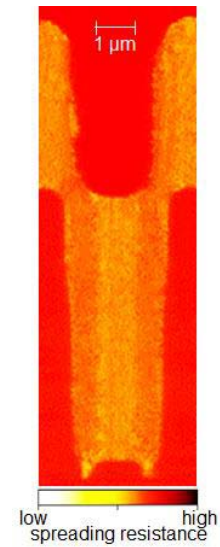


**FIGURE 1.** Flow chart of epitaxial growth processes. (a)(a') Surface reactions. (b)(b') Vapor-phase diffusion. (c) Surface diffusion.

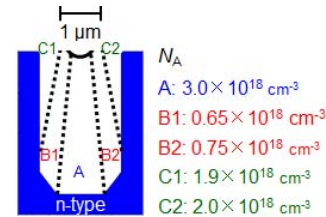
As shown schematically in Fig. 3, on the other hand, Malhan *et al.* reported that the low  $N_A$  regions (B1 and B2) are sandwiched between the high  $N_A$  regions (A/C1 and A/C2, respectively) and that the boundaries between the low and high  $N_A$  regions are inclined from the vertical direction [28]. Since faces with  $\theta$  of about  $45^\circ$  [i.e.,  $\{1\bar{1}0n\}$  ( $n \sim 4$ )] are known as facets [29], the low  $N_A$  regions (B1 and B2) in Fig. 3 are considered to be the tracks of such facets on which growing species diffused [21]. Since surface diffusion was difficult to be included in the commercial topography simulator used (Victory Process 2D [30]), this study covers growth on a rough surface (Fig. 2) only.

### A. MODEL FOR A GROWTH-RATE-SCALING FUNCTION

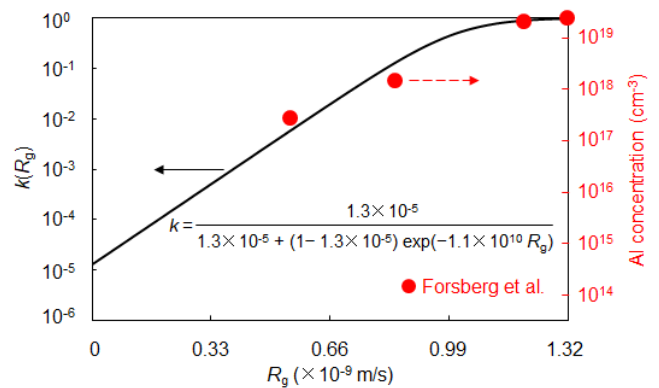
The solid circles in Fig. 4 show the reported aluminum concentration in 4H-SiC grown on (0001) substrates at surface temperature  $T$  of 1873 K [25]. With respect to surface roughness during CVD trench filling of 4H-SiC, the present authors experimentally showed that the surface on



**FIGURE 2.** Cross-sectional SSRM image of 7- $\mu\text{m}$ -deep filled trench, as seen as the  $[1\bar{1}20]$  direction, reported in [20].

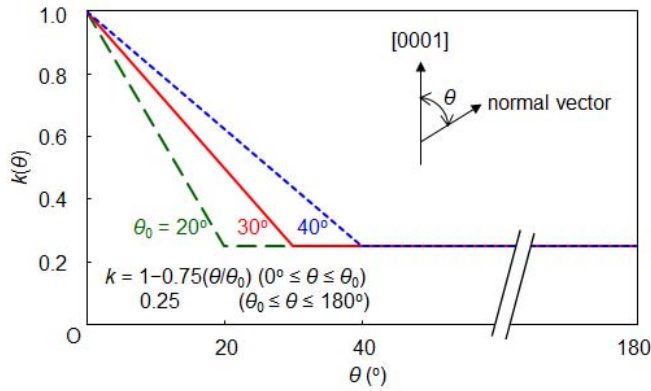


**FIGURE 3.** Schematic cross-sectional SSRM image of 3.5- $\mu\text{m}$ -deep filled trench, as seen as the  $[1\bar{1}20]$  direction, reported in [28]. Due to the difficulty in clearly reproducing the reported SSRM image, we just traced the boundaries that were drawn in [28].



**FIGURE 4.** Measured aluminum concentration (shown in the right-hand vertical axis) as a function of  $R_g$  [25] and modeled growth-rate-scaling function (shown in the left-hand vertical axis).

the mesa top was rough in the case  $T \geq 1843$  K, while it was smooth in the case  $T \leq 1823$  K [31]. We therefore considered the experimental data in Fig. 4 represent  $N_A$  in 4H-SiC grown on a rough surface and modeled  $k(R_g)$  by vertically displacing the data, as shown by the solid line. In reference to the Burton-Prim-Slichter theory, which was



**FIGURE 5. Modeled surface-normal-scaling function. Definition of  $\theta$  is shown in the inset.**

successfully applied to  $k$  in silicon grown from the melt [32],  $k(R_g)$  was fitted as

$$k(R_g) = k^e / \left[ k^e + (1 - k^e) \exp\left(-1.1 \times 10^{10} / R_g\right) \right] \text{ and} \quad (1a)$$

$$k^e = 1.3 \times 10^{-5}, \quad (1b)$$

where  $k^e$  represents  $k(R_g = 0)$  under the equilibrium condition.

