Zlatan Kulenović^{*} Ivica Kuzmanić^{**} Igor Vujović^{***}

ISSN 0469-6255 (75-80)

BRODSKO STROJARSTVO

ABOUT A CRACK IN PIEZOCERAMIC ELEMENT OF ELECTROMECHANICAL DEVICE ON THE SHIP

O pukotini u piezokeramičkom elementu brodskog elektromehaničkog uređaja

UDK 534.843-8 Pregledni članak *Review*

Abstract

The future of navigation cannot be imagined without nanotechnology. It is increasingly implemented in electronic and computer components of every modern automatic system. In manufacturing of these components such as sensors, transducers, actuators and other electromechanical devices, piezoelectric materials have been and will be used. It is well known that various defects in material, such as dislocations, cracks and inclusions can adversely influence on the integrity and performance of such devices. Therefore, it is very important that the behaviours of these defects are analyzed under real electromechanical load. These defects can be observed on very small dimensions, at atomic level. This paper analyses a screw dislocation around finite crack in a hexagonal ceramic crystal subjected to antiplane mechanical and in-plane electrical loads. The linear piezoelectric theory, complex analytic functions and conformal mapping method are used, and the forces acting on a dislocation are determined. The numerical results are obtained in MatLab and they are presented in 2D and 3D graphs.

Key words: crack, dislocation, electromechanical load, piezoceramic element

Sažetak

Budućnost pomorstva nije moguće zamisliti bez nanotehnologije. Ona se sve više primjenjuje u elektroničkim i računalnim komponentama svakog suvremenog automatiziranog brodskog sustava. U proizvodnji takvih komponenata kao što su senzori, pretvornici, aktuatori i druge elektromehaničke naprave koriste se i koristit će se i piezoelektričkim materijalima. Poznato je da različiti defekti u takvim materijalima, poput dislokacija, pukotina i uključevina, mogu znatno utjecati na integritet i rad svake piezoelektrične komponente. Poradi toga vrlo je važno da se ponašanja takvih poremećaja analiziraju pod stvarnim elektromehaničkim opterećenjem. Ovi poremećaji mogu se zamijetiti na vrlo malim dimenzijama, na atomskoj razini. U ovom je radu analizirana dislokacija oko konačne pukotine u heksagonalnom keramičkom kristalu podvrgnutomu električnom opterećenju u ravnini i mehaničkom opterećenju u ortogonalnoj ravnini. Primjenom linearne piezoelektrične teorije, funkcija kompleksne varijable i metoda konformnog preslikavanja, određene su sile koje djeluju na dislokaciju. Numerički rezultati dobiveni su u MatLabu i prikazani su 2D i 3D-grafovima.

Ključne riječi: pukotina, dislokacija, elektromehaničko opterećenje, piezokeramički element

1. Introduction

Uvod

Nanotechnology is the set of activities in design and construction on the nanometre scale structures. Difficulty with nanotechnology is in the fact that characteristics of some material depend not only on molecules (atoms), but also on the order of construction units. Many problems in design, manufacturing and development, come from the reduction in size of modern devices. That kind of problems becomes even greater if one deals with devices on nano-scale. In recent years there has been a resurgence of interest in piezoelectricity, motivated by

^{*} dr. sc. Zlatan Kulenović, red. prof., Sveučilište u Splitu, Zrinskofrankopanska 38, 21000 Split

^{**} mr. sc. lvica Kuzmanić, prof. v. šk., Sveučilište u Splitu, Zrinskofrankopanska 38, 21000 Split

^{***} mr. sc. Igor Vujović, pred., Sveučilište u Splitu, Zrinskofrankopanska 38, 21000 Split

advances in nano-structures technology [1-6]. The fracture mechanics studies on piezoelectric materials were reported actively during the last decade [8-16]. It is well known that piezoelectric materials produce an electric field when stressed and deform when subjected to an electric field. Because of that, the piezoelectric materials have been used in various applications of modern electromechanical devices such as transducers, sensors, actuators, etc. Various defects such as dislocations, cracks, cavities and inclusions may be produced in piezoelectric material during their manufacturing process [3, 4, 7, 8, 9]. These defects can adversely influence on the integrity and performance of such piezoelectric devices. Therefore, it is very important that the behaviours of these defects should be analyzed and studied in the real electrical and mechanical load fields.

