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Modeling of Threading Dislocation Density Reduction in Porous III-Nitride Layers

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In this work, we report on the results of the theoretical analysis of threading dislocation (TD) density reduction in porous III-nitride layers grown in polar orientation. The reaction-kinetics model originally developed for describing TD evolution in growing bulk layers has been expanded to the case of the porous layer. The developed model takes into account TD inclinations under the influence of the pores as well as trapping TDs into the pores. It is demonstrated that both these factors increase the probability of dislocation reactions thus reducing the total density of TDs. The mean pore diameter acts as an effective interaction radius for the reactions among TDs. The model includes the main experimentally observed features of TD evolution in porous III-nitride layers.

Key words: Reaction-kinetics model, threading dislocations, porous III-nitride layers

INTRODUCTION

III-nitride semiconductor heterostructures grown by epitaxial techniques have wide applications in solid state electronics and optoelectronics. The choice of the template for subsequent heteroepitaxial growth strongly influences the quality of the fabricated structures. The best results in this direction can be achieved by the use of bulk III-nitride monocrystalline substrates, e.g. GaN or AlN, with extremely low defect density. However, due to a high cost of such materials, heterophase templates are usually used. For heterophase templates, thick epitaxial III-nitride layers (e.g. GaN) are grown on foreign substrates (e.g. sapphire) that possess the relative mismatch in crystal lattice parameters and coefficients of thermal expansion. Such a mismatch is the main reason for mechanical stress generation in the templates. Relaxation of the stresses occurs via misfit dislocation formation at the heterophase interface that is also accompanied by threading dislocation (TD) formation in the layer interior. Threading dislocations strongly deteriorate carrier transport and optoelectronic properties of heterostructures on the base of III-nitrides.[1,2] Thus, the reduction of TD density is an essential scientific and technological issue.

The formation of an intermediate porous layer is an effective way to reduce TD density. It has been experimentally demonstrated that the use of an intermediate porous layer results in the drastic reduction of TD density in growing III-nitride layers.[3–5] Nevertheless, nowadays, there is a lack of adequate explanation of porosity influence on TD density reduction. The aim of this work was to develop a model and to perform mathematical analysis of TD density evolution in growing porous polar (as this is one of the most commercially demanded III-nitride material growth configurations) GaN layers on the base of a reaction-kinetics approach.[6,7]

MODEL DESCRIPTION

Let us consider a (0001)-oriented GaN template that includes a porous interlayer with edge TDs inside; a cross-section of the porous template is

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shown schematically in Fig. 1. For simplicity, the model geometry is chosen as an array of regular hexahedrons whose vertices are occupied by spherical pores. This allows us to parameterize the problem by three quantities: volume concentration of the pores (volume porosity) ω, average pore diameter D, and the initial TD density ρ_0. We assume that the dislocations are uniformly distributed over the volume of the material. On the basis of the above described geometry of the porous layer, one can write the following expressions for the volume porosity ω and the average distance between neighboring pores L:

$$\omega = \frac{V_p}{V} = \frac{\pi D^3}{6(L+D)^3}, \tag{1}$$

$$L = \left(\sqrt[3]{\frac{\pi}{6\omega}} - 1\right)D, \tag{2}$$

where V_p is the volume occupied by pores, and V is total volume of the material with pores.

The process of the porous layer formation and any related effects are out of view and need to be investigated further.

We divide the total TD density into three families:

(i) ρ_1 is the density of the vertical TDs, which do not get into pores and do not incline from the vertical direction due to the pore influence;
(ii) ρ_2 is the density of inclined TDs, which are not trapped by pores, but inclined from the vertical direction at an angle $\overline{\theta}$ due to the pore influence;
(iii) ρ_3 is the density of TDs, which are trapped by pores.

The actual thickness of the porous layer h is used as the evolution variable. The dislocation densities are subject to change because of mutual interactions and dislocation/pore interactions. The following reactions are of physical relevance in such dislocation/pore systems.

