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Modeling of Threading Dislocation Density Reduction in AlN/Al_2O_3 Porous Heterostructure

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Abstract. We analyze the possibility for reducing the density of threading dislocations (TDs) in a porous AlN films exploring numerical calculations of thermoelastic stresses and the reaction-kinetic model of dislocation interactions. We study the distributions of the normal and shear components of the thermoelastic stress tensor in AlN film with triangular pores grown on Al_2O_3 substrate. We find the pore parameters that affect the decrease in the TD density in the AlN film. We compare the results of theoretical calculations with experimental data on TD density reduction in porous AlN/Al_2O_3 heterostructures.

1. INTRODUCTION

Al_2O_3 still remains the most usable substrate material for III-nitride heteroepitaxy [1]. Due to significant differences in the parameters of crystal lattices and thermal expansion coefficients between film and substrate materials, in the III-nitride film grown on Al_2O_3 substrate arise large internal stresses, which can lead to the formation and evolution of various defects including threading dislocations (TDs). The presence of TDs in the film is unadvisable, since TDs strongly deteriorate carrier transport and optoelectronic properties of semiconductor heterostructures and devices based on them [1,2].

One of the most affordable ways to reduce the level of internal stresses and the density of TDs in the III-nitride films is the use of patterned substrates [3]. For instants, patterned substrates based on Al_2O_3 were successfully implemented for the growth of GaN [4] and AlN [5] films with low TD density. The technology of patterned substrates is based on the lateral overflowing pre-etched III-nitride buffer layer [6–8]. In the result of lateral overgrowth, pores are often formed in the semiconductors film interior [5].

The use of a porous layer for the subsequent growth of the film allows to reduce the level of thermoelastic stresses in the film occurring when the heterostructure is cooled after the growth process is completed [9,10]. In overall, thermoelastic stresses have a great impact, since they can control the evolution of defect structure in the process of heterostructure growth at high temperatures [11–14]. In its turn, the presence of pores in the film can directly affect the behavior of TDs. It was recently shown that the presence of triangular pores in AlN film grown on the Al_2O_3 substrate leads to a significant decrease in dislocation density in the film [5]. In this case there exist a problem in optimizing the porous film structure for achieving the lowest possible density of TDs.

In the previous analysis, reaction-kinetic models were proposed to describe TD density evolution in porous films, but most of them analyzed the influence of the spherical pores [15,16]. Thus, the purpose of this work is to construct the analytical and numerical models to estimate the effect of triangular pores on the thermoelastic stresses and the TD density reduction in AlN/Al_2O_3 heterostructure.

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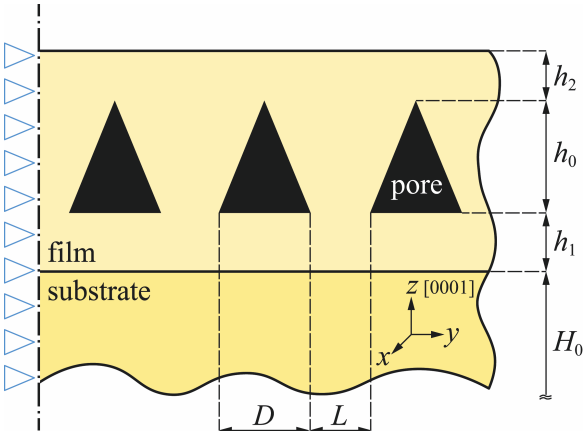

Fig. 1. Schematic representation of the cross section of AlN/Al_2O_3 heterostructure with porous film. L is the distance between neighboring pores, D is the base of the pore, h_0 is the pore height, h_1 is the distance between the pore and the film surface, h_2 is the distance between the pore and the film/substrate interface, H_0 is substrate thickness. Symmetry boundary condition $u_y = 0$ is shown with blue triangles.

2. THERMAL STRESSES IN AlN/Al_2O_3 HETEROSTRUCTURE WITH POROUS FILM

Consider a model of a film/substrate heterostructure with triangular pores in the film, see Fig. 1. Based on the experimental [5] data, we use the following parameters to describe the material properties and geometry features of the heterostructure: film material is AlN, substrate material is Al_2O_3, L is the distance between neighboring pores, D is the base of the pore, h_0 is the pore height, h_1 is the distance between the pore and the film free surface, h_2 is the distance between the pore and the film/substrate interface, H_0 is substrate thickness. Since misfit stresses relax at high growth temperatures, we calculated thermoelastic stresses, the level of which are usually not sufficient for the formation of new defects, however, these stresses can affect the evolution of previously formed defects, for example, TDs.