In this article, it was considered that the nano-scale devices consisted of piezoelectric material are used as element of pressure sensor in ship's loading process in the port. We analysed a simple continuum model of a single screw dislocation around finite crack in a hexagonal piezoelectric crystal subjected to antiplane mechanical and in-plane electrical loads. The dislocation has a line force and a line charge along its core. The linear piezoelectric theory, complex analytic functions and conformal mapping method are used, and the forces acting on a dislocation are determined. The numerical results are obtained in MatLab and they are presented in 2D and 3D graphs.

2. Formulation and solution to the problem

Formulacija i rješenje problema

The geometry of considered problem is shown in Figure 1. Suppose that a piezoelectric material is transversely isotropic, containing a charged screw dislocation around a finite crack of length 2a. A set of Cartesian coordinates (x, y, z) is attached at the center of the crack. The piezoelectric material has a hexagonal symmetry with an isotropic basal plane of xy-plane and a poling direction of z-axes. The crack is situated along the plane y = 0. A piezoelectric medium are subjected to farfield antiplane mechanical and in plane electrical loads. In this configuration, the piezoelectric boundary value problem [8, 9] is simplified considerably because only the out-of-plane displacement and in-plane electric fields exist. The constitutive relations for the piezoelectric material are [3, 15]:

$$\tau_{zi} = c_{44} \gamma_{zi} - e_{15} E_i \tag{1}$$

$$D_i = e_{15} \gamma_{zi} + \epsilon_{11} E_i \tag{2}$$

where $\tau_{zi}(x, y)$, $\gamma_{zi}(x, y)$, $E_i(x, y)$, and $D_i(x, y)$ (i = x, y) are the components of the shear

stress, shear strain, electric field, and electric displacement vectors, respectively. Also, c_{44} , e_{15} and \in_{11} are the elastic modulus, piezoelectric constant, and dielectric permittivity of piezoelectric material, respectively.



Figure 1. Geometry of the problem *Slika 1. Geometrija problema*

The electric field can be expressed as:

$$E_i = -\frac{\partial \phi}{\partial i} \quad (i = x, y)$$
⁽³⁾

where $\phi(x, y)$ is the electric potential.

Taking into consideration that the boundary conditions are: a) on the surfaces of the crack (|x| < a, y = 0): $\tau_{zy} = 0$, $D_y = 0$; b) in the far-field (x, $y = \pm \infty$): $\tau_{zy} = \tau_{\infty}$, $\gamma_{zy} = \gamma_{\infty}$, $D_y = D_{\infty}$, $E_y = E_{\infty}$, where τ_{∞} , γ_{∞} , D_{∞} , and E_{∞} are the uniform quantities, equations (1), (2) and (3), give the governing equations which can be expressed as follows:

$$\nabla^2 w = 0, \quad \nabla^2 \phi = 0 \tag{4}$$

The solution can be found by letting *w* and ϕ be the complex analytic functions such that $w = W(Z), \phi = \Phi(Z)$, where W and Φ are the

complex potentials for displacement and electric potential, respectively; Z = x + iy is a complex variable. Due to complex variable solution, a crack on the *x*-axis is constructed using the following mapping function [7, 10]:

$$\xi = \frac{1}{a} \left[Z + \sqrt{Z^2 - a^2} \right] \tag{5}$$

which transforms the circle $|\xi| = 1$ in the ξ -plane onto a finite crack of length 2a along the real axis in the z-plane.

In this case a screw dislocations subjected to a line force and a line charge, and the potential functions $W(\xi)$ and $\Phi(\xi)$ have three terms, respectively: the first corresponds to the line force or charge, the second to the screw dislocation, the third to the uniform external loads. The strain, electric field, stress, and electric

displacement can be expressed by these complex potentials, and the forces acting on a screw dislocation are given with [11, 15]:

$$F_{x} = b_{z}\tau_{zy}^{T} + \Delta\phi D_{y}^{T} + p_{z}^{S}\gamma_{zx}^{T} + q_{z}^{S}E_{x}^{T}$$
(6)

$$F_{y} = -b_{z}\tau_{zx}^{T} - \Delta\phi D_{x}^{T} + p_{z}^{S}\gamma_{zy}^{T} + q_{z}^{S}E_{y}^{T}$$
(7)

where b_z , $\Delta \phi$, p_z , and q_z are the Burgers vector, electric potential jump, line force, and line charge, respectively. Superscripts S and T represent internal domain in which a screw dislocation exists and external domain in which a crack subjected to the mechanical and electrical loads exists, respectively.