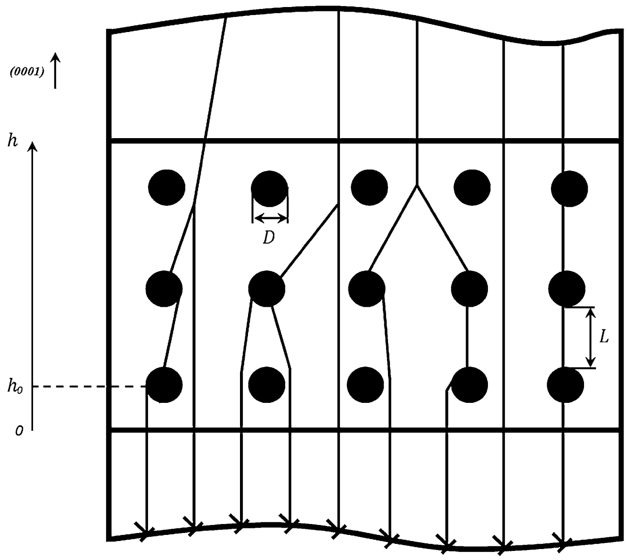

Fig. 1. Schematic cross-section of the porous layer with edge threading dislocations.

The density ρ_1 changes due to:

(1) interaction of dislocations with pores resulting in TD inclination; this is described by the rate of ρ_1 diminishing $K_1\rho_1$, which is also equal to the rate of ρ_2 increasing;
(2) getting dislocations into overlying pores, which leads to the decrease of the dislocation density ρ_1 and to the increase of ρ_3 with the same rate $K_2\rho_1$;
(3) reactions of vertical dislocations with inclined TDs, providing decreases of ρ_1 and ρ_2 with the same rate $K_3\rho_1\rho_2$;
(4) escape of vertical TDs from pores resulting in the increase of ρ_1 and the decrease of ρ_3 with the equal rate $K_4\rho_3$.

In addition to the reactions #1 and #3, the density ρ_2 changes due to the following reasons:

(5) capturing of inclined TDs by the pores, which leads to ρ_2 decreasing and ρ_3 increasing with the equal rate $K_5\rho_2$;
(6) reactions among inclined TDs, which provide ρ_2 diminishing with the rate $K_6\rho_2^2$;
(7) escape of inclined TDs from the pores, which results in ρ_2 increasing and ρ_3 decreasing with the rate $K_7\rho_3$.

The density ρ_3 changes due to #2, #4, #5 and #7 reactions, but also due to the additional reaction:

8) TD reaction inside pores, which provides ρ_3 diminishing with the rate $K_8\rho_3^2$.

The coefficients $K_1, K_2, \ldots, K_8$ are cross-sections of the reactions of dislocations with pores or with other dislocations and should be determined from microscopic models and geometric considerations.

Then, the following system of kinetic equations for the dislocation density evolution in the overgrown GaN layer can be obtained:

$$\begin{cases} \frac{d\rho_1}{dh} = -K_1\rho_1 - K_2\rho_1 - K_3\rho_1\rho_2 + K_4\rho_3 \\ \frac{d\rho_2}{dh} = K_1\rho_1 - K_5\rho_2 - K_6\rho_2^2 - K_3\rho_1\rho_2 + K_7\rho_3 \\ \frac{d\rho_3}{dh} = K_2\rho_1 + K_5\rho_2 - K_8\rho_3^2 - K_7\rho_3 - K_4\rho_3 \end{cases} \tag{3}$$

The initial conditions for the system of differential Eq. 3 are:

$$\begin{aligned} \rho_1(h_0) &= \rho_{10}, \\ \rho_2(h_0) &= \rho_{20}, \\ \rho_3(h_0) &= \rho_{30}, \end{aligned} \tag{4}$$

where h_0 is assumed to be a height of the porous layer initiation, as shown in Fig. 1.