Table I. Material parameters of AlN and Al_2O_3 that used in simulation [17–19].

Parameter	AlN	Al_2O_3
C_{11}	410 GPa	497 GPa
C_{12}	149 GPa	163 GPa
C_{13}	99 GPa	116 GPa
C_{14}	0	22 GPa
C_{33}	389 GPa	501 GPa
C_{44}	125 GPa	147 GPa
α_a	4.2×10^{-6} K^{-1}	7.5×10^{-6} K^{-1}
α_c	5.3×10^{-6} K^{-1}	8.5×10^{-6} K^{-1}

To calculate thermoelastic stresses, we used the ANSYS engineering simulation software. A half two-layer plate was chosen as the calculation model based on the symmetry of the problem (Fig. 1). The boundary conditions were set to a free surface expect symmetry plane on which the normal displacement was zero, $u_y = 0$. Thermal loads with temperature drop of 1300 °C (which is typical for AlN growth process) were implemented. The initial geometric model was divided into finite elements (PLANE 183) by an unstructured triangle mesh refined near the pore corners for obtaining smoother distributions of stresses. The number of finite elements was 25 thousand. The values of geometric parameters that we used in simulation were: L = 5 μm, D = 1.5 μm, h_0 = 3 μm, h_1 = 3.4 μm, h_2 = 3 μm, H_0 = 450 μm, the length of the heterostructure along the y axis is much greater than the distance between neighboring pores L; elastic constants C_{ij} and thermal expansion coefficients α_i that were used in simulation are given in Table I.

Fig. 2 shows the distribution of stress tensor components in AlN porous film. For analysis convenience, part of the film with three pores is shown. The presence of pores in the heterostructure leads to a redistribution of thermoelastic stresses inside the film (in a poreless film, the stress level is constant). It is seen, that the pore corners are the stress concentrators. In the region between the pores, there is a significant decrease (in

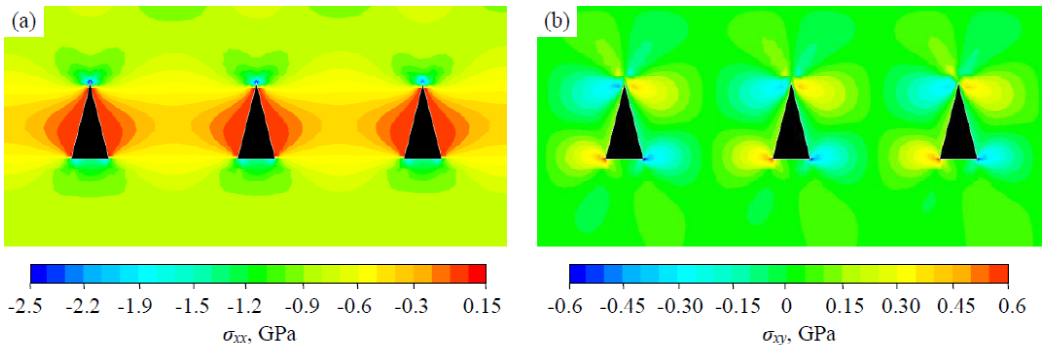

Fig. 2. Distributions of stress components in AlN porous film. Frame (a) shows normal stress tensor component σ_{xx}, frame (b) shows shear stress tensor component σ_{xy}.

absolute value) in the level of the stress component σ_{xx} (Fig. 2a). Moreover, the presence of pores in the film leads to the appearance of the shear component σ_{xy} of the stress tensor (Fig. 2b).

It should be noted that stresses change sign near the pores, which can lead to a change in the trajectory (line direction) of the TDs closest to the pores. Similar behavior of dislocations was observed experimentally [5]. Inclination of TDs can lead to reactions between dislocations, exit of dislocations on the free surface of the film, and absorption of dislocations by pores. On the other hand, the pores can emit TDs under certain conditions. The mechanisms described above can affect the TD density in the AlN film. In Section III, we present a reaction-kinetic model that describes the change in the dislocation density depending on the film porosity in AlN/Al_2O_3 heterostructure.

