Simulation of Influence of Template Size on Misfit Dislocation in Nanostructures

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***Abstract* — The paper considers a model of misfit dislocation determination to establish the dislocation free contour map for nanotemplate geometrical size. Dislocation free contour map has been obtained for GaN and GaAs nanostructures on the substrate of AlN and Si, respectively. The results of Burger dislocation determination in nanostructures are proved by experiment and show good agreement.**

Keywords — dislocation; nanostructures; template

I. INTRODUCTION

Continuing device miniaturization trend in modern industry makes it important to develop nanodevices tightly integrated with semiconductor components [1, 2]. For that purpose A3B5 compounds are most widely used, as they possess high quality properties in wide frequency range. These materials are suitable for microwave and high temperature optoelectronic devices. Thus nanostructures based on A3B5 compounds are widely studied.

Creation of complex functional devices on the single crystal is the most important trend in nanotechnology development. Though single chip Si/A^3B^5 devices were introduced in 1972 [3] and implemented in 1975 [4], Si/A^3B^5 compound found wide use thanks to deposition technology advances. As a result single chip integrated circuits are used in microwave communications as duplexers, converters, modulators, amplifiers etc [5].

Deposition technology improvement continues nowadays. One of the promising directions is method of template synthesis of aluminum anodic oxide (TAOA) [6]. This method is used to create structures in nanosized pores. TAOA film thickness varies from sub-micrometer to nanometer range. This technology was adopted to develop optoelectronic and micromechanical nanodevices [7, 8], and for multi-island single electron transistors suitable for room temperature operation [9]. Template method is one of the most promising ways to create nanostructures base on III-nitrides. Template growth of the nanostructures allows precise control over dimensions and placement of quantum dots free of defects which arise with different methods.

Therefore there is an urgent problem establishing the geometrical relationship between the size and templated nanostructures heterogeneity as well as choosing optimal parameters of nanostructures in which no dislocations occur.

This paper is focused on considering a model of misfit dislocation determination for nanostructures to establish dependence of the dislocation free contour map on nanotemplate geometrical size, namely for GaN on AlN-substrate and for GaAs on Si.

II. PROBLEM STATEMENT AND SOLUTION

The method of template synthesis of nanostructures consists of growing on the semiconductor substrate a thin film layer of nanostructures. Schematic of template nanostructures with radius R and height h (film thickness) is presented on Fig. 1.

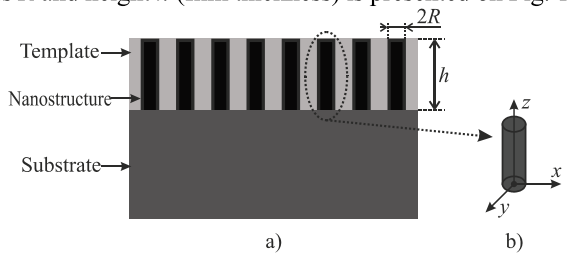

Fig. 1. Schematic of template nanostructures (a), and its part (b).

At the boundary between two media there is tension caused by the crystal lattice mismatch of the substrate and the grown nanostructures. Uniformity template's layer is determined by the degree of mismatch, which in turn depends on the radius and height of the nanostructures (see Fig. 1).

In [10] dislocation density change is calculated by:

$$p \cong \begin{cases} 0 & ,h \le h_c \\ \left(\dfrac{\varepsilon^m}{|b|}\right)^2 \bullet \left(1-\dfrac{h_c}{h}\right)^2 & ,h > h_c \end{cases}, \qquad (1)$$

where p is dislocation density per area; b is Burgers vector; h is film thickness; h_c is critical thickness; $\varepsilon^m = 2\dfrac{a_f - a_s}{a_f + a_s}$ – lattice mismatch strain; where a_f and a_s is lattice parameters of the film and substrate, respectively.

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From the dependence it's seen, that for film thicknesses less than a certain critical value h_c, strain can be considered completely elastic. Beyond this critical thickness strain relaxation becomes energetically more favorable via introduction of misfit dislocations at the mismatched film–substrate interface.

In the simulation of template nanostructures, dislocation density in the formula (1) have to include the heterogeneity of tension in a confined space. For this we consider the mechanism of rare dislocations. Suppose that an isolated dislocation is formed only along the border of the film-substrate distribution. Then the energy change with the introduction of solitary dislocation along the z-axis describes the dependence:

$$\Delta E = E_d - \int_0^h \sigma_j(x) b_j dz,$$

where E_d is the self-energy of a dislocation; σ is the stress tensor; b_j is j component of the Burgers vector.

After spatial averaging along the z coordinates value of energy change is:

$$\Delta E = E_d - h\overline{\sigma}(x)b, \qquad (2)$$

where $\overline{\sigma}(x)$ is averaging values of the stress tensor; b is Burgers vector; h is film thickness.