From the suggestion that ρ_{10} is proportional to the ratio of the pore-free section area to the complete section of the layer which is parallel to the basal plane, as well as from the assumption that below the porous layer all TDs are vertical, one can write the following expression for the initial TD densities:

$$\rho_{10} = \left(1 - \frac{\pi D^2/4}{(L+D)^2}\right)\rho_0,$$
$$\rho_{20} = 0, \tag{5}$$
$$\rho_{30} = \frac{\pi D^2/4}{(L+D)^2}\rho_0$$

where ρ_0 is the total initial TD density. Figure 2 illustrates the above-mentioned geometrical considerations.

The resulting TD density over the porous layer is $\rho_\Sigma = \rho_1 + \rho_2 + \rho_3$.

ANALYSIS OF REACTION COEFFICIENTS

The coefficients $K_1, K_2, \ldots, K_8$ of the differential equation system (3) are selected according to the following physical and geometrical considerations. First, the system (3) must satisfy the following limiting case: $h \to +\infty$ (very thick porous layer): $\rho_\Sigma(h) \to 0$. It is reasonable to assume that the number of possible reactions among TDs in the porous layer is proportional to the thickness of the layer as well as to the volume porosity, and inversely proportional to the average distance between pores. At the same average pore diameter, the smaller the distance between neighboring pores, the greater the probability for TDs to be trapped into pores. Hence, we suppose that the coefficients of the equations should contain the factor $n = \frac{h\omega}{L}$.

The coefficient K_1 is determined by how difficult it is for the external force to "move" a probe dislocation in the direction to the pore; therefore, it should be proportional to the force of dislocation attraction to the pore. In accordance with the analysis given in [8]:

$$K_1 = n\frac{G_1}{\sigma_p}\cdot\frac{1}{4\pi(1-\nu_1)}\cdot\frac{\frac{D^2}{4}}{(\bar{x})\left(\bar{x}^2 - \frac{D^2}{4}\right)}, \tag{6}$$

where $\bar{x} = \frac{L}{4} + \frac{D}{2}$, $G_1$is the shear modulus of the material, ν_1 is the Poisson ratio of the material and $_p$ is the Peierls barrier.

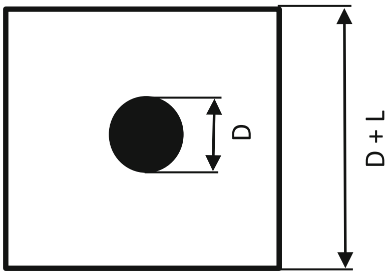

Fig. 2. Scheme for the initial TD densities ρ_{10} and ρ_{30} calculation.

The coefficients K_2 and K_5 describe the capturing of vertical and inclined TDs, respectively, by the neighboring pores. Figure 3 presents the geometrical considerations regarding the coefficient K_2 choice: in the case of D = const, the shorter the distance between neighboring pores ($L_2 < L_1$), the more the vertical TDs fall into pores, thus $K_2 \sim \frac{1}{L}$. Taking into account the factor n, we suggest that

$$K_2 = \frac{n}{L}. \tag{7}$$

Figure 4 demonstrates the geometrical considerations regarding the coefficient K_5 choice: in case D = const and θ = const the shorter the distance between neighboring pores the more inclined TDs get into pores (Fig. 4a), thus $K_5 \sim \frac{1}{L}$; in case D = const and L = const the more inclination angle θ, the larger fraction of inclined TDs is captured in the pores (Fig. 4b), thus $K_5 \sim \frac{1}{\cos\theta}$. On the base of consideration given above we suggest that

$$K_5 = \frac{n}{L\cos\bar{\theta}}, \tag{8}$$

where $\bar{\theta}$ is an average angle of dislocation inclination in the porous layer, which depends on the growth conditions and geometry of the layer. In the case of vertical TD ($\bar{\theta} = 0$) K_2 equals to K_5.