3. THREADING DISLOCATION DENSITY REDUCTION ON POROUS AlN FILM

Fig. 3 shows the film of AlN/Al_2O_3 heterostructure with TDs. As mentioned in Section II, pores can attract TDs, changing their line direction from the normal to the heterostructure growth plane, and, as a result, affect the TD density in the film. To describe such process, one can use the approach proposed in Refs. [15,16]. Artemiev et al. have constructed the reaction-kinetics model for GaN/Al_2O_3 heterostructure with spherical pores and suggested to consider the total dislocation density ρ_{tot} consisting of three components [16]:

$$\rho_{tot} = \rho_1 + \rho_2 + \rho_3, \tag{1}$$

where ρ_1 is the TD density with a vertical dislocation line direction (DLD) parallel to the [0001] crystallographic direction; ρ_2 is the TD density with DLD inclined from the [0001] crystallographic direction; ρ_3 is the density of TDs trapped by the pores. Such division of the total TD density is consistent with the conclusions and assumptions made in Section II based on thermoelastic stress field analysis.

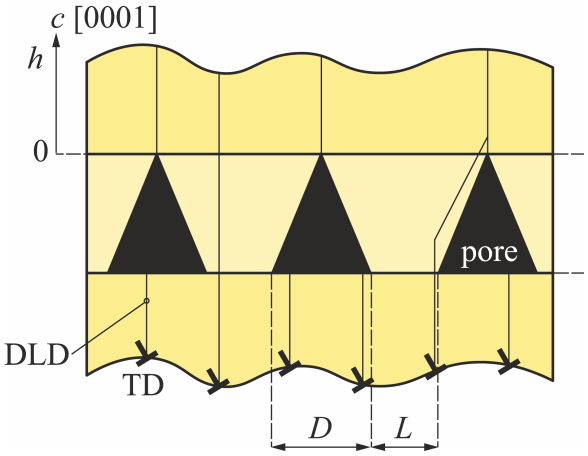

Fig. 3. Schematic representation of the cross section of a porous AlN film with TDs. *h* is the current film thickness above the porous layer. DLD is dislocation line direction threading dislocation (TD).

In the case of an AlN film with triangular pores, the reaction kinetics model that describes the evolution of TD density depending on the film thickness above the porous layer acquires the following form:

$$\begin{cases} \dfrac{d\rho_1}{dh} = -K_{I}\rho_1 - K_{II}\rho_3 + K_{III}\rho_1\rho_2 \\ \dfrac{d\rho_2}{dh} = K_{I}\rho_1 - K_{III}\rho_1\rho_2 - K_{IV}\rho_2^2 - K_{V}\rho_2, \\ \dfrac{d\rho_3}{dh} = -K_{II}\rho_3 + K_{V}\rho_2 - K_{VI}\rho_3^2 \end{cases} \tag{2}$$

where $K_{I–VI}$ are coefficients that are defined by taking into account the physical and geometric features of the system and dislocation behavior in special cases: $D \to 0$ (there are no pores in the film) $\Rightarrow \rho_{tot} \to \rho_0$ (ρ_0 is TD density in the film without pores); $h \to \infty \Rightarrow \rho_{tot} \to 0$(there are no TDs in thick films); $L \to 0$ (no film) $\Rightarrow \rho_{tot} \to 0$.

Coefficient K_I depends on the force of TD attraction to the pore and shows the number of TDs that change DLD from vertical (along the [0001] crystallographic direction) to inclined one under the pore influence. On the other hand, coefficient K_I must satisfy the limiting case: $K_I = 0$ at $D = 0$. Thus, coefficient K_I can be found as [20]:

$$K_I = \frac{G}{\sigma_p}\frac{1}{4\pi(1-\nu)}\frac{16D^2}{L(8D^2 + 6DL + L^2)}, \tag{3}$$

where σ_p is Peierls stress, G is shear modulus, ν is Poison ratio.

Coefficient K_{II} is related to the probability of the emission of vertical TDs that were trapped by pores:

$$K_{II} = \alpha\left(\frac{D}{D+L} + \frac{1}{h_0}\right), \tag{4}$$

where α shows the ratio of emitted TDs by the pore to those trapped. Due to the assumption that when two TDs (with vertical or inclined DP) are trapped, one vertical TD is emitted, then $0 < \alpha < 1$.

