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CONTRIBUTION TO SAFETY FACTOR ANALYSIS IN PIEZOELECTRIC CRACK PROBLEM

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ABSTRACT
Problem of defect such as dislocations, crack, cavities, and inhomogeneities, which may be produced in piezoelectric materials during their manufacturing process, can arise when the material is subjected to mechanical and electrical loads. Stress concentrations due to these defects can give rise to critical crack growth and subsequent mechanical failure. In fracture mechanics a crack is an absence of bonds between two neighboring atom layers. Stress distribution near the crack tip depends on the form of the fracture surface formation. In this article, stress intensity factor or safety factor has been calculated and plotted vs. stress for mode I of PZT-4 ceramic (piezoelectric material) as part of micro-sensors and nanorobots.
Keywords: Stress intensity factor, PZT ceramic, crack, dislocation, micro-sensor, nanorobot

1. INTRODUCTION
Piezoelectric materials play important role in different sensing devices, such as: electromechanical transducers, delay lines, medical, denotation and sonar equipment, microelectronic components, hydrophones, microphones, phonographs, gas igniters, strain gauges, vibration sensors, micro-pumps and positioners, smart structures [1]. Tactile sensor based on piezoelectric resonance is used in robotics [2]. Designs of integrated distributed sensor and active distributed vibration actuator for elastic or flexible robot structures are presented in [3]. Utilization of PZT as an actuator for micro-mobile robot is elaborated in [4]. In marine, piezoelectric materials are used for different sensing devices. Sometimes, some of devices can play a vital role in navigating dangerous seas. If device fails, lives can be in danger. Material damage is also possible. Modern trends show research interest for applications in NEMS and nanorobots also.
This article presents results on stress intensity factor (safety factor) for microstructure produced from piezoelectric material (PZT ceramic), which is possibly used in micro-sensors and NEMS.

2. PROBLEM FORMULATION AND SOLUTION
Stress intensity factor describes mathematical stress and deformation distribution in the top of the crack. Physically, stress intensity factor is the measure the intensity of rise of stress in observed space. In fracture mechanics a crack is an absence of bonds between two neighboring atom layers. Stress distribution near the crack tip depends on the form of the fracture surface formation. Figure 1 shows mode I of deformation geometry. Mode I is defined by separation of the fracture surface symmetrically in regard to the primary crack plane (“crack opening”): $u = u(r, \varphi)$, $v = v(r, \varphi)$, $w = 0$.

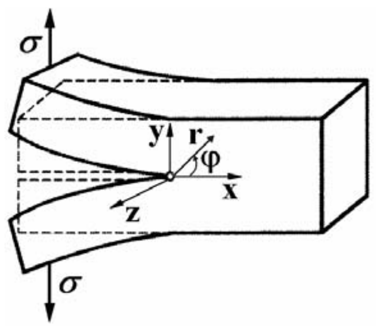

Figure 1. Illustration of mode I

In polar-cylindrical coordinate system (r, φ, z), general expressions for components of the tensor of mechanical stress state are written [5]:

$$\sigma_{i,j}(r,\varphi,z) = \frac{1}{\sqrt{2\cdot r\cdot \pi}}\cdot\left[K_I(z)\sigma_{i,j}^{I}(\varphi) + K_{II}(z)\sigma_{i,j}^{II}(\varphi) + K_{III}(z)\sigma_{i,j}^{III}(\varphi)\right] \quad (1)$$

where K_I, K_{II}, K_{III} are stress intensity factors for modes I, II and III.
The stress intensity factor is a measure of the stress magnitude in the neighborhood of the crack tip. It is defined for a known stress state and geometry. For a fictitious infinite body with a central crack of length 2*a* loaded along three perpendicular directions, K_I is expressed as [5, 6, 7]:

$$K_I = \left(\lim_{x\to a^+}\sqrt{2\pi(x-a)}\right)\cdot \sigma_y \Big|_{y=0}^{x} \quad (2)$$

