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### ANALYSIS OF STEP-VELOCITY DEPENDENCES OF CARBON CONCENTRATION IN c- AND m-PLANE GAN HOMOEPITAXIAL LAYERS

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Reported step-velocity dependences of carbon concentration in c- and m-plane GaN homoepitaxial layers were successfully reproduced based on a step-edge segregation model with the following assumptions: 1) the diffusion coefficient of carbon in GaN is  $2\times10^{-13}$  cm²/s (@  $1000^{\circ}\text{C}-1100^{\circ}\text{C}$ ); 2) the length of time before the carbon concentration at the step-edge site reaches its equilibrium value is sufficiently shorter than the meantime until a carbon atom incorporated at the kink site moves through the step-edge site to the surface site.

#### I. Introduction

Toward the realization of an advanced energy-saving society, group-III-nitride semiconductors have been used for highly efficient electronic<sup>1,2)</sup> and optical devices.<sup>3)</sup> For the performance improvement of such devices, it is necessary to reduce the carbon impurity, which is known to create deep levels.<sup>4–9)</sup> In the case of GaN power devices with breakdown voltage exceeding 1 kV, the carrier concentration in the n-type drift layer has to be lower than  $1 \times 10^{16}$  cm<sup>-3</sup>.<sup>10)</sup> Metalorganic vapor-phase epitaxy (MOVPE) under unoptimized growth conditions, however, results in carbon concentration on the order of  $10^{16}$  cm<sup>-3</sup> in GaN layers.<sup>11)</sup> In the case of green laser diodes, on the other hand, the growth temperature  $T_g$  for p-type (Al)GaN layers has to be low (about 900°C) to avoid thermal degradation of high-In content InGaN/GaN multi-quantum wells.<sup>12)</sup> Such low  $T_g$  during MOVPE induces severe carbon incorporation, resulting in high-resistivity p-(Al)GaN.<sup>13)</sup>

With respect to the understanding of impurity segregation, MOVPE growth on vicinal surfaces should be effective on the basis that an impurity can segregate not only at the surface site, <sup>14)</sup> but also at the step-edge sites (Fig. 1). In the case of nitrogen segregation during liquid-phase epitaxy of GaP, Nishinaga et al. proposed a step-edge segregation

model in which part of the impurity atoms incorporated at the kink site is assumed to escape from the step-edge site. 15,16) They expressed the

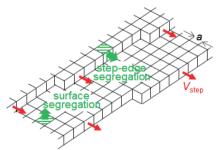


Fig. 1. Schematic illustration of step-edge and surface segregation on a growing stepped surface.  $V_{\rm step}$ : average step velocity; a: lattice constant.

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$$k = k_{\text{surf}} + (k_{\text{step}} - k_{\text{surf}}) \exp(-D / V_{\text{step}} a), \tag{1}$$

where  $k_{\text{surf}}$  and  $k_{\text{step}}$  are the equilibrium segregation coefficients at the surface and stepedge sites, respectively, D is the diffusion coefficient in the solid,  $V_{\text{step}}$  is the average step velocity, and a is the lattice constant. Equation (1) holds when the length of time before the impurity concentration at the step-edge site reaches its equilibrium value,  $\tau_{\text{step}}$ , is sufficiently shorter than the meantime until an impurity incorporated at the kink site moves through the step-edge site to the surface site,  $\tau$ .

Considering a large strain around the carbon occupying a gallium site ( $C_{Ga}$ ) in GaN (because of the bond length of  $C_{Ga}$  being 18%–26% shorter than the GaN bulk bond length), <sup>4,17-19</sup> Mochizuki et al. assumed that the segregation coefficient of  $C_{Ga}$  is less than unity. <sup>20)</sup> They also assumed that the concentration ratio of carbon adatoms to gallium adatoms in the vicinity of the step-edge site was about the same as the concentration ratio of carbon adatoms to gallium adatoms at the surface site and rewrote Eq. (1) as <sup>20)</sup>

$$N = N_{\text{surf}} + (N_{\text{step}} - N_{\text{surf}}) \exp(-D / V_{\text{step}} a), \tag{2}$$

where N is the carbon concentration in GaN layers,  $N_{\rm surf}$  is the equilibrium carbon concentration at the surface site, and  $N_{\rm kink}$  is the equilibrium carbon concentration at the kink site. In the case of polar c-plane GaN homoepitaxial layers [Fig. 2(a)], they reproduced the reported experimental results<sup>21-23)</sup> using Eq. (2) with  $D = 2 \times 10^{-13}$  cm<sup>2</sup>/s and a = 0.30 nm.<sup>20)</sup>

In the case of non-polar m-plane GaN homoepitaxial layers [Fig. 2(b)], on the other hand, Yamada et al. experimentally reported the dependence of N on  $V_{\text{step}}$ . Accordingly, in this report, the reported  $V_{\text{step}}$  dependence of N in m-plane GaN layers is analyzed and compared to the reported analysis for the  $V_{\text{step}}$  dependence of N in c-plane GaN layers. <sup>24)</sup>

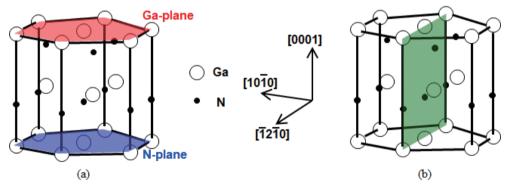


Fig. 2. (a) Polar c-plane and (b) nonpolar m-plane in the GaN wurtzite crystal unit cell.

#### II. Analysis

The surface atomic density in the solid, n, is  $0.61 \times 10^{15}$  cm<sup>-2</sup> on an m-plane and 1.14  $\times 10^{15}$  cm<sup>-2</sup> on a c-plane. <sup>25)</sup> By simply assuming the simple cubic lattice shown in Fig. 1,  $a = (m^{-0.5})$  is calculated to be 0.40 nm on an m-plane and 0.30 nm on a c-plane. As shown in Fig. 3, D of  $2 \times 10^{-13}$  cm<sup>2</sup>/s well reproduces the results for c- (i.e., Ga-, N-) and m-plane growths.

#### III. Discussion

Cao et al. measured the concentration-depth profiles of carbon implanted into GaN at doses of  $3-5\times10^{14}$  cm<sup>-2</sup> and found that D is less than  $2 \times 10^{-13}$ cm<sup>2</sup>/s even after annealing at 1450°C.<sup>26)</sup> Judging from the similar D fitted in the case of  $T_g$ of 1000°C<sup>24</sup>)–1100°C<sup>21</sup>) (Fig. 3), consider the step-edge segregation model is adequate describing carbon segregation during MOVPE of GaN.

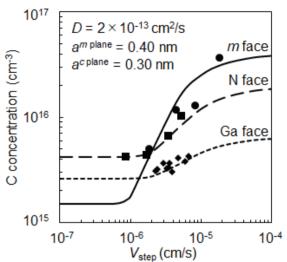


Fig. 3. Step-velocity dependences of carbon concentration fitted to the reported results. 21~24)

#### **IV. Conclusions**

Based on the step-edge-segregation model, the reported step-velocity dependences of carbon concentration in c- and m-plane GaN homoepitaxial layers were reproduced by assuming  $D = 2 \times 10^{-13}$  cm<sup>2</sup>/s (@ 1000°C-1100°C) and  $\tau_{\text{step}} << \tau$ .

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