Coefficient K_{III} characterizes the probability of reactions between vertical and inclined TDs that have not trapped by the pores or emitted from them. Reactions between TDs are possible when the distance between TDs becomes less than reaction radius r_{react}:

$$K_{III} = r_{react}, \tag{5}$$

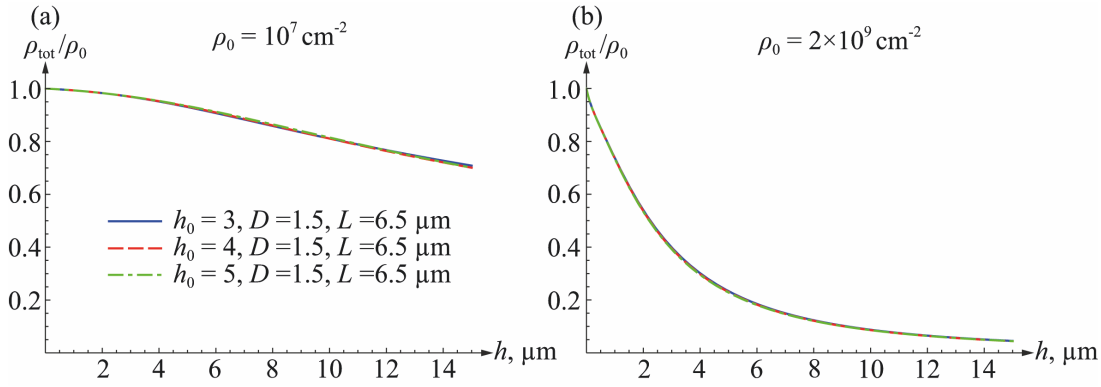

Fig. 4. Dependences of the normalized TD density ρ_{tot}/ρ_0 on the AlN film thickness h above the porous layer. (a) initial density of TDs $\rho_0 = 10^7$ cm^{-2} and (b) $\rho_0 = 2\times10^9$ cm^{-2}. The solid, dash and dash-dotted curves correspond to the dependence obtained at a pore height h_0 = 3, 4 and 5 μm, respectively. Pore base D = 1.5 μm, distance between neighboring pores L = 6.5 μm.

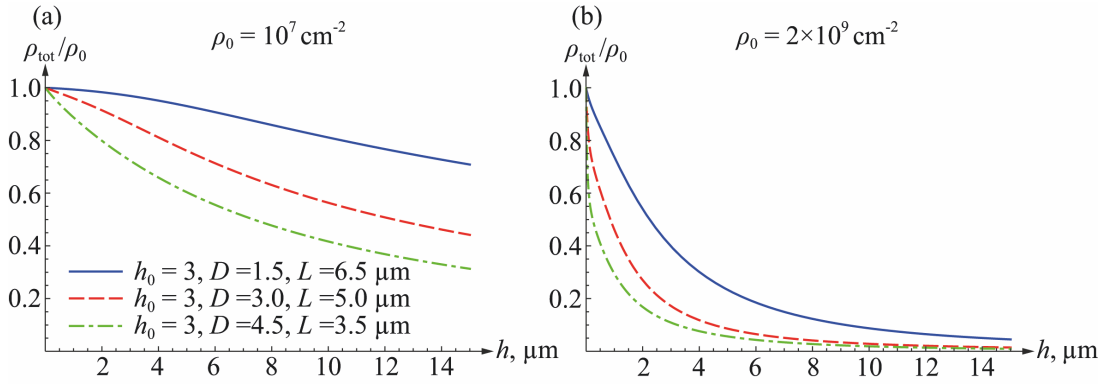

Fig. 5. Dependences of the normalized TD density ρ_{tot}/ρ_0 on the AlN film thickness h above the porous layer. (a) initial density of TDs $\rho_0 = 10^7$ cm^{-2} and (b) $\rho_0 = 2\times10^9$ cm^{-2}. The solid, dash and dash-dotted curves correspond to the dependence obtained at pore base D = 1.5 μm and distance between neighboring pores L = 6.5 μm, D = 3.0 μm and L = 5.0 μm, D = 4.5 μm and L = 3.5 μm, respectively. Pore height h_0 = 3 μm.

for definiteness r_{react} was taken equal to 100 nm.

The coefficient K_{IV} is related to the probability of reactions among inclined TDs that do not trapped by the pores. In contrast to the coefficient K_{III}, the probability of a reaction between inclined TDs increases, since in this case not one but two TDs move at an angle, therefore, the entering of inclined TDs to reaction zone is more possible:

$$K_{IV} = mr_{react}, \tag{6}$$

where $m > 1$.