Find the value for the energy of the dislocation E_d. In [11] for 3-D nanostructures is obtained:

$$E_d = E_{d,\infty} + \sum_{n=1}^{\infty} (E_I(4Rn) - E_I((2n-1)2R)), \qquad (3)$$

where $E_{d,\infty}$ is the self-energy of the dislocation in infinite environment; n is the order of system; E_I is interaction energy between dislocations, which is described by:

$$E_I(d) = \frac{\mu b_1^2}{4\pi(1-\nu)}\left(\ln(4a^2+1) + 4a^2\frac{4a^2+3}{(4a^2+1)^2}\right) +$$

$$+ \frac{\mu b_2^2}{4\pi(1-\nu)}\left(\ln(4a^2+1) - 4a^2\frac{4a^2+1}{(4a^2+1)^2}\right) + \frac{\mu b_3^2}{4\pi}\ln(4a^2+1),$$

where $a = h/d$, d is distance between the imaginary dislocations.

As can be seen in a key aspect of the mathematical analysis is to determine the tension tensor. For today to determine the value of this tensor, there are several approaches. In particular, in [12] tension tensor describes the analytical expression. However, ratios h/R values exceeding 0.2, the accuracy of measurements goes beyond ± 20%. In [13] as tension tensor using Fourier polynomials of Lagrange:

$$\{u_j(x_1,x_2,x_3), \sigma_{ij}(x_1,x_2,x_3)\} = \sum_{k=0}^{N} \{u_j^{(k)}(x), h^{-1}\sigma_{ij}^{(k)}(x) P_k(\zeta)\},$$

where $x = (x_1, x_2)$ is point average plane of the plate; $u_j^{(k)}(x)$ and $\sigma_{ij}^{(k)}(x)$ are expansion coefficients (moments); h is isotropic plate thickness; $P_k(\zeta)$ is finite Fourier polynomials of Lagrange; N is natural number. Use as a tension tensor decomposition in Fourier series leads to unnecessarily large computational cost.

To avoid the above disadvantages, we used an approach based on the determination of the average stress [14] as:

$$\overline{\sigma} = k\varepsilon^m g(h/R),$$

where $k = 2\mu\frac{1+\nu}{1-\nu}$ – the biaxial modulus, where μ is the Lame constant; ν is the Poisson ratio. The expression for $g(h/R)$ is empirically fit to:

$$g(h/R) = \frac{1}{\alpha(h/R)}(1 - e^{-\alpha(h/R)}),$$

where coefficient α was calculated using the commercial software package ABAQUS.

In our work was made numerical experiment for determining coefficient α. Modeling was done using the mathematical package MATLAB using the least squares method.

Inserting (3) into (2) we obtain the relation for the calculation of the critical thickness h_c emerging deployment:

$$h_c(R) = \frac{E_d(h_c/R)}{kb\varepsilon^m g(h_c/R)} \qquad (4)$$

From expression (4) can be seen that the critical height is a function of the created nanostructures the ratio of its size and range. This equation can be solved only numerically.

III. Verification Model

To verify our model, we used the model data curves relatively dislocational-free relief from [14] at different stages of the lattice mismatch. In Fig. 2 comparative analysis of our model with model data for relatively dislocation-free relief is presented. Lattice mismatch degree (Δε) is 1.67%, 2.51%, 4.1%.

In Figs. 3 a and 4 a shows the dependence obtained by numerical simulation of nanostructures based on GaN, grown on AlN-substrate with lattice mismatch degree 2.57% and GaAs, grown on Si-substrate with lattice mismatch degree 4.08%, respectively. The model parameters are: lattice parameter of the GaAs film a_f = 0.57 nm; lattice parameter of the Si substrate a_s = 0.54 nm; Poisson ratio ν = 0.35; Lame constant (shear modulus) μ = 148.1 GPa; Burgers vector b = 0.5 nm; lattice mismatch strain ε^m = 1.57%; biaxial modulus k = 615.85 GPa; distance between the imaginary dislocations d = 1 μm.

