DE GRUYTER OPEN

Journal of MECHANICAL ENGINEERING – Strojnícky časopis,
VOL 67 (2017), NO 2, 61 - 68

STU SjF

THE EFFECTS OF PIEZOELECTRICITY MATRIX CONSTANTS ON THE CHARGE OF A THIN MEMBRANE

KOVÁČ Tomáš[1], HORVÁT František[1], HUČKO Branislav[1], JANČO Roland[1], MUSIL Miloš[1]

[1]*Slovak University of Technology in Bratislava, Faculty of Mechanical Engineering, Institute of Applied Mechanics and Mechatronics, Nám. Slobody 17,812 31 Bratislava, Slovakia, email: branislav.hucko@stuba.sk*

Abstract: This article is devoted to the comparison of the influence of the piezoelectric matrix properties on the magnitude of the resulting charge when a thin piezoelectric membrane of circular cross section, made from aluminium gallium nitride (Al-GaN), is loaded. The size of change of the electric charge was determined by the numerical analysis and the by the change of the properties of the piezoelectric matrix. The matrix constants were obtained from various sources introduced in world databases.

KEYWORDS: piezoelectric, gallium nitride, constitutive equations, average, variance, deviation

1 Introduction

Thin Al-GaN membranes have different configurations for their application. In the case of a membrane of a circular cross section (as shown in Fig 1, in the analysed device), it is most common for the measurement of pressure. To apply pressure onto the membrane, it must be fixed around its circumference. The internal structure of piezoelectric materials is highly dependent on their manufacturing process, which then is reflected on their properties. Even a small change in the properties of the piezoelectric material can lead to more pronounced changes in the electrical charge obtained in the so called direct piezoelectric effect, or the change in the properties can lead to significantly different deformations in an inverse piezoelectric effect. Using a numerical methods, we can predict the behaviour of the pressure sensors. It is possible to simulate the different properties of the Al-GaN material and to obtain the assumed values of the electrical charge, respectively the deformation of the material. The first part of the article is devoted to the comparison of the results of 10 sets with different material constants for the aluminium gallium nitride material. Applied material constants were taken from research reports and contributions introduced in world databases [1-16]. In the second part of the article, we compare the obtained results with the results measured during the experiment [17].

2 The investigated model

The numerical model is based on a thin membrane used in experimental measurements. The configuration and geometrical properties of the membrane are shown in Fig. 1. It is made of a piezoelectric Al-GaN layer over GaN. The ratio of each corresponding layer is 99.9524% GaN overlaid with 0.0476 % Al-GaN. The membrane is circular with a diameter of 750 μm. The membrane is placed over a ceramic substrate measuring 350 x 350 μm. The thickness of each layer is 4.22 μm and 0.02 μm for GaN and Al-GaN respectively. Once a charge is created, a thin 2D layer of electron gas is produced between the layers and it acts as a transmitter for the

DOI: 10.1515/scjme-2017-0018, Print ISSN 0039-2472, On-line ISSN 2450-5471

current across the membrane. This layer influences the magnitude of the piezoelectric charge which occurs on the surface of the Al-GaN layer.

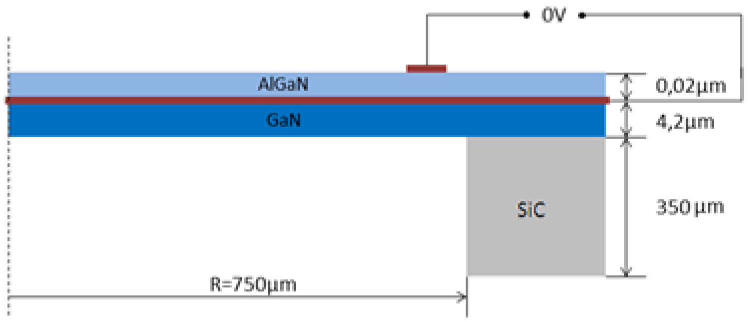

Fig. 1 Dimensions of the equivalent model of the membrane

3 General description of piezoelectric materials

The solution of piezoelectric problems requires a physical and electrical description of the material. These can be divided into two general equations. Mechanical properties are given by equation (1) while the electric properties are given in equation (2) with respect to dielectrics.

