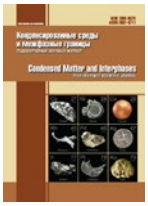

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Elastic stresses in bimorph piezocantilevers based on epitaxial wide-band III-nitrides

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Abstract

Objectives: In this work, the elastic properties of bimorphous piezocantilevers based on epitaxial AlN/AlN (AlGaN/AlN/AlGaN/AlN/AlGaN) structures were studied using computer modeling. These structures allow for the simultaneous manifestation of direct and inverse piezoelectric effects and the excitation of various types of acoustic waves. Given the high thermal resistance and thermal stability of these materials, it is assumed that such cantilevers could serve as a basis for the subsequent creation of various sensors designed to operate in high-temperature and chemically aggressive environments.

Experimental: In static and infra-low-frequency modes, the reverse piezoelectric effect manifests as bending deformations and associated elastic stresses. To pre-estimate the magnitude of these stresses, which have a multidirectional character at the hetero-interfaces of the layers, a simple mathematical model was constructed, which allows establishing the magnitude of these stresses and their relationship with the geometric and elastic parameters of the console.

Conclusions: Based on the model, a computational algorithm was developed in the MATLAB environment, which allows determining the dependence of elastic stresses, including the ratio of the thicknesses of the active layers. Such a dependence has the form of a curve with a maximum, which is reached at the ratio of the thicknesses of the layers m = 1.5, at the same time, the value of these stresses practically does not depend on the ratios of the values of the elastic constants of the layer materials (for the cases of AlGaN/AlN and GaN/AlN). It is assumed that such estimates will be useful for the preliminary design and optimization of the geometry of piezoelectric sensors.

Keywords: High-temperature functional electronics, Wide-bandgap semiconductors; Epitaxial technologies; Multilayer AlN/AlGaN structures; Bimorph cantilever, Bending deformations, Elastic stresses

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Упругие напряжения в биморфных пьезокантилеверах на основе эпитаксиальных широкозонных III-нитридов

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Аннотация

Цель статьи: В настоящей работе методом компьютерного моделирования проведено исследование упругих свойств биморфных пьезокантилеверов, сформированных на базе эпитаксиальных AlN/AlN (AlGaN/AlN/AlGaN/AlN/AlGaN) структур, допускающих возможность совместного проявления прямого и обратного пьезоэффектов и возможность возбуждения акустических волн различных типов. Учитывая высокую термостойкость и термостабильность параметров этих материалов, предполагается, что такие кантилеверы могли бы послужить основой для последующего создания различных сенсоров, ориентированных на работу в высокотемпературных условиях и в условиях химически агрессивных сред.

Экспериментальная часть: В статических режимах и в режимах работы в области инфранизких частот основным проявлением обратного пьезоэффекта является появление изгибных деформаций и связанных с ними упругих напряжений. Для предварительной оценки величины этих напряжений, имеющих на гетерограницах слоев разнонаправленный характер, была построена простая математическая модель, позволяющая установить величину этих напряжений и их связь с геометрическими и упругими параметрами консоли. *Выводы:* На основе модели в среде MATLAB был разработан вычислительный алгоритм, который позволяет определить зависимость упругих напряжений, в том числе и от соотношения толщин активных слоев. Такая зависимость имеет вид кривой с максимумом, который достигается при отношении толщин слоев m = 1.5, в тоже время от отношений значений упругих констант материалов слоев (для случаев AlGaN/AlN и GaN/AlN) величина этих напряжений практически не зависит. Предполагается, что подобные оценки будут полезными для предварительного проектирования и оптимизации геометрии пьезоэлектрических сенсоров.

Ключевые слова: высокотемпературная функциональная электроника, широкозонные полупроводники; эпитаксиальные технологии; многослойные AlN/AlGaN-структуры; биморфный кантилевер, изгибные деформации, упругие напряжения

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1. Introduction

The development and technological implementation of the component base for sensor elements focused on operation in high-temperature conditions (including monitoring of geothermal zones, diagnostics of the current state of nuclear reactors) is becoming increasingly relevant, as it is expected to contribute to increasing the reliability of predictions of the onset of destructive earthquakes or accidents at geothermal power plants.