After solving this symmetric problem, the equations which presented the forces on a screw dislocation located in arbitrary position around a crack are obtained as follows:

$$F_{x} = -\left[b_{z}\left(c_{44}A_{1} + e_{15}B_{1}\right) + \Delta\phi\left(e_{15}A_{1} - \epsilon_{11}B_{1}\right)\right] \cdot \left\{-\frac{1}{\sqrt{r_{1}r_{2}}}\sin\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \frac{r}{2r_{1}r_{2}}\right] \\ \left[\sin(\theta - \theta_{1} - \theta_{2}) + \cos\theta \tan\left(\frac{\theta_{1} + \theta_{2}}{2}\right)\right] \right\} - \left[b_{z}\left(c_{44}A_{2} + e_{15}B_{2}\right) + \Delta\phi\left(e_{15}A_{2} - \epsilon_{11}B_{2}\right)\right] \cdot \\ \cdot \left\{\frac{m}{\sqrt{r_{1}r_{2}}}\cos\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \frac{r}{2r_{1}r_{2}}\left[\cos(\theta - \theta_{1} - \theta_{2}) + \cos\theta\right] \right\} - \frac{2}{a}\left[b_{z}\left(c_{44}A_{3} + e_{15}B_{3}\right) + \\ + \Delta\phi\left(e_{15}A_{3} - \epsilon_{11}B_{3}\right)\right] \cdot \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left(p_{z}A_{1} - q_{z}B_{1}\right)\left\{\frac{1}{\sqrt{r_{1}r_{2}}}\cos\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \\ - \frac{r}{2r_{1}r_{2}}\left[\cos(\theta - \theta_{1} - \theta_{2}) - \cos\theta\right]\right\} - \left(p_{z}A_{2} - q_{z}B_{2}\right)\left\{-\frac{m}{\sqrt{r_{1}r_{2}}}\sin\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \frac{r}{2r_{1}r_{2}}\right] \\ \cdot \left[\sin(\theta - \theta_{1} - \theta_{2}) - \cos\theta\tan\left(\frac{\theta_{1} + \theta_{2}}{2}\right)\right]\right\} - \frac{2}{a}\left(p_{z}A_{3} - q_{z}B_{3}\right)\left\{\frac{r}{\sqrt{r_{1}r_{2}}}\sin\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] \right]$$
(8)

$$F_{y} = -\left[b_{z}\left(c_{44}A_{1} + e_{15}B_{1}\right) + \Delta\phi\left(e_{15}A_{1} - \epsilon_{11}B_{1}\right)\right] \cdot \left\{\frac{1}{\sqrt{r_{1}r_{2}}}\cos\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \frac{r}{2r_{1}r_{2}} \cdot \left[\cos(\theta - \theta_{1} - \theta_{2}) + \cos\theta\right]\right\} - \left[b_{z}\left(c_{44}A_{2} + e_{15}B_{2}\right) + \Delta\phi\left(e_{15}A_{2} - \epsilon_{11}B_{2}\right)\right] \cdot \left\{-\frac{m}{\sqrt{r_{1}r_{2}}}\sin\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \frac{r}{2r_{1}r_{2}}\left[\sin(\theta - \theta_{1} - \theta_{2}) - \cos\theta\tan\left(\frac{\theta_{1} + \theta_{2}}{2}\right)\right]\right\} + \frac{2}{a} \cdot \left[b_{z}\left(c_{44}A_{3} + e_{15}B_{3}\right) + \Delta\phi\left(e_{15}A_{3} - \epsilon_{11}B_{3}\right)\right] \cdot \left[\frac{r}{\sqrt{r_{1}r_{2}}}\sin\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] - \left(p_{z}A_{1} - q_{z}B_{1}\right) \cdot \left\{-\frac{1}{\sqrt{r_{1}r_{2}}}\sin\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \frac{r}{2r_{1}r_{2}}\left[\sin(\theta - \theta_{1} - \theta_{2}) + \cos\theta\tan\left(\frac{\theta_{1} + \theta_{2}}{2}\right)\right]\right\} - \left(p_{z}A_{2} - q_{z}B_{2}\right) \cdot \left\{\frac{m}{\sqrt{r_{1}r_{2}}}\cos\left(\frac{\theta_{1} + \theta_{2}}{2}\right) - \frac{r}{2r_{1}r_{2}} \cdot \left[\cos(\theta - \theta_{1} - \theta_{2}) + \cos\theta\right]\right\} - \frac{2}{a}\left(p_{z}A_{3} - q_{z}B_{3}\right) \cdot \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right]\right\} - \left(p_{z}A_{3} - q_{z}B_{3}\right) \cdot \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right]\right\} - \left(p_{z}A_{3} - q_{z}B_{3}\right) \cdot \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right) + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right) + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right)\right] + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right) + \left[\frac{r}{\sqrt{r_{1}r_{2}}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right) + \left[\frac{r}{\sqrt{r_{1}r_{2}}\cos\left(\theta - \frac{\theta_{1} + \theta_{2}}{2}\right) + \left[\frac{r}{\sqrt{r$$