$$S = \frac{\sigma}{Y} \quad \left[\frac{\mathrm{m}}{\mathrm{m}};\frac{\mathrm{N}}{\mathrm{m}^2};\frac{\mathrm{N}}{\mathrm{m}^2}\right] \tag{1}$$

$$D = \varepsilon . E \quad \left[\frac{\mathrm{C}}{\mathrm{m}^2};\frac{\mathrm{F}}{\mathrm{m}};\frac{\mathrm{V}}{\mathrm{m}}\right] \tag{2}$$

where: S is the strain, σ is stress, Y is Young's modulus, D is the electric displacement, ε is the permittivity of the dielectric and E is the electric field. As the piezoelectric effect deals with both, it is necessary to combine the electric and mechanical properties into an electro mechanical description given by (3).

$$S = \frac{\sigma}{Y} + d.E \quad \left[\frac{\mathrm{m}}{\mathrm{m}};\frac{\mathrm{N}}{\mathrm{m}^2};\frac{\mathrm{N}}{\mathrm{m}^2};\frac{\mathrm{m}}{\mathrm{V}};\frac{\mathrm{N}}{\mathrm{m}^2}\right] \tag{3}$$

$$D = d.\sigma + \varepsilon^{\sigma}.E \quad \left[\frac{\mathrm{C}}{\mathrm{m}^2};\frac{\mathrm{C}}{\mathrm{m}^2};\frac{\mathrm{N}}{\mathrm{m}^2};-;\frac{\mathrm{N}}{\mathrm{m}^2}\right] \tag{4}$$

where d – piezoelectric deformation constant with respect to electric field E. In the absence of mechanical stress, d in equation (4) represents the electric charge per unit stress over area. If the electric field is zero giving the permittivity ε^{σ} of the material subjected to constant stress. Equation (3) describes the inverse piezoelectric effect. The membrane is subject to an external electric field which results in the total strain S. Equation (4) describes the direct piezoelectric effect. Mechanical stress applied to the body in combination with the piezoelectric constant and presence of electric field, results in the creation of a charge and a corresponding displacement D.

To coincide with the direction of polarization (3) and (4) can be rewritten as:

$$S_i = s_{ij}.\sigma_j + d_{mi}.E_m \tag{5}$$

$$D_m = \mathrm{d}_{mj}.\sigma_j + \varepsilon_{mk}.E_k \tag{6}$$

where: indexes i, j = 1,2,3,...,6 and m, k = 1,2,3 and represent the individual orientations in the coordinate system [1].

In cases where the material is polarized in direction *z*, the material is understood to be transversely isotropic. A material polarized in such a way simplifies equations (5) and (6). Further description requires the application into matrix form which a finite element software such as ANSYS can easily formulate.

4 Finite elements and meshing

In order to do the calculations for the piezoelectric study, it was necessary to define each element to calculate the mechanical and piezoelectric properties. Mechanical properties were defined by 8 node, PLANE183 elements. The element is suitable for axisymmetric problems. The Al-GaN layer was represented by PLANE223 elements. This is the electrically active layer. It consists of the same 2D 8 node element which defines 4 degrees of freedom at each node. The properties allow for solutions with large deformations caused by piezoelectricity. 2D elements PLANE183 and PLANE223 are represented in Fig. 2.

