Epitaxial AlN/AlN bimorph piezocantilevers for geothermal monitoring

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Abstract. The problem of early and reliable prediction of earthquakes, which can lead to catastrophic consequences, is far from being solved, so it remains extremely topical. The next step towards its solution, as it is supposed, could be the creation of a network of sensors located in the hot deep layers of geothermal systems and capable of continuous monitoring of geophysical parameters characterizing the activity of magma. In this paper we propose the use of matrices of thermally stable bimorph piezocantilevers formed on the basis of epitaxial AlN/AlN structures and allowing the possibility of excitation of acoustic waves of various types as a universal platform for the subsequent creation of various sensors capable of operating in high-temperature and chemically aggressive environments. Since in static modes the main manifestation of the inverse piezo effect is the appearance of bending deformations, for preliminary estimation of the geometrical parameters of such cantilevers, a mathematical model of the change in the deflection value was constructed, and a computational algorithm (MATLAB environment) was developed to make it possible to obtain the optimal ratios between the thicknesses of active AlN layers from the point of view of minimizing the control stresses.

1 Introduction

The problem of reliable and early prediction of earthquakes (it is enough to recall the devastating cataclysms in Turkey (1939), Armenia (1988), Haiti (2010), which can lead to catastrophic consequences and numerous human casualties, is still far from its final solution. It is well known that one of the most effective approaches aimed at further progress in the right direction is the creation of monitoring systems, and it has already become obvious that the seismoacoustic sensor networks being created are not able to provide the desired completeness of the necessary information that would provide the possibility of long-term and reliable forecasts regarding all the features of the behavior of magmatic structures.

Many characteristic signs preceding global tectonic cataclysms (changes in the composition and intensity of volcanic gas release or changes in the composition of liquid medium, appearance of specific features in the spectra of background deep seismic waves) can be revealed only by monitoring deep underground layers, the geophysical parameters of which reflect changes in magmatic activity to a greater extent.

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Geothermal systems formed in areas of magmatic activation of the Earth's crust (for instance, Geysers (California, USA); Himalayan geothermal belt (Tibet, China), Larderello (Italy); or Ebeko volcano (South Kamchatka, Russia) [1-3]) appear to be convenient geologic objects from the point of view of clarifying the peculiarities of deep magmatic processes, as well as technical possibilities for direct penetration into deep layers. They consist of rather loose fracture-pore geological structures formed at depths up to 10 kM and filled with hot mineral solutions and superheated dry steam under high pressure and with temperatures up to 500ºC÷700ºC. For this reason, all sensor elements intended for operation in such monitoring systems should be initially oriented for operation not only in high-temperature conditions, but also in chemically aggressive environments.

At the same time, at present it is possible to distinguish quite an extensive class of sensors united by the presence of a structural unit including a piezoelectric bimorph microcantilever (cantilever element), the resonance properties of which make it possible to realize a wide variety of highly sensitive sensor devices. To date, sensors for pressure [4,5], viscosity and chemical composition of liquid medium [6-8], radiation sensors and gas analyzers [9,10], as well as vibration sensors and energy harvesting devices have already been created [11-13].

However, despite the fact that most of the listed sensor elements were developed using well-developed industrial ceramics of the segmentoelectric type (PZT composites) and featured high values of piezo coefficients, they have a number of significant disadvantages, the main of which is temperature limitations leading to loss of piezoelectric properties at $T \geq 300$ ºC.

At the same time, some wide-gap semiconductor materials (including, ε-Ga_2O_3 , ZnO and, especially, AlN), epitaxial technologies for the production of which have advanced significantly in recent years, are chemically inert and heat-resistant piezoelectrics, and AlN is featured by exceptional heat resistance, which makes it possible to preserve the invariability of its dielectric parameters in the specified temperature range with a large margin.

Therefore, the development of various technologies for obtaining multilayer structures on the basis of such materials, which in the future could become the basis for the subsequent creation of single-crystal bimorph microcantilevers and even their matrices by postepitaxial methods, seems to be actual.