Many characteristic features that necessarily precede global tectonic cataclysms (such as changes in the composition of volcanic gases or changes in the concentration of salts in a liquid medium) can only be detected through contact diagnostics of deep (geothermal) underground zones, where temperatures can reach 500 °C.

At the same time, among the sensors that are sensitive to various types of stimuli and have been implemented to date, there is a class of devices that contain a piezoelectric bimorph

microcantilever (console element), whose frequency properties, depending on its geometric design, allow for the creation of a wide range of highly sensitive sensor devices.

To date, sensors have been developed and studied for detecting pressure differences [1, 2], measuring viscosity and determining the chemical composition of a liquid medium [3–5], monitoring radiation levels, gas analysis, and vibration [6–10]. Most of these sensors use ferroelectric ceramics with a temperature limit of 300 °C.

At the same time, piezomaterials such as AlN and AlGaN have exceptional chemical inertness and thermal stability up to 900–1000 °C, and the technologies for their production, including those for multilayer epitaxial structures that could serve as a basis for microcantilevers, have already been developed.

Given the high cost of epitaxial processes and the fact that cantilever operation induces elastic stresses, it is desirable to obtain a preliminary assessment of its maximum values using computer modeling techniques to avoid potential damage.

The purpose of this work was to calculate the magnitude of the elastic stresses that occur during the bending deformation of bimorphic AlN/AlN and AlN/AlGaN consoles, depending on the thickness of the layers. To achieve this, a computational algorithm (using MATLAB) was developed to obtain the optimal ratios between the thicknesses of the active layers.

2. Materials and structure

Aluminum nitride was chosen as the material for these sensor elements for the following reasons. As a wide-band semiconductor (hexagonal wurtzite lattice, band gap Eg = 5.9 eV), AlN has exceptional chemical stability, as well as the highest known thermostability of parameters (electrical conductivity, piezoelectric modules, dielectric constant, and dielectric loss factor), which retain their original values at least up to 1000 °C [11, 12].

It is assumed that among the various epitaxial technologies developed so far (MBE, MOS), the HVPE (Hydride Vapor Phase Epitaxy) method is the most suitable, as, unlike other methods focused on nano- and submicron layers, this method is characterized by high growth rates, allows for the production of layers in a wide range of thicknesses, and provides an economic feasibility for producing layers up to 300 μm or more [13, 14].

The post-epitaxial formation of a cantilever node with three electrodes involves a pre-existing epitaxial structure of the GaAlN/AlN/GaAlN/AlN/GaAlN type, where the active dielectric AlN layers form the basis of the bimorphic cantilever, and the thin conductive GaAlN layers act as passive electrodes, ensuring the equipotentiality of the hetero-interfaces along the cantilever length.

In addition, the formation of a suspended cantilever requires the presence of a special technological layer, known as a "sacrificial" layer (e.g., doped GaN or InGaN layers), which is initially formed directly on the substrate, preceding the main structure, and which is partially removed from the sub-console space at a certain stage, except for small regions that ensure a monolithic connection between the cantilever and the substrate. Various technologies can be used to remove the necessary areas of the sacrificial layer, including ion milling, but local electrochemical etching (for example, in a KOH solution) appears to be the simplest and most effective method.

3. Calculation of elastic stresses

It is assumed that the cantilever microelement formed on the basis of a multilayer epitaxial structure contains two active dielectric AlN-layers, and, in addition, contains thin conducting AlGaN layers (lower, interlayer and upper), which act as electrodes and ensure equipotentiality along the entire length of the cantilever (Fig. 1). Further, it is assumed that the thickness of the electrodes is less than the thickness of the active AlN-layers, and two cases are considered: 1) the case of extremely thin electrodes, when the presence of the AlGaN layer has almost no effect on the deformation of the active AlN layers, and 2) the thickness of the electrode is comparable to the thickness of the AlN, and the elastic stresses will be calculated for model structures such as AlN/AlGaN (AlN/GaN).