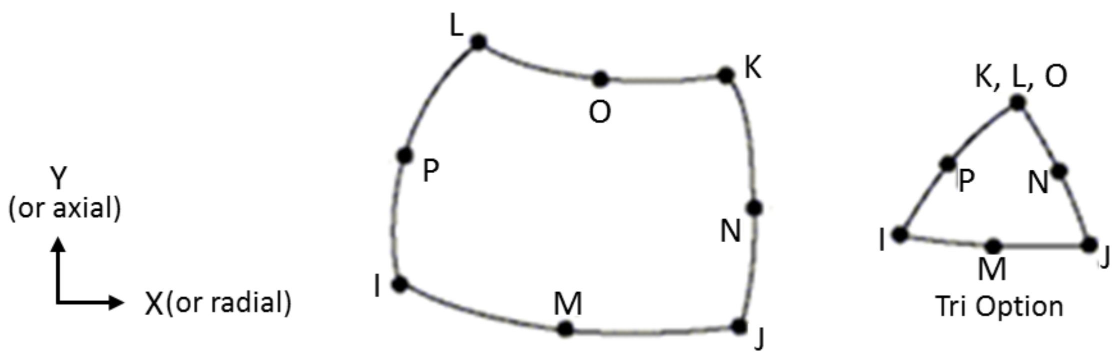

Fig. 2 Geometry of the 2-D elements PLANE183 and PLANE223 [3]

The finite element model was constructed as an axisymmetric problem with mapped meshing. To accommodate midplane effects, a minimum of three elements over any given thickness was used. The meshed model can be observed in fig. 3.

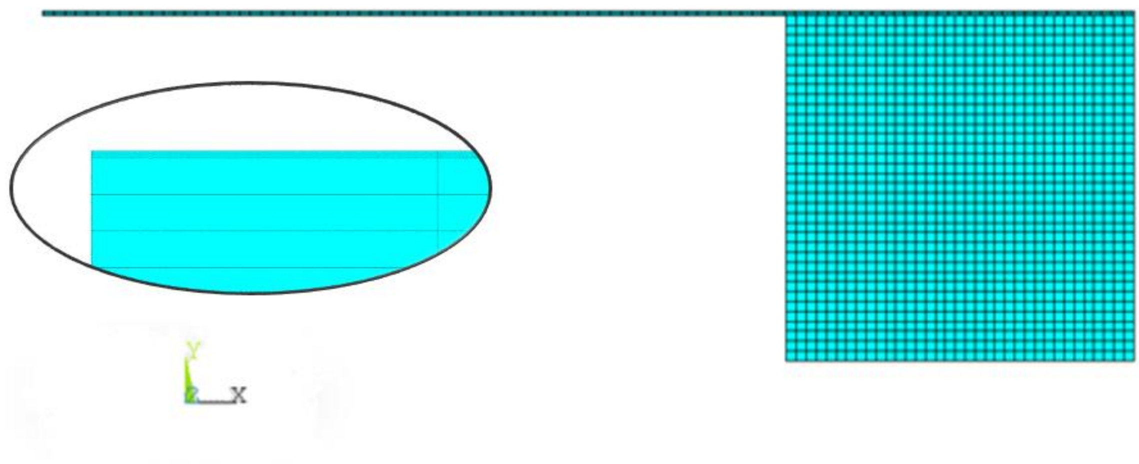

Fig. 3 A finite element mesh of the membrane model with edge detail (left bubble)

5 Comparing the numerical calculations

Investigating the effects of changing piezoelectric constants of Al-GaN and observing their behavior was based on the results of a numerical evaluation. Investigating the effect of the changes in the input constants e31, e33 and e15 of the piezoelectric matrix on the numerically calculated results was the primary focus of our study.

The variations of constants are based on findings in 10 different publications which have formulated these constants based on experimental evaluation. Their results can be seen in Tab.1.