However, taking into account the considerable labor-intensiveness of epitaxial processes, a preliminary at least rough estimation of some basic parameters of layers, which can be carried out by computer modeling methods, is advisable. The purpose of this work was to calculate the curvature and deflection value of a bimorph AlN / AlN cantilever depending on the thickness of the layers and the value of the electric field. For this purpose, we developed a computational algorithm (MATLAB environment), which makes it possible to obtain, in addition, the optimal ratios between the thicknesses of active layers from the point of view of minimizing the control stresses.

2 Materials and structure

Among other conditions, which should be met by the material on the basis of which it would be possible to develop this family of sensors, the main ones are its belonging to the family of piezoelectrics and long-term thermostability of parameters in the temperature range up to 700ºC.

As it is well known, the piezo effect (change of crystal polarization and the appearance of electric charges on opposite faces under the action of external deformations) is typical for some classes of crystals (in particular, having a lattice such as perovskite, wurtzite or pseudowurtzite); the opposite piezo effect consists, respectively, in the spontaneous deformation of the crystal under the influence of an applied electric field.

The basis for the choice of aluminum nitride as a material suitable for the creation of such sensor elements are the following considerations. As a wide-area semipro-water (hexagonal lattice of wurtzite type, forbidden zone width E_g = 5.9eV), AlN has exceptional chemical resistance, as well as the highest among the known piezoelectrics thermostability of parameters (electrical conductivity, piezomoduli, dielectric constant, dielectric loss coefficient), which retain their original values at increasing temperatures, at least to 1000ºC [14,15].

In addition, an important advantage of AlN in the considered perspective is its technological compatibility with other wide-gap materials such as GaN, Ga_2O_3 or SiC, which makes it possible to epitaxially produce multilayer structures with different sets of layers and with an acceptable level of perfection of their hetero-boundaries.

It is assumed that among the various epitaxial technologies developed to date (MBE, MOS), the HVPE (Hydride Vapor Phase Epitaxy) method is the most acceptable, since, unlike others focused on nano- and submicron layers, this method is featured by high growth rates, makes it possible to obtain layers in a wide range of thicknesses, and provides economic feasibility of obtaining layers up to 300 μm and more [16, 17].

Post-epitaxial formation of a cantilever node with three electrodes implies the presence of a pre-derived epitaxial structure of GaAlN/AlN/GaAlN/AlN/AlN/GaAlN type, in which active dielectric AlN layers form the basis of a bimorphic cantilever, and thin conducting GaAlN perform the passive role of electrodes, providing equipotentiality of hetero-boundaries along the length of the cantilever.

In addition, the formation of a dangling cantilever requires a special technological so-called “sacrificial” layer (for instance, doped GaN or InGaN layers), which is initially formed directly on the substrate, preceding the main structure, and which at a certain stage is partially removed from the sub-cantilever space, except for small areas that provide a monolithic connection between the cantilever and the substrate. To remove the necessary areas of the sacrificial layer it is possible to use various technologies, including the ion milling method, but the simplest and quite effective is local electrochemical etching (for instance, in KOH solution).

It is obvious that within the framework of the proposed approach it is also possible to create cantilever matrices, which after additional individualization of each cantilever (application of chemically specific coatings, change of cantilever length) opens the way for creation of multifunctional sensor groups united in a single single chip and capable of multi-parametric environmental diagnostics.

However, in order to perform a substantive evaluation of the desired geometrical parameters of the initial epitaxial structure, using the relationship between the deflection value and the applied electric field as one of the criteria of the cantilever effectiveness, it is advisable to perform preliminary computer modeling of its bending deformation, which, as it is supposed, will make it possible to find out the optimal ratio of active layer thicknesses as well.

3 Elementary theory of bimorph piezocantilever and deflection calculation

It is assumed that the cantilever microelement (cantilever), formed on the basis of a multilayer epitaxial structure, contains two active dielectric AlN layers and, in addition, contains thin conducting AlGaN layers (bottom, interlayer and top), which act as electrodes and provide equipotentiality along the entire length of the cantilever (Fig. 1). It is further assumed that the thickness of the electrodes is much less than the thickness of the active AlN layers, so that these layers have no appreciable influence on the mechanical behavior of the cantilever, and their presence will not be taken into account in further calculations.