The coefficient K_4 describes the escape of TDs from of pores:

$$K_4 = \alpha(K_2 + K_5), \tag{9}$$

where α is the factor which defines how many of the TDs trapped by pores will come out vertical, hence $0 < \alpha < 1$. The coefficient K_7 describes the inclined exit of TDs out of pores:

$$K_7 = \gamma(K_2 + K_5), \tag{10}$$

where γ is the factor which defines how many of the TDs trapped by pores will come out as inclined ones, hence $0 < \gamma < 1$.

The coefficients K_3, K_6 and K_8 characterize reactions among TDs:

$$K_3 = r_{\mathrm{react}}, \tag{11}$$

where r_{react} is the effective cross-section parameter of the reactions between the inclined and vertical TDs. The coefficient K_6 describes reactions between two inclined TDs outside pores:

$$K_6 = m \cdot r_{\mathrm{react}}, \tag{12}$$

where $m > 1$ because the probability of reaction between two inclined TDs is higher than between the inclined and vertical ones.[7] The coefficient K_8 is responsible for the annihilation of two TDs inside pore, which thus effectively increases the radius of the dislocation reaction. Therefore, we suppose that K_8 is proportional to the pore size:

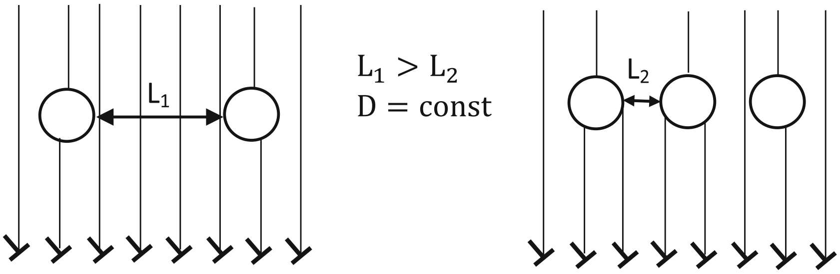

Fig. 3. Schematics explaining the choice of the coefficient K_2: the probabiliy of capturing vertical TDs into pores is inversely proportional to the average distance between neigbouring pores.