Tab. 1 Input constants based on findings from various authors

no.	e31	e33	e15	Ref.
1	-0.58	1.55	-0.48	[5]
2	-0.6	1.446	-0.364	[6]
3	-0.6	1.46	-0.48	[7]
4	-0.38	1.26	-0.33	[8]
5	-0.82	2.1	-0.48	[9]
6	-0.33	0.7	0.29	[10]
7	-0.22	0.44	-0.22	[11]
8	-0.36	1	-0.3	[12]
9	-0.33	0.67	-0.37	[13]
10	-0.49	1	-0.33	[14]

The axisymmetric finite element model was built / performed / modelled in ANSYS Multiphysics. The loading and boundary conditions can be observed in fig.4. Using the coupling function, it was possible to calculate the electric charge. A pre-stress based on displacement is applied in the first load step to simulate the clamping of the membrane and it results in an in-plane stress of 40 MPa. The second load step applies pressure perpendicularly to the membrane itself at magnitudes of 1, 5, 10 and 20 kPa.

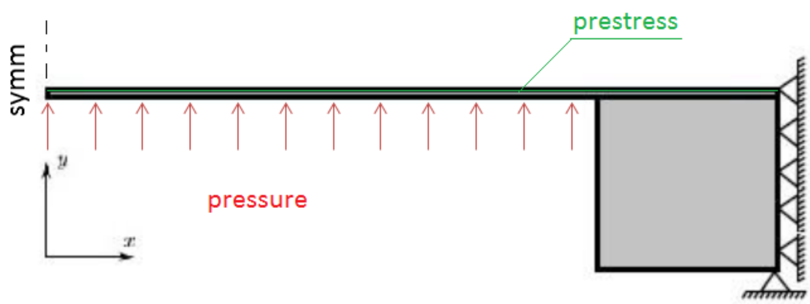

Fig. 4 Boundary and loading conditions in the model

6 Comparison of the results

Forty numerical simulations were performed utilizing the varying material constants of aluminum gallium nitride and loading conditions discussed in parts 4 and 5 of this article. Each set of material constants was numerically calculated for four loading conditions. The goal of each simulation was to determine the magnitude of the electrical charge. The results of all ten sets of material constants and their corresponding charges are displayed in tab. 2. Experimental data was also provided and can be seen at the end of tab. 2. Graphical representation of these results can be seen in fig. 5.

Tab. 2 Values obtained from experimental measurements and simulation results

Simulation data	p [kPa]	1	5	10	20
1	charge Q [pC]	2.2643	10.512	18.904	31.66
2		2.2487	10.439	18.773	31.439
3		2.257	10.477	18.843	31.556
4		1.6293	7.5648	13.604	22.784
5		3.1468	14.609	26.272	43.998
6		1.1802	5.4783	9.8523	16.499
7		0.77102	3.5788	6.4362	10.778
8		1.428	6.6296	11.923	19.967
9		1.1624	5.3957	9.7038	16.25
10		1.7291	8.0259	14.434	24.172
Experimental data		1.0388	5.6272	13.7016	25.2063