### B. MODEL FOR A SURFACE-NORMAL-SCALING FUNCTION

The ratio of the low  $N_A$  to the high  $N_A$  in Fig. 2 was reported to be 0.25, although the values of  $N_A$  were not measured [20]. Since the  $C/Si$  was less than unity [20], the effect of incorporation of nitrogen donors [26] seemed to affect the measured  $k(\theta = 90^\circ)$  of 0.25. According to the experiments by Forsberg *et al.*,  $k(\theta = 180^\circ)$  was also considered to be small [25].  $k(\theta)$  was therefore fitted simply as

$$k(\theta) = 1 - 0.75(\theta/\theta_0) \quad (0^\circ \leq \theta \leq \theta_0) \text{ and} \quad (2a)$$

$$0.25(\theta_0 \leq \theta \leq 180^\circ). \quad (2b)$$

Eqs. (2a) and (2b) are shown in Fig. 5 in the cases  $\theta_0 = 20^\circ$ ,  $30^\circ$ , and  $40^\circ$ .

### III. SIMULATION

Based on the result in Fig. 2, a 7- $\mu\text{m}$ -deep trench having 0.5- $\mu\text{m}$ -deep sub trenches (Fig. 6) was numerically investigated. Since the conditions for the trench-filling growth were not described in detail [20], the following conditions for the boundary-layer model in topography simulation [11] were tentatively assumed:

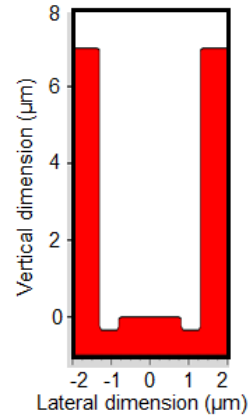
$$C^e(\infty) = 8.775 \times 10^{-9} \text{ kmol/m}^3, \quad (3a)$$

$$C^0 = 8.952 \times 10^{-9} \text{ kmol/m}^3, \quad (3b)$$

$$L_L = 1.5 \text{ mm}, \quad (3c)$$

$$T = 1923 \text{ K}, \text{ and} \quad (3d)$$

$$\gamma = 0.1 \text{ J/m}^2, \quad (3e)$$



**FIGURE 6. Initial structure used for topography simulation. The trench is 7  $\mu\text{m}$  deep and the sub trenches are 0.5  $\mu\text{m}$  deep.**

where  $C^e(\infty)$  and  $C^0$  are vapor-phase concentrations of growing species in the vicinity of an infinite plane and at the top of the boundary layer, respectively,  $L_L$  is the thickness of the boundary layer, and  $\gamma$  is the surface free energy of 4H-SiC during growth [11]. The effective vapor-phase diffusivity of growing species ( $D^{\text{eff}}$ ) was determined from the growth rate on an infinite plane ( $R_0$ ), which was chosen as an input parameter.

$R_g$  was determined from the following equations: [11]

$$\partial\varphi/\partial t + R_g(\partial\varphi/\partial x + \partial\varphi/\partial y) = 0, \quad (4)$$

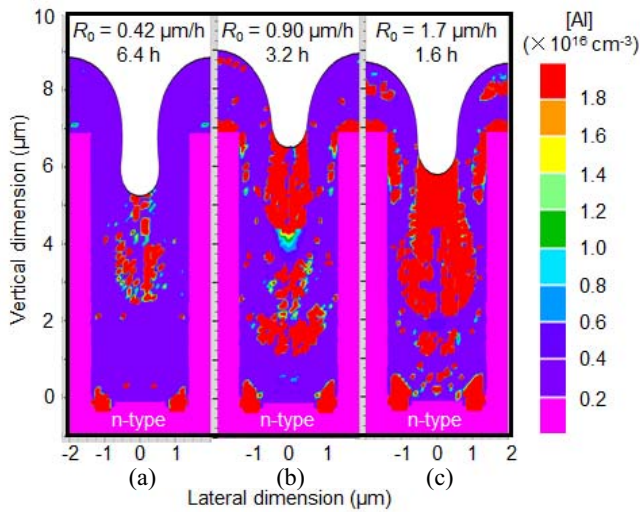
$$R_g = \left[ -D^{\text{eff}} \left( C|_{\text{growing surface}} - C^e(r) \right) / \partial n \right] V_m, \text{ and} \quad (5)$$