Using Westergaard's [8] solution and complex variable $Z = x + iy$, K_I is given with:

$$K_I = \sigma\sqrt{\pi\cdot a} \quad (3)$$

The solution of mechanical stress and strain distribution problem in a stressed piezoelectric material can be found if for vector of electric displacement (D_i), vector of electric field (E_k), tensor of mechanical stress (σ_{ij}) and tensor of strain (ε_{kl}), relationship can be established. In curvilinear system of coordinates, the governing linear piezoelectric equations, in the absence of volume forces and free electric charges, may be written as:

$$D_i = e_{ikl}\varepsilon_{kl} + d_{ik}^{\varepsilon}E_k \quad (4)$$

$$\sigma_{ij} = c_{ijkl}^{E}\varepsilon_{kl} - e_{kij}E_k \quad (5)$$

where indexes: i, j, k, and l, take values 1, 2, and 3. In polar-cylindrical system of coordinates (r, φ, z), equations (4) and (5) changes form for hexagonal crystal system into:

$$\begin{bmatrix} D_r \\ D_\varphi \\ D_z \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix}\cdot\begin{bmatrix} \varepsilon_r \\ \varepsilon_\varphi \\ \varepsilon_z \\ 2\varepsilon_{\varphi z} \\ 2\varepsilon_{rz} \\ 2\varepsilon_{r\varphi} \end{bmatrix} + \begin{bmatrix} d_{11}^{\varepsilon} & 0 & 0 \\ 0 & d_{11}^{\varepsilon} & 0 \\ 0 & 0 & d_{33}^{\varepsilon} \end{bmatrix}\cdot\begin{bmatrix} E_r \\ E_\varphi \\ E_z \end{bmatrix} \quad (6)$$

$$\begin{bmatrix}\sigma_r\\ \sigma_\varphi\\ \sigma_z\\ \tau_{\varphi z}\\ \tau_{rz}\\ \tau_{r\varphi}\end{bmatrix}=\begin{bmatrix}c_{11}^E & c_{12}^E & c_{13}^E & 0 & 0 & 0\\ c_{12}^E & c_{11}^E & c_{11}^E & 0 & 0 & 0\\ c_{13}^E & c_{13}^E & c_{33}^E & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44}^E & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44}^E & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{c_{11}^E-c_{12}^E}{2}\end{bmatrix}\cdot\begin{bmatrix}\varepsilon_r\\ \varepsilon_\varphi\\ \varepsilon_z\\ 2\varepsilon_{\varphi z}\\ 2\varepsilon_{rz}\\ 2\varepsilon_{r\varphi}\end{bmatrix}-\begin{bmatrix}0 & 0 & e_{31}\\ 0 & 0 & e_{31}\\ 0 & 0 & e_{33}\\ 0 & e_{15} & 0\\ e_{15} & 0 & 0\\ 0 & 0 & 0\end{bmatrix}\cdot\begin{bmatrix}E_r\\ E_\varphi\\ E_z\end{bmatrix} \tag{7}$$

For boundary conditions on the crack surface with normal in circular direction, when $\varphi = \pm\,\pi$, it is assumed that: $D_\varphi = 0$ (in the spots of crack surface), $\sigma_\varphi = 0$, $\tau_{\varphi r} = 0$ (in radial direction), $\tau_{\varphi z} = 0$ (in axial direction).
In this work, stress intensity factor is simulated for mode I. Solution of derived equations is performed using analytical Laurent's series functions of complex variable, have a form, i.e [6, 9]:

$$D_z = \frac{2e_{31}}{c_{11}+c_{12}}\sum_{n=0}^{\infty} n r^{\frac{n}{2}-1} A_n \cos\left(\left(\frac{n}{2}-1\right)\cdot\varphi\right) \tag{8}$$

$$\sigma_r = \frac{1}{2}\sum_{n=0}^{\infty} n r^{\frac{n}{2}-1}\left[\left(3-\frac{n}{2}\right)A_n \cos\left(\left(\frac{n}{2}-1\right)\cdot\varphi\right)-B_n\cos\left(\left(\frac{n}{2}+1\right)\cdot\varphi\right)\right] \tag{9}$$

where some of the series members can be obtained as: $A_1 = \dfrac{-d_{11}p_z + e_{15}q_z}{2\pi\left(c_{44}\varepsilon_{11}+e_{15}^2\right)}$, $A_2 = -\dfrac{b_z}{2\pi}$,

$B_1 = -\dfrac{d_{11}p_z + c_{44}q_z}{2\pi\left(c_{44}d_{11}+e_{15}^2\right)}$, $B_2 = -\dfrac{\Delta\varphi}{2\pi}$.