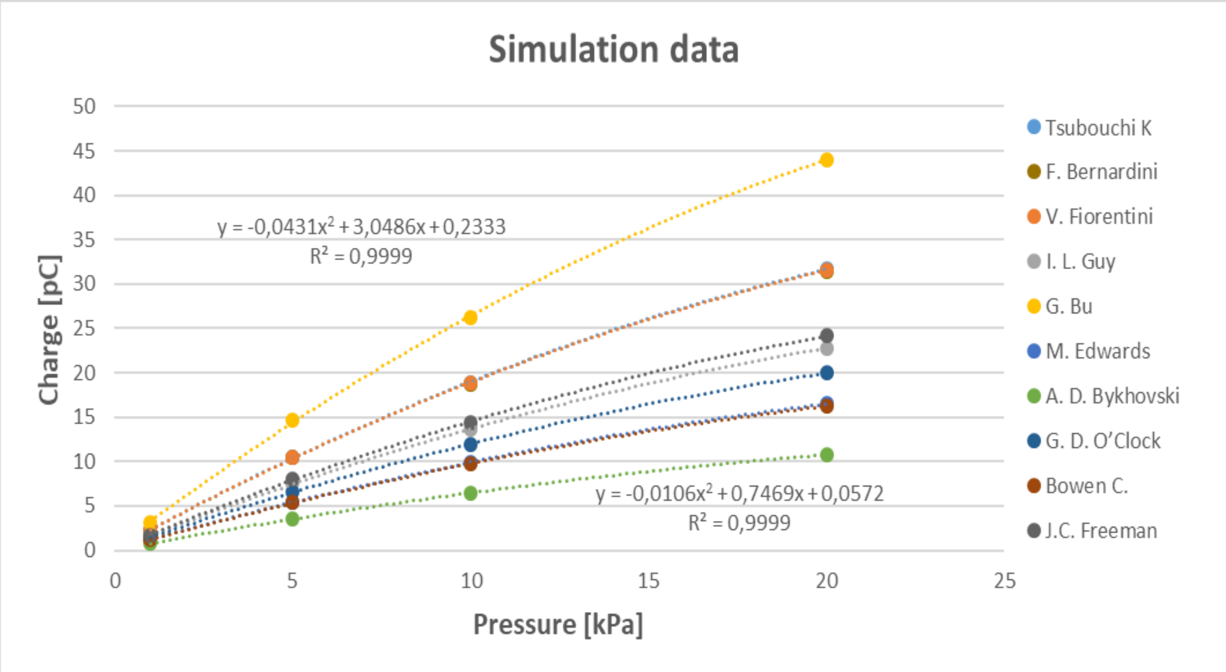

Fig. 5 Graphical representation of the simulation results

Fig. 5 above shows the magnitude of the charge which was numerically calculated by ANSYS Multiphysics for four different load cases. Between each point a 2nd degree polynomial regression curve was overlaid onto the data. To maintain clarity in the graph, only the edge curve equations are shown. Some statistically significant values, such as maximum charges, minimum charges, average values and variation coefficients, are clearly shown in Tab. 3.

Tab. 3 Statistical values of the results

Pressure [kPa]	Relative maxima of the charge value [pC]	Relative minima of the charge value [pC]	Average [pC]	Coefficients of variation [%]
1	3.1468	0.77102	1.783242	25.08406
5	14.609	3.5788	8.27101	116.1832
10	26.272	6.4362	14.87453	208.9278
20	43.998	10.778	24.9103	349.9209

The average values in tab. 3 where compared with experimental results [17] which can be seen in fig. 6.

