of etching v_p, entering into formula (2), will be higher for the face (0001). Hence, and according to formula (2), the etch pits, formed on the dislocations, will be wider and deeper.

In this connection we mention, that in the vicinity of the emergence of dislocations and on the faces (0001) and $(1\bar{1}01)$, the relation between gaseous flows of the components, V/III, may be violated, see Eq. (1).

5. Thermodynamics and kinetics of the nucleation of V-defects in polar and semipolar epitaxial GaN films

A large body of models describing the nucleation of etch pits on dislocations, are fully considered in the monograph [17]. Among them the Cabrera [22] and Schaarwehter [23] models hold the lead. According to the Cabrera model, the formation of a disk-shaped (or coin-shaped) etch pit results in a decrease in free energy by $hA\kappa \ln r/r_0$, where $A = G^{GaN}b^2/4\pi$, G^{GaN} is a shear modulus of GaN; b is the Burgers vector of dislocations in GaN; $\kappa = 1/(1-\nu)$; ν is the Poisson coefficient of GaN; and r_0 is a radius of the dislocation nuclei, beyond which the theory of elastic continuum is valid, r and h are a radius and a depth of an etch pit, respectively. Schaarwehter [23] has shown that the Cabrera model holds only beyond the dislocation nucleus, which is not, however, proved experimentally. He proposed to take for calculations another form of the potential, namely, the potential of the form $hA\kappa(r/r_0)$, i.e. the deformation energy, along Schaarwehter, increases linearly with radius, not logarithmically as it does in the Cabrera model. As a result, Schaarwehter has derived the expressions for the critical radius r'_{cr} and the free energy $\Delta F'_d\ (r'_{cr})$ of an etch pit nucleated on dislocations. These dependences are of the form:

$$r'_{cr} = \frac{\gamma\Omega}{\Delta\mu}\left(1 - \frac{A\kappa}{2\pi\gamma r_0}\right) = \sqrt{p}r_{cr}, \tag{3}$$

$$\Delta F^*_d(r'_{cr}) = p\Delta F^*(r_{cr}). \tag{4}$$

Here $p = \left(1 - \frac{A\kappa}{2\pi\gamma r_0}\right)^2 = \left(1 - \frac{r_F}{r_0}\right)^2$; $r_F = \kappa G^{GaN}b^2/8\pi^2\gamma$ is the Frank radius; γ, surface energy; Ω, a volume per atom, in our case, per a molecule of GaN; $\Delta\mu = \mathrm{kT}\ln C/C_o$; C_o, the concentration of saturation in the vapor phase; C, the concentration of the matter at the place of emergence of dislocations; $r_{cr} = \gamma\Omega/\Delta\mu$, the critical size of an etch pit, formed on the smooth surface, without regard for the dislocation energy; $\Delta F^*(r_{cr}) = \pi h\gamma^2\Omega/\Delta\mu$, the free energy of formation of an etch pit of depth h on the crystal surface, without considering the dislocation energy.

The expression for the chemical potential $\Delta\mu$, entering into formulas (2) and (3), is applicable to one -component systems only. It is can, however, be generalized, by invoking the recently developed theory of nucleation of a new phase in chemical reactions [24], in which the chemical affinity ξ plays a role of the quantity $\mathrm{kT}\ln C/C_o$. In our case, with regard for the reaction (1) of formation of GaN, for the chemical affinity ξ we have the expression

$$\xi = kT \ln \frac{P_{H_2}P_{GaCl}}{P_{NH_3}K_p^{GaN}}, \tag{5}$$

where $\mathrm{K_p^{GaN}} = P^0_{H_2}P^0_{HCl}/P^0_{NH_3}$ is the equilibrium constant of the chemical reaction (1); $P^0_{H_2}, P^0_{GaCl}, P^0_{NH_3}$ are the pressures of hydrogen, gallium chloride and ammonia, respectively, which are equilibrium at temperature of the synthesis; $P_{H_2}, P_{GaCl}, P_{NH_3}$ are the operating pressures [at which the synthesis of GaN occurs along the reaction (1)]. One should keep in mind, that on dissolving of the surface, the operating pressures in the gaseous phase may be comparable (or even lower) to the equilibrium pressures in the vicinity of the dislocation

nucleus.