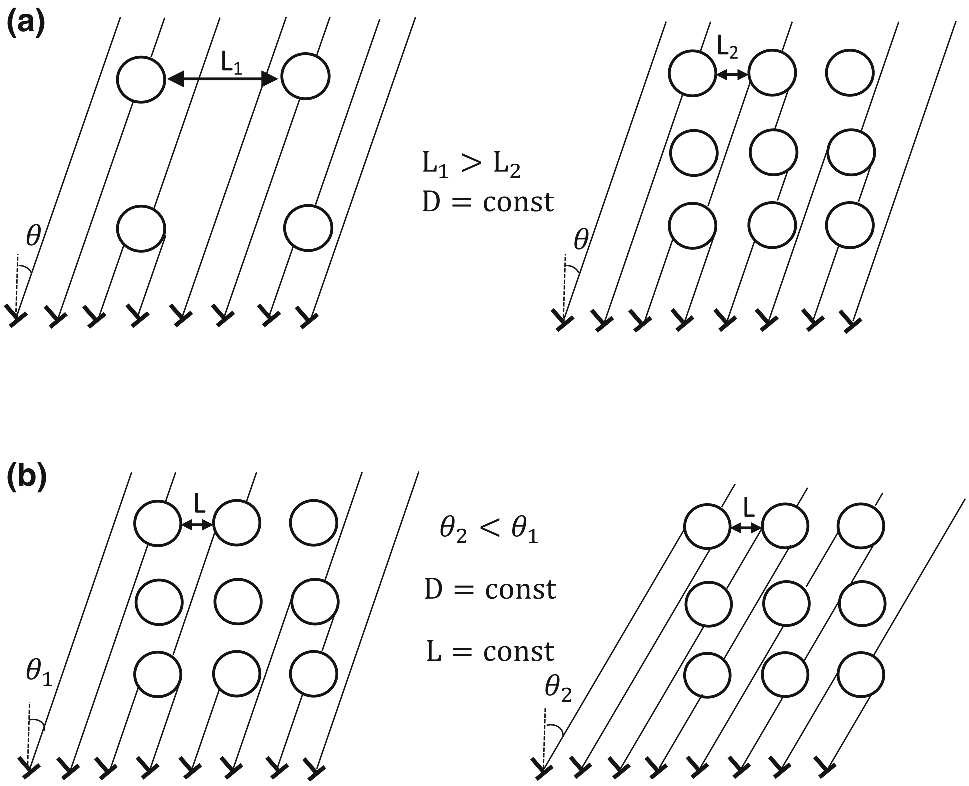

Fig. 4. Schematics explaining the choice of the coefficient K_5: the probabiliy of getting inclined TDs into pores is inversely proportional to the average distance between neigbouring pores (a) as well as to cosinus of the inclination angle (b).

$$K_8 = nD. \tag{13}$$

RESULTS AND DISCUSSION

Let us analyze the resulting total TD density in GaN grown layer on the basis of the model described above with following typical parameter values: $\nu_1 = 0.26$, $\frac{G_1}{\sigma_p} \cong 250$, $D = 0.25\ \mu$m, $\alpha = 0.5$, $\gamma = 0.5$, $\theta = 45°$,$r_{\text{react}} = 100$ nm, $m = 2$.[3,7,9] The initial density of the TDs and the volume concentration of pores are variable parameters: $\rho_0 = 10^8 \Upsilon 10^{10}$ cm^{-2}, $\omega \leq 0.5$. It should be noted that maximum volume porosity that we consider in the framework of our model can be calculated with (1). It equals to 0.52. The greater volume porosity causes the change in the geometry of the model and is out of the consideration.

Figures 5 and 6 show the dependence of the relative TD density on the porous layer thickness for the initial TD densities $\rho_0 = 10^8$ cm^{-2}, $\rho_0 = 10^9$ cm^{-2} and $\rho_0 = 10^{10}$ cm^{-2} and volume porosity 0.25 and 0.5, respectively.

Figure 7 demonstrates the dependence of the relative TD density (ρ_Σ/ρ_0) on volume porosity for the initial TD densities $\rho_0 = 10^9$ cm^{-2} and $\rho_0 = 10^{10}$ cm^{-2}, and $h = 5\mu$m.

The obtained dependences demonstrate that the model satisfies the specified limiting case of a very thick porous layer: $\rho_\Sigma(h) \to 0$ when $h \to +\infty$.