The equations (8) and (9) are translated into MatLab simulation code in m-type script. For the numerical analysis, basic values of piezoceramic material parameters are:

 $b_z = 1 \cdot 10^{-9}$ (m) - Burgers vector; $\Delta \phi = 1$ (V) - electrical potential jump; $p_z = 10$ (N/m) - line force; $q_z = 1 \cdot 10^{-8}$ (C/m) - line charge; $c_{44} = 2,3 \cdot 10^{10}$ (N/m²) - elastic modulus; $e_{15} = 17$ (C/m²) - piezoelectric constant; $\in_{11} = 150,4 \cdot 10^{-10}$ (C/Vm) - dielectric permittivity;

$$\begin{aligned} A_1 &= \frac{-\epsilon_{11} p_z + e_{15} q_z}{2\pi (c_{44} \epsilon_{11} + e_{15}^2)}; \ A_2 &= -\frac{b_z}{2\pi}, \ A_3 &= -\frac{a}{2} \gamma_{\infty}, \\ B_1 &= -\frac{e_{15} p_z + c_{44} q_z}{2\pi (c_{44} \epsilon_{11} + e_{15}^2)}, \ B_2 &= -\frac{\Delta \phi}{2\pi}, \quad B_3 &= \frac{a}{2} E_{\infty} \end{aligned}$$

real constants; $\gamma_{\infty} = 9.5 \cdot 10^{-5}$ - shear strain; $E_{\infty} = 2 \cdot 10^5$ (V/m) - electric field; a = 1 $\cdot 10^{-2}$ (m) for the Fig. 2., and a = 1 $\cdot 10^{-8}$ (m) for the Fig. 3.

We took three a/r ratios: 0,5 , 1 and 2, for both cases (three curves in every diagram).

3. Results

Rezultati

The results are obtained in Mat Lab 5.3 on PC Windows's platform and presented in Fig. 2 - 6. Mat Lab

uses matrix formats even for scalar values. In some calculations that fact was making forces' expression difficult to apply. Modifications are used in order to obtain wanted results and did not affect the correctness of the final results. Without modifications it would not be possible to plot diagrams presented in the figures. Both micro and nano-structures were simulated. Results of simulation on microstructures are shown in Figure 2. Results of simulation at nano-scala are shown in Figure 3. The obtained results for nano-structures are better seen if presented as zoomed part of diagrams (see Figure 3a. and 3b.)





b)

Figure 2. Numerical results of the Mat Lab simulation for microstructures:
a) in x-direction, b) in y-direction
Slika 2. Numerički rezultati simulacije mikrostruktura u MatLabu:
a) u smjeru x-osi, b) u smjeru y-osi





Figure 3. Specific force vs. angle – simulation results on nanostructures:

a) in x-direction (zoom x-axe: 0.01-1.58; zoom y-axe: 0.5-



Slika 3. Specifična sila u ovisnosti o kutu - simulacijski rezultati na nanostrukturama:

a) u smjeru x-osi (povećani dio po x-osi: 0,01-1,58; po yosi: 0,5-2,9), b) u smjeru y-osi (povećani dio po x-osi 0,02-1,56; po y-osi: 0,1-1,56)



Figure 4. Specific forces and line charges in 3D presentation Slika 4. Specifične sile i linijski naboji predstavljeni u 3D



Figure 5. 3D graph of force F_x , line charge q_z and angle θ Slika 5. 3D graf ovisnosti sile F_x , linijskog naboja q_z i kuta θ



Figure 6. 3D graph of force F_y , line charge q_z and angle θ Slika 6. 3D graf ovisnosti sile F_y , linijskog naboja q_z i kuta θ

Results show that force F_x tends to be negative at small dislocation angels. When angle increases, force F_x rises linearly. However, force F_y is of non-linear character (see Figure 2). The greatest gradient is observed in case r = a, for force in both x and y-direction (see Figure 3). Force F_y tends asymptotically to infinity

when dislocation angle θ is close to 0. So, it is possible that lower angles in y-direction lead to break of material's structure. Furthermore, lower angles of dislocation produce higher force in x-direction, which leads to break the material, because the force tends to infinity. This is possible in nano-structures, one deal with atomic-size structures and nuclear forces takes over any other force. 3D representations of any combination (F, q, θ) are presented as arcs (see Figures 4, 5, 6).