An asymmetrical connection of a pair of AlGaN electrodes (for example, the bottom and interlayer electrodes) to an external source

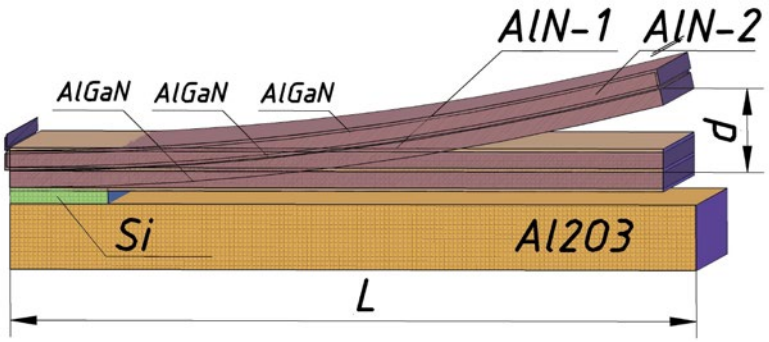

Fig. 1. Schematic representation of a cantilever formed based on an epitaxial AlGaN/AlN/AlGaN/AlN/AlGaN structure obtained on a Si substrate and using an additional Al_2O_3 support

with a voltage of U_1, and the resulting electric field E_1 (or $D_1 = \varepsilon E_1$) leads to the appearance of deformations that are transverse to the field, determined by the module d_{31}. In the case of a rigid connection between the layers, this causes the second AlN layer to be forced to deform. Since such deformations will be different for each of the AlN layers when averaged over the thickness, the resulting additional stresses will cause the cantilever to bend. Further calculations will be based on the approach developed for thermoelasticity problems [15].

The main forces that arise in the layers when the stress U_1 changes are represented by the corresponding changes in the tensile force (F_1) and the compressive force (F_2), which are opposite in sign and equal in magnitude (force F), as well as by the bending moments M_1 and M_2, where:

$$M_1 = (Y_1\ J_1)/R \text{ and } M_2 = (Y_2\ J_2)/R. \quad (1)$$

Here Y_1 and Y_2 are the elastic moduli, J_1 and J_2 are the inertia moments for two arbitrary cross-sections and R is the radius of curvature of the bending.

In further calculations, the following numerical values of the AlN parameters will be used: the dielectric constant ε = 8.5, the transverse piezomodule d_{31} = -2.0 pm/V and the elastic modulus Y = 308 GPa [14].

Next, let w_1 and w_2 be the thickness values of the layers, and taking into account the smallness of the thickness of the GaAlN-electrodes, we will assume that the total thickness of the cantilever is $w \approx w_1 + w_2$. For cross-sections that are close to a square, the moments of inertia of the two AlN layers are, respectively, equal to:

$$J_1 = w_1^3/12 \text{ и } J_2 = w_2^3/12, \quad (2)$$

then the corresponding products $Y_1 \cdot J_1$ and $Y_2 \cdot J_2$ will characterize the bending stiffness of the layers.

Since no external forces are applied to the system and it is in equilibrium, the following equation holds:

$$\frac{Fw}{2} = M_1 + M_2 \text{ or } \frac{Fw}{2} = \frac{Y_1\ J_1 + Y_2 J_2}{R} \quad (3)$$

In addition, at the interphase boundary of two piezo layers (more precisely, inside a thin conductive GaAlN layer), there must be a neutral surface on which the deformations (relative changes in size due to the application of external stress U_1) of these layers are mutually equal, which allows us to formulate the following equation:

$$\begin{aligned} &d_{31} \cdot \varepsilon \cdot E_1\ + F_1/(Y_1 w_1) + w_1/2R = \\ &= d_{31} \cdot\ \varepsilon \cdot E_1\ + F_2/(Y_2 w_2) + w_1/2R. \end{aligned} \quad (4)$$

This equation allows us to establish a relationship, firstly, between the radius of curvature of the cantilever R and the geometric and elastic parameters of the layers of the console, and, in addition, with the values of the external voltage applied to the GaAlN-electrodes. Next, it is advisable to introduce the following notations for the thickness ratios $w_1 / w_2 = m$ and the modulus ratios $Y_1 / Y_2 = k$.

