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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 2×10^{-13} cm^2/s (@ 1000°C−1100°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[1,2] and optical devices.[3] For the performance improvement of such devices, it is necessary to reduce the carbon impurity, which is known to create deep levels.[4–9] 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 1×10^{16} cm^{-3}.[10] Metalorganic vapor-phase epitaxy (MOVPE) under unoptimized growth conditions, however, results in carbon concentration on the order of 10^{16} cm^{-3} in GaN layers.[11] 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.[12] Such low T_g during MOVPE induces severe carbon incorporation, resulting in high-resistivity p-(Al)GaN.[13]

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,[14] 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

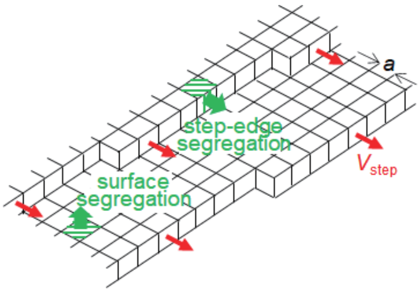

Fig. 1. Schematic illustration of step-edge and surface segregation on a growing stepped surface. V_{step}: average step velocity; a: lattice constant.

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segregation coefficient, k, as

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

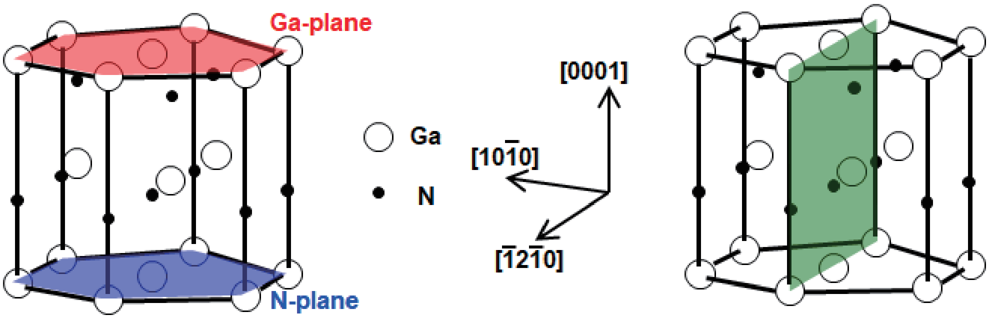
where k_{surf} and k_{step} are the equilibrium segregation coefficients at the surface and step-edge sites, respectively, D is the diffusion coefficient in the solid, V_{step} is the average step velocity, and a is the lattice constant. Equation (1) holds when the length of time before the impurity concentration at the step-edge site reaches its equilibrium value, τ_{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, τ.

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),[4,17-19] Mochizuki et al. assumed that the segregation coefficient of C_{Ga} is less than unity.[20] 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[20]

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

where N is the carbon concentration in GaN layers, N_{surf} is the equilibrium carbon concentration at the surface site, and N_{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[21-23] using Eq. (2) with $D = 2\times10^{-13}$ cm^2/s and $a = 0.30$ nm.[20]

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_{step}. Accordingly, in this report, the reported V_{step} dependence of N in m-plane GaN layers is analyzed and compared to the reported analysis for the V_{step} dependence of N in c-plane GaN layers.[24]



(a) (b)

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 0.61×10^{15} cm^{-2} on an m-plane and 1.14×10^{15} cm^{-2} on a c-plane.[25] By simply assuming the simple cubic lattice shown in Fig. 1, a ($= n^{-0.5}$) 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 2×10^{-13} cm^2/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^{-2} and found that D is less than 2×10^{-13} cm^2/s even after annealing at 1450°C.[26] Judging from the similar D fitted in the case of T_g of 1000°C[24]–1100°C[21] (Fig. 3), we consider the step-edge segregation model is adequate for describing carbon segregation during MOVPE of GaN.

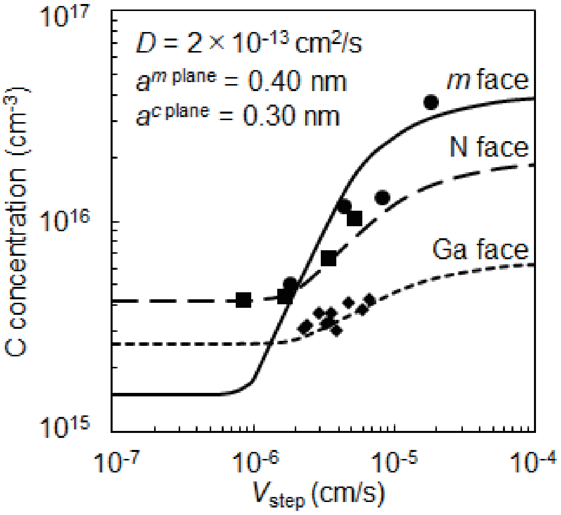


Fig. 3. Step-velocity dependences of carbon concentration fitted to the reported results.[21~24]

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 $D = 2\times10^{-13}$ cm^2/s (@ 1000℃−1100℃) and $\tau_{\mathrm{step}} \ll \tau$.

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