$$C^e(r) = C^e(\infty) \exp(\gamma V_m / RT r), \quad (6)$$

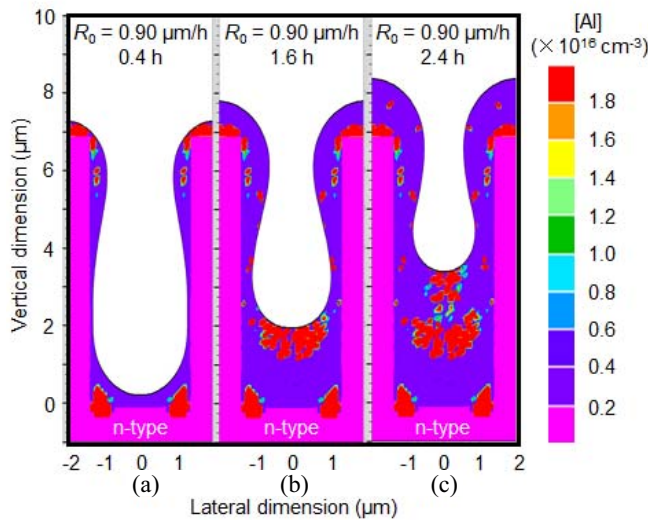
where  $\varphi(x, y)$  is a level-set function defined as a function of the signed distance from the point  $(x, y)$  to the growing surface,  $\mathbf{n}$  is the vector normal to the growing surface,  $C^e(r)$  is the equilibrium vapor-phase concentration of growing species in the vicinity of a growing surface with a radius of curvature  $r$ ,  $V_m$  is the molar volume of 4H-SiC ( $1.25 \times 10^{-5} \text{ m}^3/\text{mol}$ ) [33], and  $R$  is the ideal gas constant. Eq. (6) is known as the Gibbs–Thomson effect [34]. Eqs. (4) and (5) were solved by methods that use the high-order nonoscillatory schemes for Hamilton–Jacobi equations [35].

### IV. RESULTS AND DISCUSSION

In the case that  $k$  can be assumed to be independent of  $\theta$  and  $C/Si$ , the maximum doping level of aluminum ( $N_{\text{max}}$ ), which corresponds to  $N_A$  at  $k = 1$ , was assumed to be  $3.0 \times 10^{17} \text{ cm}^{-3}$  to give  $N_A$  of  $2.0 \times 10^{16} \text{ cm}^{-3}$  that was assumed for device simulation in [20]. As shown in Fig. 7(b), the use of  $R_0 = 0.90 \mu\text{m/h}$  reproduces the result in Fig. 2 qualitatively. When  $R_0$  is lower (i.e.,  $0.42 \mu\text{m/h}$ ),  $N_A$  in the region around the trench bottom is too low [Fig. 7(a)]. When  $R_0$  is higher (i.e.,  $1.7 \mu\text{m/h}$ ), on the other hand, the width of the regions (with low  $N_A$ ) close to the trench sidewalls is too narrow [Fig. 7(c)]. Figs. 8(a)–(c) shows topography changes over growth time in the case  $R_0 = 0.9 \mu\text{m/h}$ . During the initial stage of trench filling, the



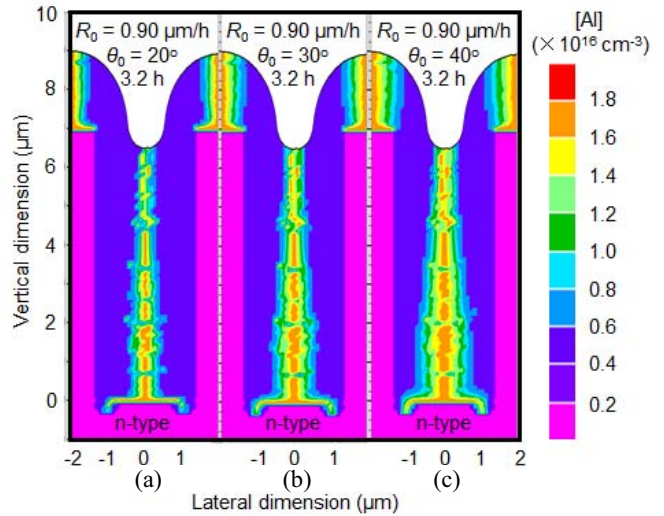
**FIGURE 7.** Simulated isoconcentration contours of aluminum in (a) 6.4-h ( $R_0 = 0.42 \mu\text{m/h}$ ), (b) 3.2-h ( $R_0 = 0.90 \mu\text{m/h}$ ), and (c) 1.6-h ( $R_0 = 1.7 \mu\text{m/h}$ ) grown 4H-SiC filled trenches when  $k$  is a function of  $R_g$  only.