Coefficient K_V characterizes the probability of inclined TDs to be trapped by pores, and can be found from film geometry:

$$K_V = 1/h_0. \tag{7}$$

Finally, coefficient K_{VI} is related to the probability of annihilation of two TDs that were trapped by a pore. The coefficient can be given as pore size:

$$K_{VI} = D. \tag{8}$$

The initial conditions for the system of differential equations (2) at $h = h_0$ are chosen as:

$$\begin{aligned} \rho_{10} &= \rho_1(h_0) = \frac{L}{D+L}\rho_0, \\ \rho_{20} &= \rho_2(h_0) = 0, \\ \rho_{30} &= \rho_3(h_0) = \frac{D}{D+L}\rho_0, \end{aligned} \tag{9}$$

where ρ_0 is the initial density of TDs in AlN/Al_2O_3 heterostructure without pores and corresponds to a typical experimental value of 2×10^9 cm^{-2} [5]).

The total TD density ρ_{tot} was calculated for the porous AlN film taking into account the following parameters: $\nu = 0.26$; $G/\sigma_p = 65$; $\alpha = 0.5$; $r_{react} = 100$ nm; $m = 2$ [5,21–23]. The values of pore height h_0, pore base D, distance between neighboring pores L, and initial TD

density ρ_0 were varied to estimate their impact on the total TD density ρ_{tot}.

Fig. 4 shows the dependences of the normalized total TD density ρ_{tot}/ρ_0 on the AlN film thickness h above the porous layer for the initial density of TDs $\rho_0 = 10^7$ cm^{-2} (Fig. 4a) and $\rho_0 = 2\times10^9$ cm^{-2} (Fig. 4b) with different pore height $h_0 = 3\div5$ μm. The pore base D was taken equal to 1.5 μm, and the distance between neighboring pores $L = 6.5$ μm.

It can be seen from Fig. 4 and Eqs. (4), (7), that the pore height h_0 has almost no effect on the total dislocation density ρ_{tot}. For AlN film thickness h about 15 μm above the porous layer, the TD density decreases to 10^8 cm^{-2}, which is consistent with the experimental value of 3×10^8 cm^{-2}[5]. The initial TD density ρ_0 significantly affects the value of the total TD density ρ_{tot} in AlN film with pores. The higher the initial TD density, the more the rate of decrease of the dislocation density with increasing thickness of the porous film. Also, this conclusion coincides with the conclusion made earlier for GaN films with spherical pores [15,16].

Fig. 5 shows the dependences of the total normalized TD density ρ_{tot}/ρ_0 on the AlN film thickness h above the porous layer for the initial density of TDs $\rho_0 = 10^7$ cm^{-2} (Fig. 5a) and $\rho_0 = 2\times10^9$ cm^{-2} (Fig. 5b) with different pore base D 1.5÷4.5 μm, and distance between neighboring pores $L = 3.5\div6.5$ μm. The pore height h_0 was taken equal to 3 μm. Due to this choice of parameters, the periodicity of the pore ($D + L$) remains unchanged and is equal to 8 μm for dependences shown in Fig. 4 and Fig. 5.

Fig. 5 illustrates that the pore base D and the distance between neighboring pores L have a much stronger effect on the total TD density ρ_{tot} than the pore height h_0. The lower the initial TDs density, the less the rate of decrease of the dislocation density with increasing the porous film thickness. In the case of a sufficiently high initial TD density $\rho_0 = 2\times10^9$ cm^{-2}, it is possible to achieve a decrease in the total dislocation density ρ_{tot} by two orders of magnitude in film with $L = 3.5$, $D = 4.5$ μm and $h = 15$ μm. In the case of initial TD density $\rho_0 = 10^7$ cm^{-2} the total dislocation density decreases less noticeably – that is only to 3.1×10^6 cm^{-2}.

4. CONCLUSIONS

A numerical model that describes thermoelastic stresses in AlN/Al_2O_3 heterostructure with a porous film, and a reaction-kinetic model that describes the evolution of the TD density in this heterostructure depending on the porosity of the film have been proposed. It has been shown that the presence of triangular pores in the film leads to the appearance of shear component of the thermoelastic stress tensor in the film. It has been confirmed that pore corners act as stress concentrators. It has been also shown that the presence of a stress gradient near the pores can affect the behavior of TDs.

Calculations using the reaction-kinetic model have demonstrated that the density of TDs decreases after their passing through the porous layer. It has been shown that the pore height has no effect on the total TDs density, in contrast to the density of pores in the film. It has been found that for the base of the pore $D = 4.5$ μm and the distance between neighboring pores $L = 3.5$ μm, the total TDs density in the AlN film ($h = 15$ μm) decreases by two orders of magnitude in comparison to the initial TDs density about 10^9 cm^{-2}. Thus, the larger the base of the triangular pore and the lower distance between neighboring pores, the lower the total TD density in the AlN film grown on a sapphire substrate.

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