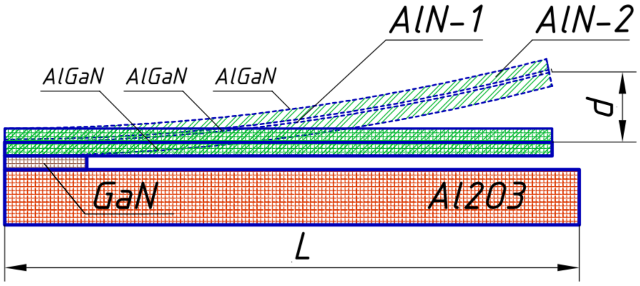

Fig.1. Schematic representation of the deflection of a bimorph piezocantilever formed on the basis of a six-layer GaN/AlGaN/AlN/AlGaN/AlGaN/AlN/AlGaN structure epitaxially produced on an Al_2O_3 substrate

Unsymmetrical connection of a pair of AlGaN electrodes (for instance, the bottom and interlayer electrodes) to an external source with voltage U_1, and the emerging electric field E_1 (or $D_1 = \varepsilon E_1$) leads to the appearance, including transverse to the field deformations defined by the modulus d_{31}, which, in the case of rigid connection of the layers, causes forced deformation of the second AlN layer as well. Since such deformations will be different for each of the AlN layers, the resulting additional stresses will lead to bending of the cantilever.

The main forces occurring in the layers during the stress change are U_1, are represented by the tensile force (F_1) and the compressive force (F_2), and

$$|F_1| = |F_2| = F \tag{1}$$

and the corresponding bending moments M_1 and M_2, where

$$M_1 = \frac{Y_1 J_1}{\rho} \quad and \quad M_2 = \frac{Y_2 J_2}{\rho} \tag{2}$$

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

In the simplest case for unalloyed AlN layers, it is obvious that $Y_1 = Y_2$, However, with possible use of isovalent doping (in particular, doping with scandium, which increases the values of piezomoduli), the values of elastic moduli may not coincide, so the formulated objective will be solved in general for different parameters of both piezo-active layers. In further calculations the following numerical values of AlN parameters will be used: dielectric constant ε=8.5, transverse piezomodulus d_{31} = -2.0 pm/V and elastic modulus Y=308 GPa [14].

Furthermore, let w_1 and w_2 be the values of layer thicknesses, and taking into account the smallness of GaAlN-electrode thickness, we will assume that the total thickness of the cantilever – $w \approx w_1 + w_2$. For cross-sections with a shape close to square, the moments of inertia of the two AlN layers are, respectively, equal to

$$J_1 = \frac{w_1^{\ 3}}{12} \quad and \quad J_2 = \frac{w_2^{\ 3}}{12} \tag{3}$$

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 is valid:

$$\frac{1}{2} F\, w = M_1 + M_2$$

or

$$\frac{1}{2} F\, w = \frac{Y_1 J_1 + Y_2 J_2}{\rho} \tag{4}$$

In addition, at the boundary of the two layers (more precisely, inside the thin conducting GaAlN layer) there must exist a neutral surface on which the deformations (relative changes of dimensions caused by the application of external voltage U_1) of these layers are mutually equal, which makes it possible to make the following equation:

$$d_{31} \cdot \varepsilon \cdot E_1 + \frac{F_1}{Y_1 b_1} + \frac{b_1}{2\rho} = d_{31} \cdot \varepsilon \cdot E_1 + \frac{F_2}{Y_2 b_2} + \frac{b_2}{2\rho} \tag{5}$$

which can be transformed to the following, more convenient form

$$\frac{w}{2\rho} + \frac{2(Y_1 J_1 + Y_2 J_2)}{w\rho} \cdot \left(\frac{1}{Y_1 w_1} + \frac{1}{Y_2 w_2} \right) = d_{31} \cdot \varepsilon \cdot E_1 \tag{6}$$

and which makes it possible to relate the radius of curvature of the cantilever ρ, on the one hand, to its geometric and elastic parameters, and, on the other hand, to the values of the field E_1 and, respectively, the external voltage applied to the GaAlN electrodes.