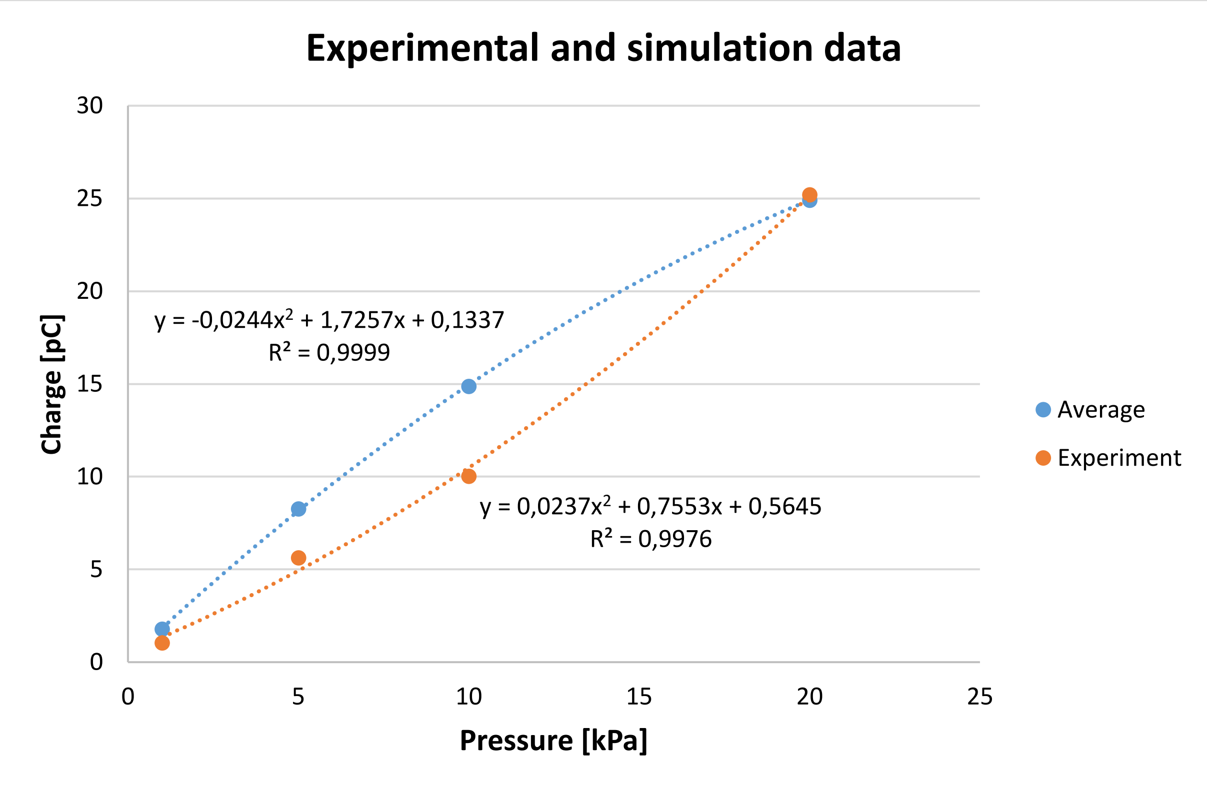

Fig. 6 Graphical representation of the average values (simulated) and experimental results

7 CONCLUSIONS

Based on the results of the numerical simulations performed in the ANSYS Multiphysics software and the comparison of these results with the results obtained by the experiment, several conclusions can be drawn. It is worth mentioning that with increased loading there is a deviation in the charge values. Based on the number of simulations and statistically calculated results, relatively large differences were observed between the individual results. Fig. 5 and Tab. 3 show variations between the individual sets of constants. There are several reasons for these differences. The most likely one is the fact that the piezoelectric material is transversally isotropic i.e. its properties are markedly different in one direction than in other directions. The statistically significant constant therefore is the e33 constant in the piezoelectric matrix. As supported by the data (Tab. 1), this constant has the largest differences between each set. These differences correlate with those shown in Fig. 5 of this article. These results are also significantly different from the results of the comparison of GaN material properties, as shown in [16].

It can be concluded that the accuracy of the determination of the maturity matrix constants for the GaN materials has minimal effect on the ultimate precision. However, in the case of the piezoelectric matrix for AlGaN material, even small inaccuracies will have a significant effect on the results.

At the same time, there is a relative correlation between the simulation results and the results obtained experimentally (Fig. 6) for load pressure values of 1 and 20 kPa. On the other hand, at the loading pressures of 5 and 10 kPa, the values do not show a good correlation with the obtained results. The lack of correlation could be due to several factors, such as the imperfections of the equipment used for experimental measurements, the inaccurate determination of the mechanical and electrical properties of the material under investigation, and, last but not least, the simplifications used in the membrane model. Given the results, it can also be stated that the membrane behaves like a rigid body at low load pressures. It is confirmed by the values that are relatively similar when the lowest and highest load pressures are applied. Verifying this assumption would require additional experimental measurements and subsequent repetition of numerical simulations.

ACKNOWLEDGMENTS

The authors would like to express their gratitude to the following grants for their financial support: VEGA 1/0712/14 and KEGA 060STU-4/2016.

REFERENCES

[1] M. Kermani, M. Moallem, R. Patel. Applied Vibration Suppresion Using Piezoelectric Materials, New York: Nova Science Publishers, Inc., **2008**, ISBN-13: 978-1-60021-896-5, 176 p.