Values of some parameters are: $a = 10^{-2}$ [m], Burgers vector $b_z = 10^{-9}$ [m], dielectric permittivity $d_{11} = 150\cdot 10^{-10}\left[\dfrac{C}{Vm}\right]$, line force $p_z = 10\left[\dfrac{N}{m}\right]$, line charge $q_z = 10^{-8}\left[\dfrac{C}{m}\right]$, matrix of elastic constants, piezoconstants and dielectric constants tensor are respectively:

$$\left[C_{ij}^E\right]=\begin{bmatrix}13{,}9 & 7{,}78 & 7{,}43 & 0 & 0 & 0\\ 7{,}78 & 13{,}9 & 7{,}43 & 0 & 0 & 0\\ 7{,}43 & 7{,}43 & 11{,}5 & 0 & 0 & 0\\ 0 & 0 & 0 & 2{,}56 & 0 & 0\\ 0 & 0 & 0 & 0 & 2{,}56 & 0\\ 0 & 0 & 0 & 0 & 0 & 3{,}06\end{bmatrix}\cdot 10^{10}\left[\frac{N}{m^2}\right],$$

$$\left[e_{ij}\right]=\begin{bmatrix}0 & 0 & 0 & 0 & 12{,}7 & 0\\ 0 & 0 & 0 & 12{,}7 & 0 & 0\\ -5{,}2 & -5{,}2 & 15{,}1 & 0 & 0 & 0\end{bmatrix}\left[\frac{C}{m^2}\right] \text{ and } \left[d_{ij}^{\varepsilon}\right]=\begin{bmatrix}6{,}46 & 0 & 0\\ 0 & 6{,}46 & 0\\ 0 & 0 & 5{,}62\end{bmatrix}\cdot 10^{-9}\left[\frac{F}{m}\right].$$

3. RESULTS

Numerical calculations and simulation is performed on PC in MatLab program package. Results of the calculations for the safety factor of the PZT-4 ceramic material are shown in Figure 2. Ratios *a/r* are taken from 0.2 to 3 with 0.01 step. The result is the surface of safety factors for stress and angle. Similar results (for different piezoelectric materials) can be obtained by introducing different elastic, piezoelectric and dielectric constants.

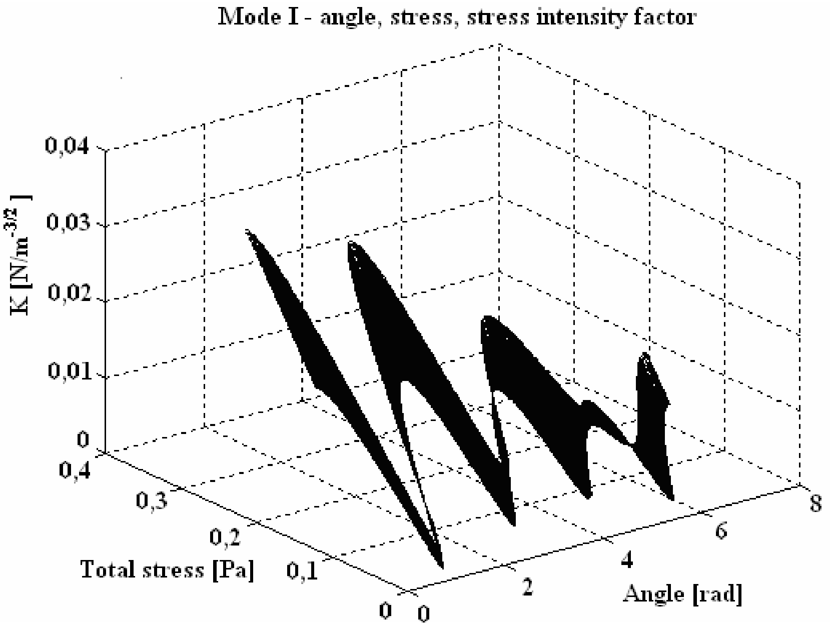

Figure 2. PZT-4 ceramic's simulation results - total stress and stress intensity factor for r = 0,2a to 3a

If someone wants to perform calculations in different scale (mini, micro, nano), only desired values of the geometry properties have to be changed. The results presented are obtained for microstructures.

4. CONCLUSIONS

The problem is solved by LEFM, because plastic area around the crack is too small to influence the final conclusions, which is supported by most teams dealing with this problems and references. From the obtained results, one can conclude that the existence of a crack in a stressed piezoelectric material leads to a stress redistribution and concentration, and the tensors of mechanical and piezoelectric stress at the crack tip become infinitely large. This "point of stress singularity" occurs in the most sensitive point to fracture.

In cases of NEMS, additional problem is limited usage of LEFM, because plastic area around crack cannot be considered to small. That presents additional complexity in nanotechnology and it is broad area of future researches.

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