$$\frac{1}{\rho} = \frac{d_{31} \cdot \varepsilon \cdot E_1}{\frac{w}{2} + \frac{2(Y_1 J_1 + Y_2 J_2)}{w} \left(\frac{1}{Y_1 w_1} + \frac{1}{Y_2 w_2} \right)} \tag{7}$$

Ratios of thicknesses and elastic moduli

$$\frac{w_1}{w_2} = m \qquad \frac{Y_1}{Y_2} = n \tag{8}$$

$$\frac{1}{\rho} = \frac{6 \cdot d_{31} \cdot \varepsilon \cdot (E_1)(1+m)^2}{w \cdot \left[3(1+m)^2 + (1+mn)\left(m^2 + (mn)^{-1} \right) \right]} \tag{9}$$

$$\frac{1}{\rho} = \frac{24 \cdot d_{31} \cdot \varepsilon \cdot E_1}{w \cdot \left(14 + n + n^{-1} \right)} \tag{10}$$

For the particular case n = 1 we have:

$$\frac{1}{\rho}=\frac{3\cdot d_{31}\cdot\varepsilon\ \cdot E_1}{2w} \tag{11}$$

Finally, using the obtained values of the radius of curvature of the cantilever, the deflection of its end can be calculated:

$$d(2\rho-d)=(L/2)^2 \quad \text{then} \quad 2d\rho=L^2/4 \quad \text{or} \quad d = L^2/8\rho \tag{12}$$

On the basis of these relations, dependences of the deflection value on the ratio of layer thicknesses m, and on the ratio of their elastic moduli n can be obtained, which provides the possibility of developing recommendations for evaluating the optimal parameters of the layers, providing the maximum value of deflection d (Fig. 2).

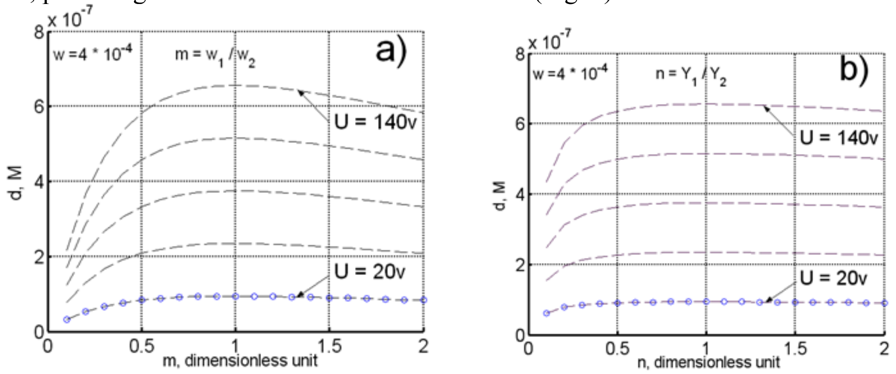

Fig. 2. Dependence of cantilever end deflection value on the ratio $m = w_1 / w_2$ (**a**) and from the relationship $n = Y_1 / Y_2$ (**b**).

In performing these calculations, the following approximations were used.

Firstly, it is assumed that the thickness of the GaAlN electrodes is much less than the thickness of any of the AlN layers. Next, the total thickness of the cantilever is assumed to be much smaller than its length. Finally, the initial mechanical stresses and their corresponding deformations resulting from technological cooling and due to differences in the values of thermal expansion coefficients, which additionally break the symmetry of the layers, were not taken into account in these calculations.

The algorithm development and calculations were performed in MATLAB environment.

4 Conclusions

The increasing intensity of tectonic processes, observed in recent decades and sometimes leading to destructive cataclysms, necessitates the implementation of work aimed at creating a distributed network of geothermal sensors, which, in addition to seismology methods, could contribute to improving the predictive ability of long-term earthquake prediction. At the same time, the achieved level of development of epitaxial technologies of wide-area nitrides, and especially AlN, already makes it possible to create sensors capable of working in hot zones of geothermal systems. Therefore, further progress towards the creation of a full-fledged element base for high-temperature functional electronics, including (in the future) also aimed at single-chip integration of AlN with other heat-resistant materials designed, for instance, for the creation of microcircuits oriented to digital operations (such as SiC or Ga_2O_3), seems topical [18-20].

5 Conflict of interest.

The authors claim that they have no conflict of interest.

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