[2] J. Erhart. Základy piezoelektřiny pro aplikace, Brno: Ústav automatizace a měřici techniky VUT v Brne, **2011**. URL: http://www.crr.vutbr.cz/system/files/brozura_06_1112.pdf

[3] Ansys Polyflow User’s Guide, https://www.sharcnet.ca/Software/Ansys/16.2.3/en-us/help/poly_pf/poly_pf.html

[4] A. Erturk, D. J. Inman. Piezoelectric energy harvesting. First edition. Wiley Publication, **2011**, 402 p., ISBN: 978-0-470-68254-8.

[5] K. Tsubouchi, N. Mikoshiba. Zero-Temperature-Coefficient SAW Devices on AlN Epitaxial Films. *IEEE Trans. Sonics Ultrason.* **1985** (32), No. 5, 634 – 644.

[6] F. Bernardini, V. Fiorentini, D. Vanderbilt. Spontaneous polarization and piezoelectric constants of III-V nitrides. *Phys. Rev. B* **1997** (56), No. 15-16, R10024(R)

[7] F. Bernardini, V. Fiorentini. First-principles calculation of the piezoelectric tensor d/sup to or from / of III-V nitrides. *Appl. Phys. Lett.* **2002** (80), 4145 - 4147

[8] I. L. Guy, S. Muensit, E. M. Goldys. Extensional piezoelectric coefficients of gallium nitride and aluminum nitride. *Appl. Phys. Lett.* **1999** (75), 4133 - 4135

[9] G. Bu, D. Ciplys, M. Shur, L.J. Schowalter, S. Schujman, R. Gaska, Surface acoustic waves in single crystal bulk aluminum nitride, *Appl. Phys. Lett. submitted* **2003**.

[10] M. Edwards. Material for Robus Gallium Nitride. Additional Report. Remperature Dependent Properties of GaN. University of Bath, **2009**, 1 – 7. URL: http://www.morganproject.eu/documents_public/Temp-Dependent%20Properties%20of%20GaN%20&%20Related%20Materials.pdf.

[11] A. D. Bykhovski, V. V. Kaminski, M. S. Shur, Q. C. Chen, and M. A. Khan, *Appl. Phys. Lett.* **1996** (68), 818.

[12] G. D. O’Clock, M. T. Duffy. Acoustic surface wave properties of epitaxially grown aluminum nitride and gallium nitride on sapphire. *Appl. Phys. Lett.* **1973** (23), No. 2, 55.

[13] C. Bowen, D. Allsopp, R. Stevens, P. Shields, W. Wang. Modelling and designing GaN piezoeolectric MEMS. In: *Second International Conference on Multi-Material Micro Manufacture*, Grenoble. **2006**.

[14] J.C. Freeman. Basic Equations for the Modeling of Gallium Nitride (GaN) High Electron Mobility Transistors. **2003**, *NASA/TM-2003-211983*.

[15] P. Staňák, J. Sládek, V. Sládek. Analysis of piezoelectric semiconducting solids by meshless method, *Journal of Mechanical Engineering - Strojnícky časopis* **2015** (65), No. 1, 77 – 92.

[16] T. Kováč, F. Horvát, M. Čekan, B. Hučko, M. Szarvas, J. Dzuba, G. Vanko. Numerical solution of aluminum galium nitride membrane in finite element analysis. *15th Conference on Applied Mathematics APLIMAT 2016 Proceedings*, Bratislava 2016, **2016**, 700 - 710.

[17] J. Dzuba, G. Vanko, O. Babchenko, T. Lalinský, F. Horvát, M. Szarvas, T. Kováč, B. Hučko. Strain induced response of AlGaN/GaN high electron mobility transistor located on cantilever and membrane. *ASDAM 2016 - Conference Proceedings, 11th International Conference on Advanced Semiconductor Devices and Microsystems,* art. no. 7805936, **2017**, 227 - 230.