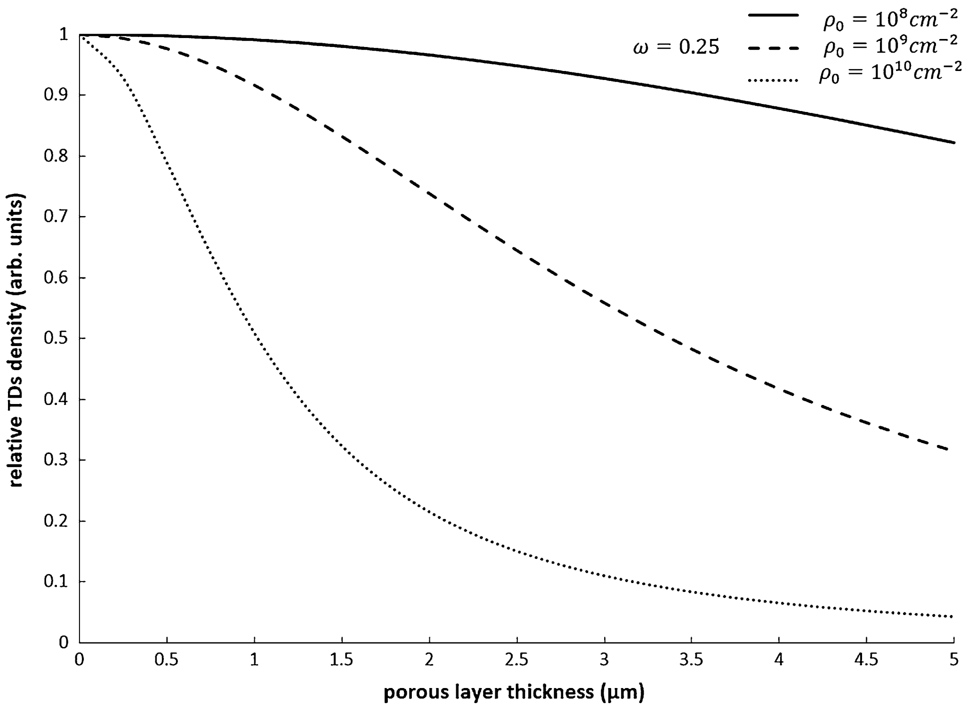

Fig. 5. The dependence of the relative TD density on the porous layer thickness for the initial TD densities ρ_0 = 10^8 cm^{-2}, ρ_0 = 10^9 cm^{-2} and ρ_0 = 10^{10} cm^{-2} and volume porosity = 0.25.

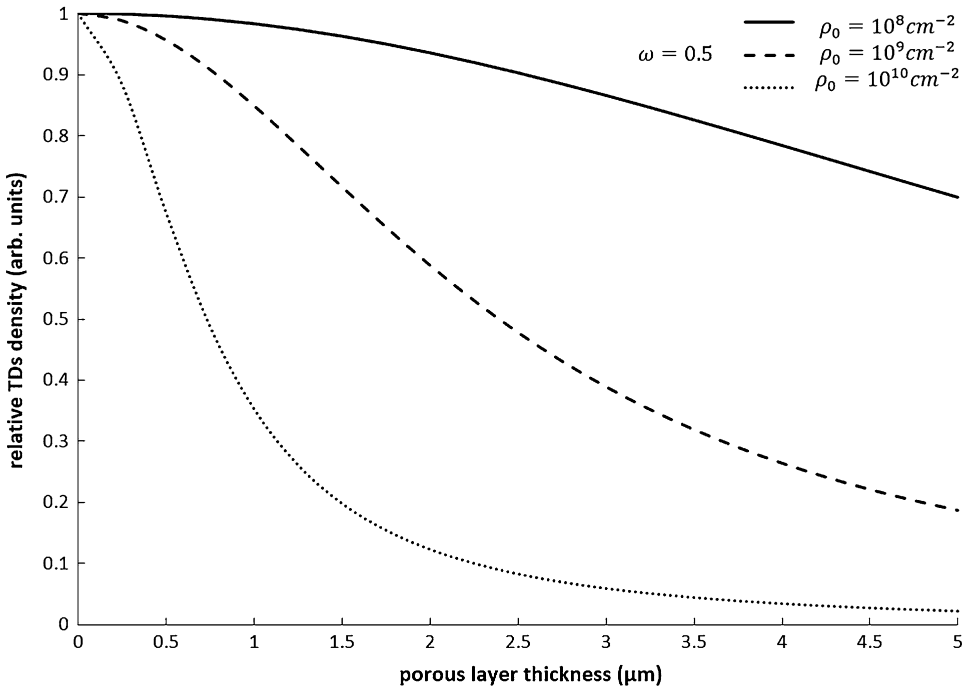

Fig. 6. The dependence of the relative TD density on the porous layer thickness for the initial TD densities ρ_0 = 10^8 cm^{-2}, ρ_0 = 10^9 cm^{-2} and ρ_0 = 10^{10} cm^{-2} and volume porosity = 0.5.