4. Conclusion

Zaključak

An engineering revolution is currently underway in that devices at the nanometre scale are fabricated. In recent years there has been a resurgence of interest in piezoelectricity, motivated by advances in nanostructures technology. Piezoelectric materials (i.e. piezoceramic) are very popular in integrity calculations, because of their wide usage, for example in modern ship's automatic system. If nano-sale crack appears in nowadays sensors, it will not have significant impact on the performance of the device before spread. However, nano-scale crack in nano-device will totally destroy the structure of the device, not to mention its function.

In this work, it was considered that the nano-scale devices consisted of piezoelectric material were used as element of pressure sensor in ship's loading process in the port. We analysed a simple continuum model of a single screw dislocation around finite crack in a hexagonal ceramic crystal subjected to mechanical and electrical load. The dislocation has a line force and a line charge along its core. The linear piezoelectric theory, complex analytic functions and conformal mapping method are used, and the forces acting on a dislocation are determined by Mat Lab simulation. There is much room left for discussion, because of unity between macro world and nanoworld. The forces have been increased by 9000 times in x-direction and 8570 in y-direction simple by entering nano-scale dimensions.

The problem considered is symmetric. However, antisymmetric problem and different shape of the crack are also analyzed in the world. Further research should include more realistic details of charge and force. For better numerical interpretation, scientists will need to perform a series of expensive fundamental experiments.

References

Literatura

- P. W. Atkins, *Molecular quantum mechanics*, Oxford University Press, Oxford, 1997.
- [2] M. A. Reed, Molecular-scale electronics, Proceedings of the IEEE, 87 (2001), pp. 652-658.
- [3] D. A. Belincourt, D. R. Curran, H. Jaffe, *Piezoelectric* and piezomagnetic materials and their function in transducers, Academic press, New York, 1984.
- [4] I.Kuzmanić, R. Vlašić, I. Vujović, *Materials in electrical engineering (in Croatian)*, Split College of Maritime Studies, Split, 2001.
- [5] D. G. Gordon, et all, Overview of nanoelectronic devices, MITRE, McLean, 1997.
- [6] I. Vujović, I. Kuzmanić, Z. Kulenović, New Ceramic Pressure Sensors, Proc. of 46th International Symposium ELMAR-2004, Zadar 2004, pp. 502-506.
- [7] J. P. Hirth, I. Lothe, *Theory of dislocations*, John Wiley and Sons, New York, 1982.
- [8] H. A. Sossa, On the fracture mechanics of piezoelectric solids, Int. J. Solids Struct. 29 (1992), 2613-2622.
- [9] Z. Suo, C. M. Kuo, D. M. Barnett, J. R. Willis, Fracture mechanics for piezoelectric ceramics, J. Mech. Phys. Solids, 40 (1992), 739-765.
- [10] W. F. Deeg, The analysis of dislocation, crack, and inclusion problems in piezoelectric solids, Ph. D. thesis, Stanford University, Stanford 1980, USA.
- [11] J. H. Kwon, K. Y. Lee, Electromechanical Effects of a Screw Dislocation Around a Finite Crack in a Piezoelectric Material, J. Appl. Mech., 69 (2002), pp. 55-62.
- [12] T. Y. Zhang, J. C. Li, Image forces and shielding effects of a screw dislocation near a finite-length crack, Mater. Sci. Eng. 142(1991), pp. 35-39.
- [13] Y. E. Pak, Crack extension force in a piezoelectric medium, J. Appl. Mech., 57 (1990), pp. 647-653.
- [14] W. Q. Chen, T. Shioya, H. J. Ding, An antisymetric problem of a penny-shaped crack in a piezoelectric medium, Arch. Appl. Mech. 71(2001), pp. 63-73.
- [15] I. Vujović, Z. Kulenović, I. Kuzmanić, Some numerical results on screw dislocation around finite crack in a piezoelectric material, Proc. of 7th International Research/Expert Conference TMT 2003, Loret de Mar 2003, Spain, pp. 749-752.
- [16] I. Vujović, Z. Kulenović, I. Kuzmanić, Numerical example of interaction of two dissimilar piezoelectric materials, 8th International Research/Expert Conference TMT 2004, Neum 2004, B&H, pp. 227-230.

Rukopis primljen: 26.11.2004.