Let us estimate the Frank radius for the faces (0001) and $(1\bar{1}01)$ of GaN. In epitaxial layers with wurtzite structure of a lattice, the dislocations of three types are observed: the edge dislocations (mixed dislocations (b_m) and screw nano-tubes (b_{nano}). The corresponding Burgers vectors are:

$b_e = \frac{1}{3}(11\bar{2}0)$, $\left(b_e = a, b_e^2 = a^2\right)$; $b_m = \frac{1}{3}(11\bar{2}3)$, $(b_{rmm} = \sqrt{c^2 + a^2}, b_m^2 = 3.66a^2)$;

$b_s = [0001]$, $(b_s = c, b_s^2 = 2{,}66a^2)$; $b_{nano} = n \times b_s$,

parameter n may take the following values n=1,2,3… and a=0,312 nm; c=0,519 nm. The values of the shear modulus G^{GaN}, of the Poisson coefficients ν of GaN, and of surface energies γ for planes (0001) and $(1\bar{1}01)$ are given in the paper [19]: $G^{GaN}_{(0001)} \approx 113$GaP, $G^{GaN}_{(1\bar{1}01)} \approx 90$GaP, $\nu_{(0001)} \approx 0.336$; $\nu_{(1\bar{1}01)} \approx 0.187$, $\gamma_{(0001)} \approx 4.41\, Jm^{-2} \gamma_{(1\bar{1}01)} \approx 3.23\, Jm^{-2}$. We note, that for $\gamma_{(1\bar{1}01)}$ we used the value of the surface energy calculated in [19] for the face $(11\bar{2}0)$ since from the crystallographic view point, the faces $(1\bar{1}01)$ and $(11\bar{2}0)$ differ insignificantly. As a result, for the Frank radius on the surface (0001), in the case $n = 1$, we have $r_F^{(0001)} \approx 5.5 \cdot 10^{-11} m$. When $n = 2$, $r_F^{(0001)} \approx 3 \cdot 10^{-10} m$. The Frank radius on the plane $(11\bar{2}0)$ is $r_F^{(0001)} \approx 2.8 \cdot 10^{-11} m$. One can assume for estimates that r_0 is of the order of the Burgers vector for the given face.

For the face $(1\bar{1}01)$ the factor $\sqrt{p}$ in formula (3) takes the following values: for the plane (0001) at n=1, $\sqrt{p}_{(0001)} \approx 0.88$. For the plane $(11\bar{2}0)$ - $\sqrt{p}_{(11\bar{2}0)} \approx 0.91$. By Schaarwehter theory [23], when the ratio $r_F/r_0 < 0.5$ holds, the etch pits are nucleated in accord with the classic theory. In this case, the value of the surface energy is changed only and should be renormalized, according to (3), as $\gamma' = \gamma \cdot \sqrt{p}$. Since $\sqrt{p} < 1$, the critical size of the pit, at the same value of the chemical affinity, will be less, than that calculated without regard for effects of dislocations on the nucleation. The nucleation barrier will also be decreased (4), resulting in higher velocity of the nucleation compared with the case of a smooth surface. In our case, as follows from the above-given estimates, the ratio $r_F/r_0 < 0.5$ takes place. Thus, in order to estimate the critical size and the nucleation velocity of etch pits, one should use the renormalized value of γ. If the condition $r_F/r_0 < 0.5$ holds both on the plane $(1\bar{1}01)$ and on the plane (0001), then, at the same value of the chemical affinity, the etch pits will be nucleated more intensively on the plane $(1\bar{1}01)$ where their critical sizes will be less. The reason is that the surface energy of an etch pit on the plane $(1\bar{1}01)$ is less than on the plane (0001). It is appropriate to note, that we ignored the lateral faceting of the etch pits. In a general case, taking it into account, we could come to the opposite result. In our model we assumed that the etch pits have a shape of plane disks.