Then the following expression for the value of the radius of curvature can be obtained:

$$\frac{1}{R} = \frac{6 \cdot d_{31} \cdot \varepsilon \cdot (E_1)(1+m)^2}{w \cdot \left[3(1+m)^2 + (1+mk)\left(m^2 + (mk)^{-1}\right)\right]} \quad (5)$$

It is obvious that the maximum elastic (normal) stress T, increasing with an increase in the electric field strength, will be observed

precisely at the interphase. In this regard, it should be noted that even in the absence of forced bending deformation, a significant elastic stress already initially exists at the layer boundary, which appears due to the mismatch of the lattice parameters of AlN and AlGaN, as well as the inequality of their coefficients of thermal expansion, and which can reach tens of MPa and more [16]. It is assumed that the operating modes of the cantilever will be such that the additional stress created by the piezoelectric deformation will be significantly lower and will be further considered as an additive.

This additional stress consists of two components: first, the stress caused by the axial force, and second, the stress caused by bending. For the AlN_1 layer, this stress can be determined using the following expression:

$$T = \frac{F}{w_1} + \frac{w_1 Y_1}{2R}. \quad (6)$$

Or, using the ratio (4), we can obtain:

$$T = \frac{2}{R}\left[\frac{1}{ww_1}\left(Y_1 J_1 + Y_2 J_2\right) + \frac{w_1 Y_1}{4}\right], \quad (7)$$

or

$$T = \frac{1}{R}\frac{1}{6}\left[\frac{1}{w}\left(Y_1 w_1^{\,2} + Y_2\left(\frac{w_2}{m}\right)^2\right) + 3Y_1 w_1\right]. \quad (8)$$

Substituting the expression for the radius of curvature (5) into this formula, the following expression can be obtained for the additional elastic stress at the layer boundary:

$$T = \frac{d_{31}\cdot\varepsilon\cdot\left(E_1\right)\left(1+m\right)^2}{w\cdot\left[3\left(1+m\right)^2 + \left(1+mk\right)\left(m^2 + (mk)^{-1}\right)\right]}\times$$
$$\times\left[\frac{1}{w}\left(J_1 w_1^{\,2} + \left(\frac{Y_2}{m}\right)w_2^{\,2}\right) + 3Y_1 w_1\right]. \quad (9)$$

The corresponding calculations performed in the MATLAB environment allowed us to establish the $T(m)$ dependence under the condition w = Const(40 μm), which takes the form of curves with a maximum that is reached at $m = 1.5$ (Fig. 2). These curves correspond to different values of the Y_2 moduli of elasticity (350 GPa, 335 GPa, 320 GPa), which, in turn, approximately correspond to AlN, AlGaN, and GaN.

In addition, from the above relations for the radius of curvature R, and from the equations that relate it to the length of the console L [17]:

$$d(2R-d) = (L/2)^2 \text{ или } 2dR = L^2/4 \quad (10)$$

the final equation for the deflection of the end of the console can be obtained:

$$d = L^2/8R. \quad (11)$$

Just like the radius of curvature R, this deviation will obviously depend on the ratio of the layer thicknesses m. For cases of different total thickness w and different values of the Y_2 elastic moduli, the values of this deviation are presented in Fig. 3. It is clear that the maximum deviation should not exceed the height of the undercantilevered area, which imposes certain restrictions on w and the field strength E. It is assumed that considering these restrictions will also help to reduce the risks of mechanical damage and increase the sensor's fault tolerance.

The following approximations were used in these calculations. Firstly, it is assumed that the thickness of the GaN electrodes is significantly smaller than the thickness of any of the AlN layers. Secondly, it is assumed that the total thickness of the cantilever is much smaller than