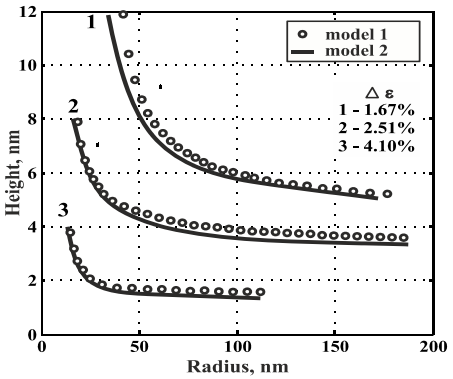
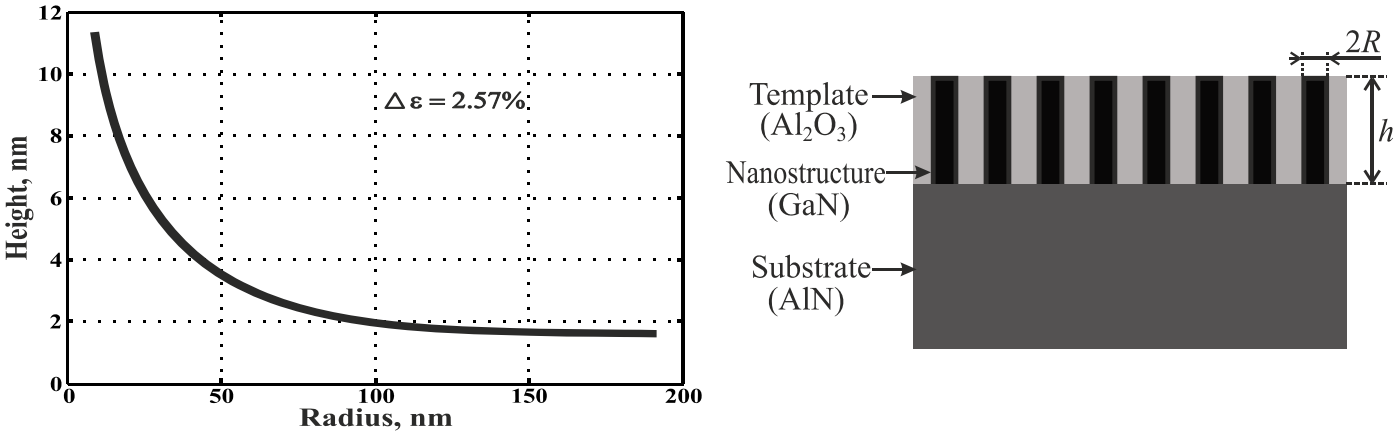
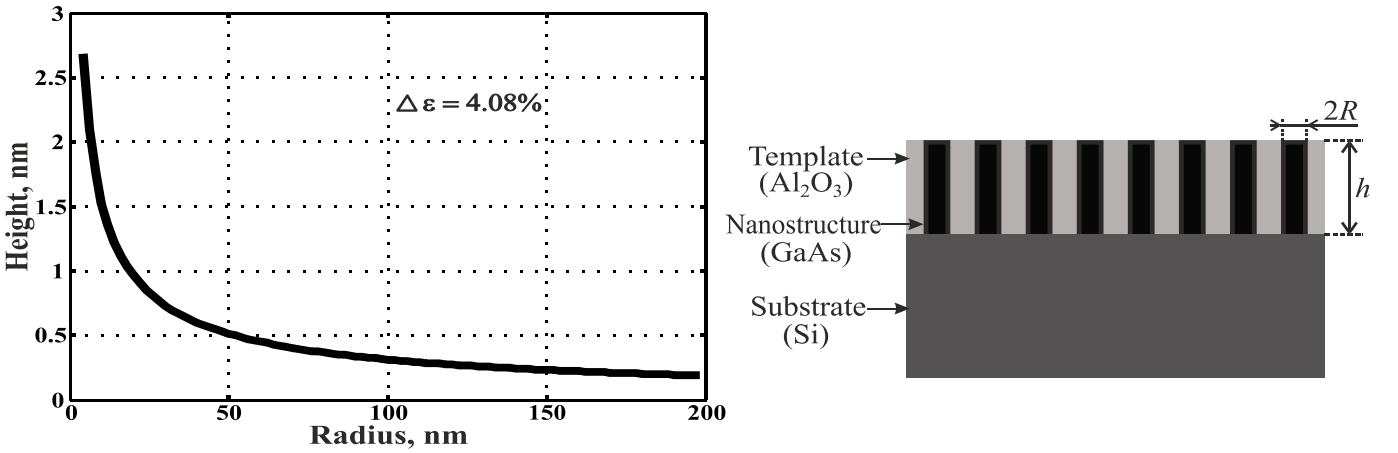


Fig. 2. Curves of relatively dislocation free map for lattice mismatch degree 1.67%, 2.51%, 4.1%, respectively.



a b

Fig. 3. Dislocation free contour map (a) and topology of GaN nanostructure on AlN substrate (b).



a b

Fig. 4. Dislocation free contour map (a) and topology of GaAs nanostructure on Si substrate (b).

IV. Conclusion

The nanostructure dislocation determination model has been considered. Dislocation free contour map has been obtained for GaN and GaAs nanostructures on the substrate of AlN and Si, respectively.

The model was verified by comparing with experimental data. Difference between those does not exceed 5 %.

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