Furthermore, it is seen that the higher the initial TD density, the more the rate of decrease of the dislocation density with increasing thickness of the porous layer. This may be due to the fact that at higher initial density of TDs the probability for them to meet with each other as well as with pores

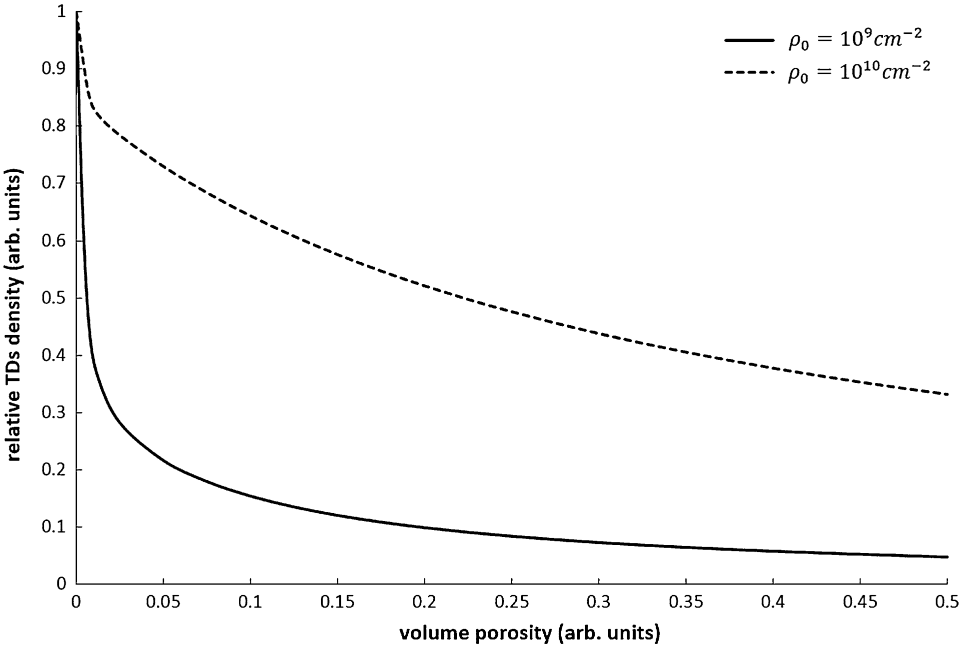

Fig. 7. The dependence of the relative TD density on volume porosity for the initial TD densities $\rho_0 = 10^9$ cm^{-2} and $\rho_0 = 10^{10}$ cm^{-2} for the case with $h = 5\mu$m.

increases. It is shown in Fig. 6 that even low porosity less than 10% leads to sufficient TD density reduction for the layer thickness of several microns. It should be noted that for the same value of the porosity the change of pore diameter in the range 50–150 nm does not influence much the dependences of the TD density on the layer thickness. In general, for the initial TD density of 10^9–10^{10} cm^{-2} the use of the intermediate porous layer with the thickness in range 1–4 μm and the volume porosity of 10–50% results in the TD density reduction of 50–95%. Further increase of the porous layer thickness becomes ineffective. In the case of high porosity of about 50% very rapid decrease of the TD density is observed already at a thickness of about 300 nm, in good agreement with the experimental results.[10]

CONCLUSIONS

Evolution of threading dislocation density in growing porous GaN layer has been theoretically considered on the base of the reaction-kinetics approach. The obtained results have demonstrated that the use of growing porous layer is effective for diminishing the initial threading dislocation density. Rate of decrease in TD density in growing layer strongly depends on the initial TD density and level of the volume porosity. Even low volume porosity less than 10% leads to sufficient TD density reduction. The initial dislocation density of 10^9–10^{10} cm^{-2} decreases by 50–95% in the grown porous GaN layer with the thickness of 1–4 μm and porosity of 10–50%. With a further increase in the thickness of the porous layer, the TD density changes very slowly.

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