When the nucleation occurs on nano-tubes with, we have $r_F/r_0 \approx 0.6$ and, according to the paper [23], different scenarios of the pit growth can develop, depending on the chemical affinity value. Thus, when $r_F/r_0 \approx 0.6$, there exists some critical potential difference $\Delta\mu^*$ which has the same dimension as the chemical affinity does. This potential difference is of the form:

$$\Delta\mu^* = \frac{2\pi^2\gamma^2\Omega}{\kappa G^{GaN} b^2}. \tag{6}$$

When $\xi > \Delta\mu^*$, the barrier for dissolution does not need to exist. In this case the pits will be formed as a result of the spontaneous nonstationary dissolution. When $\xi = \Delta\mu^*$, there may

occur either the stationary spiral dissolution around the screw dislocation, or the repeated process of the two-dimensional formation of nuclei, initiated by edge dislocations. Let us estimate the quantity $\Delta\mu^*$. By using the above-calculated data on the shear modules, surface energies, Burgers vectors and other parameters, we find that for the face (0001) with nano-tubes, at $n = 2$, $\Delta\mu^*_{(0001)} = 1 \cdot 10^{-19} J$. We have grown the GaN film at 1080 °C. At this temperature the affinity is $\xi \sim 0.14 \cdot 10^{-19} J$, and, hence, the condition $\xi \ll \Delta\mu^*$ turned out to hold. This is to say that the stationary process of layer-spiral etching of the plane (0001) around the screw dislocations takes place. This conclusion is fully sustained by the image of the V-defect with a characteristic layer-spiral relief, shown in Fig. 1. Such a result is evidence in favor of the decisive role of nano-tubes in the course of etching of the GaN(0001) plane. In the presence of nano-tubes, the etching on the plane is governed by the mechanism of the layer-spiral dissolution of the film.

On such dissolving, the morphology of the pit will be symmetric. The pit will dissolve fast, and its diameter and depth exceed significantly the sizes of the pit nuclei on the $(1\bar{1}01)$ surface, since on this surface etch pits are nucleated in accord with common classic mechanism, though with renormalized surface energy.

As a result, the growth velocity and the sizes of V-defects on the surface of polar GaN(0001) will be large, compared with that on the surface of semipolar GaN$(1\bar{1}01)$. It is precisely these phenomena that we observed in the experiment. In essence, the pit on the GaN(0001) surface dissolves (in an opposite sense) similarly to the growth of crystal: the role of the growth center is played, in this case, by a screw dislocation.

As is well known, in such conditions, the crystal will grow at arbitrary small oversaturations. For its growth there is no need for the two-dimensional nucleation of steps. The steps are formed by screw dislocations.

6. Conclusions

The studies have revealed the following:

1. V-defects, formed on the surface of polar GaN(0001), synthesized on AlN/SiC/Si(111) heterostructure, are regularly hexagons.
2. V-defects on the surface of semipolar GaN$(1\bar{1}01)$, synthesized on AlN/SiC/Si(100) heterostructure, exhibit the asymmetric morphology and are extended along the $\langle 11\bar{2}3 \rangle$ direction.
3. The dislocation nano-tubes, formed by screw dislocations, play a decisive role in the formation of V-defects on the GaN(0001) surface. In the presence of nano-tubes, the etching on the plane (0001) is governed by the mechanism of the layer-spiral dissolving of the film.
4. V-defects on the surface of semipolar GaN$(1\bar{1}01)$ are originated according to the common classic mechanism of nucleation of a new phase, though with the renormalized value of the surface energy γ. The renormalized value of γ depends on elastic properties of a medium (a film material) and on the value of Burgers vector of dislocations present on a given surface.

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