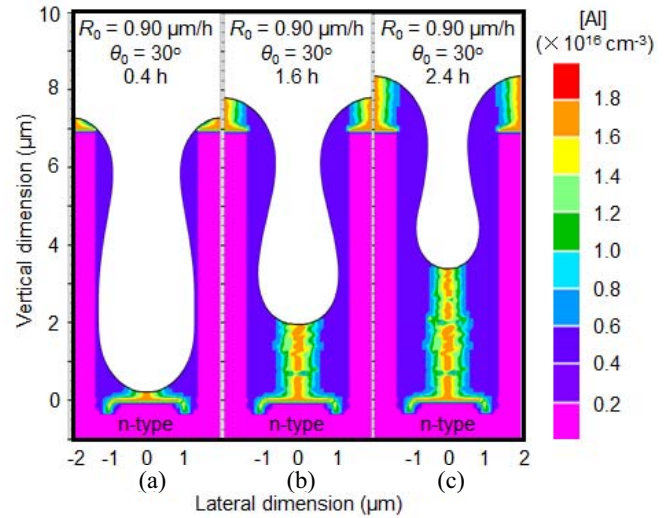
**FIGURE 8.** Simulated isoconcentration contours of aluminum in (a) 0.4-h, (b) 1.6-h, and (c) 2.4-h grown 4H-SiC filled trenches when  $R_0$  is  $0.90 \mu\text{m/h}$  and  $k$  is a function of  $R_g$  only.

regions with  $r < 0$  (in the subtrenches and around the corners of the trench bottom) are filled rapidly due to Eqs. (5) and (6), resulting in high  $N_A$  there [Fig. 8(a)]. The region with  $r < 0$  then moves to the center of the trench [Fig. 8(b)]. Since the center region comes to have high  $R_g$ , it continues to have high  $N_A$  [Figs. 8(c) and 7(b)].

In contrast, the case that  $k$  can be assumed to be independent of  $R_g$  and  $C/Si$  is considered to correspond to the case of  $R_g$  being too high.  $N_{\text{max}}$  was therefore assumed to be  $2.0 \times 10^{16} \text{ cm}^{-3}$ . As shown in Fig. 9(c), the use of  $\theta_0 = 40^\circ$  results in the sloped boundaries between the low and high  $N_A$  regions. In the cases  $\theta_0 = 20^\circ$  or  $30^\circ$ , on the other hand, the boundaries become relatively vertical [Figs. 9(a) and 9(b)],



**FIGURE 9.** Isoconcentration contours of aluminum in 3.2-h grown trenches simulated by assuming  $\theta_0$  of (a)  $20^\circ$ , (b)  $30^\circ$ , and (c)  $40^\circ$  when  $R_0$  is  $0.90 \mu\text{m/h}$  and  $k$  is a function of  $\theta$  only.



**FIGURE 10.** Simulated isoconcentration contours of aluminum in (a) 0.4-h, (b) 1.6-h, and (c) 2.4-h grown 4H-SiC filled trenches when  $R_0$  is  $0.90 \mu\text{m/h}$  and  $k$  is a function of  $\theta$  only.

which are similar to the SSRM image in Fig. 2. However, the width of the high  $N_A$  region is narrower than that in Fig. 2. Topography changes over growth time are thus shown in Figs. 10(a)-(c) in the case  $\theta_0 = 30^\circ$  only. From the initial stage of trench filling [Fig. 10(a)],  $N_A$  becomes large both in the subtrenches and in the region on the mesa top.

The comparison between these two cases is the advantage of the latter. For further investigation, however, computational fluid dynamics simulation (based on the detailed growth conditions) and quantitative analysis of the experimental observation (Fig. 2) are needed in both models for  $k(R_g)$  and  $k(\theta)$ . Additional experiments can also improve these functions of one variable to  $k(R_g, \theta, C/Si)$  contours for practical topography simulation, which should contribute

to reducing the development time for 4H-SiC SJ devices fabricated using CVD trench filling.

Note that the filled sub trenches with high  $N_A$  will lead to local electric-field concentration in reverse-biased SJ devices. To avoid that prospect, either fabricating sub trench-free trenches or making a start of trench-filling growth by a thin n-type layer should be required.

## V. CONCLUSION

Aluminum doping during 4H-SiC CVD trench filling was numerically modeled. As a first order approximation, growth-rate- and surface-normal-scaling functions were determined from the reported experimental results. The resultant iso-concentration contours of aluminum were qualitatively agreed with the reported SSRM image. Improvement of the proposed models based on additional experiments should accelerate development of high-voltage 4H-SiC SJ devices.

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