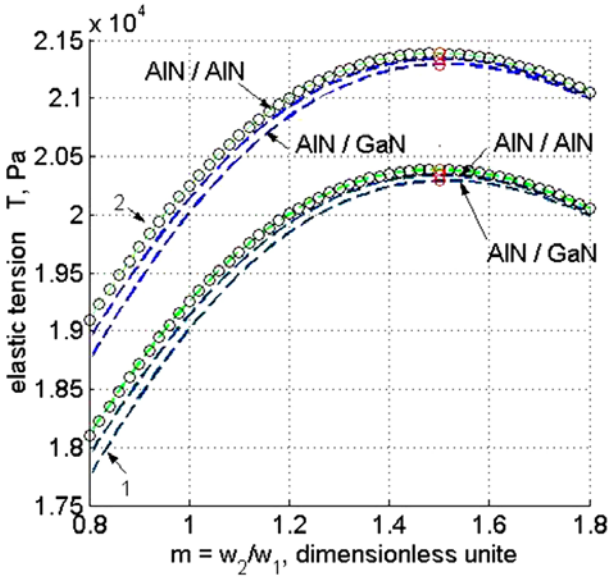

Fig. 2. Dependence of elastic stresses near heterojunctions on the layer thickness ratio w_1/w_2 for a total layer thickness w = 40 μm and the field strength for family: 1) $E = 1.1\cdot10^4$ V/cm (U = 44 V) and for family 2) $E = 1.22\cdot10^4$ V/cm (U = 49 V).

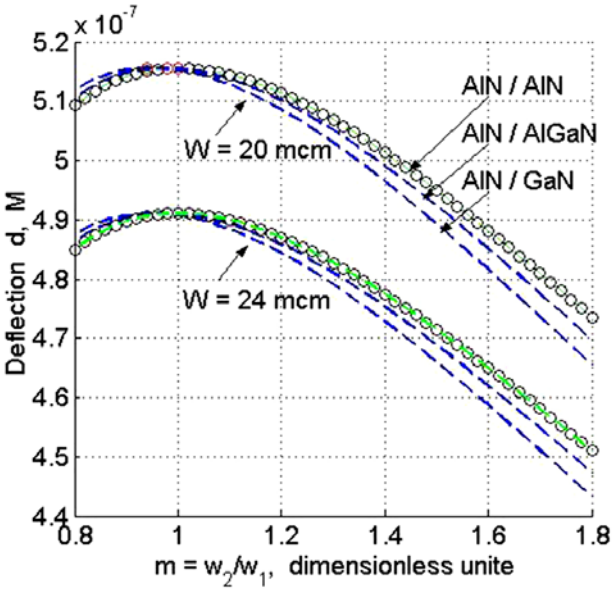

Fig. 3. Dependences of the cantilever tip deflection w_1/w_2 for various values of w and three elastic moduli (for AlN, AlGaN, and GaN) at a field strength of $E = 1.1 \cdot 10^4$ V/cm

its length. Finally, the initial mechanical stresses and corresponding deformations resulting from the technological cooling process and the differences in thermal expansion coefficients were not taken into account in these calculations.

Taking into account that the technological process of obtaining a basic epitaxial structure is very labor-intensive and requires the use of expensive components that are directly proportional to the total thickness of the resulting layers, it is assumed that even such approximate estimates will contribute to a more rational planning of the thickness of the w_1 and w_2 layers of the resulting structures.

4. Conclusion

The solution of the problem of creating various sensors designed to operate in high-temperature conditions and in chemically aggressive environments remains extremely relevant. One of the promising approaches is the use of piezocantilevers formed using epitaxial structures based on the high-temperature piezomaterial AlN. Since the key effect for the operation of such cantilevers in the static mode is bending under the influence of an electric field (reverse piezoelectric effect), a mathematical model was constructed to calculate the value of elastic stresses. Based on the model, a computational algorithm was developed in the MATLAB environment, which allows establishing the relationship between the ratio of the thicknesses of the active piezoelectric layers and the magnitude of the elastic stresses that appear at the interlayer boundaries. It is assumed that the developed tool can be used for the preliminary design and optimization of the geometry of the cantilever-type sensors, which can also be easily extended to other technologically feasible piezoelectric heterostructures, such as AlN/SiC (see [18, 19] for more information).

Authors' contributions

Panyutin E. A. – research concept, development of necessary algorithms and computational programs (MATLAB environment), and writing of the text. Sharofidinov Sh. Sh. – discussion of issues related to the technological feasibility of the proposed cantilever designs and conducting test epitaxial processes to obtain the necessary epitaxial structures.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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