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ON SCREW DISLOCATION NEAR A CRACK IN PZT MATERIAL UNDER ELECTROMECHANICAL LOAD

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ABSTRACT
The piezoelectric materials have been widely used in modern electromechanical devices and engine systems. It is well known that various effects in material, such as dislocations, cracks and inclusions can adversely influence the integrity and performance of such devices/systems. Therefore, it is very important that the behaviors of these defects are analyzed under real electromechanical load. In this work is analyzed a simple continuum model of a single screw dislocation near a finite crack in a hexagonal piezoelectric crystal subjected to electromechanical load. 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 for piezoelectric PZT ceramic material are obtained in MatLab and they are presented in 2D and 3D graphs.
Key words: screw dislocation, crack, force, PZT ceramic material

1. INTRODUCTION
Piezoelectric materials produce an electric field when stressed and deform when subjected to an electric field. Such an intrinsic coupling of course has attracted wide industrial applications of piezoelectric materials in mechanical engineering, shipbuilding, marine engineering, electronic, etc. Typical examples include electromechanical transducers, delay lines, denotation devices, sonar equipment, microelectronic components, dynamic strain gages, vibration sensors, and the newly emerging smart (adaptive) structures. The defects, such as dislocations, cracks, cavities, and inhomogeneities may be produced in piezoelectric materials during their manufacturing process. When the materials are subjected to mechanical and electrical loads, stress concentrations due to these defects can give rise to critical crack growth and subsequent mechanical failure. These problems are pointed out at nano-scale dimensions. Therefore, it is very important that the behaviors of these defects are analyzed under real electromechanical load. In this work is analyzed a continuum model of a single screw dislocation near a finite crack in piezoelectric material and the forces acting on a dislocation are determined.

2. MATEMATICAL MODEL AND SOLUTION
Suppose that a piezoelectric material is transversely isotropic and containing a charged screw dislocation around a finite crack of length $2a$ as shown in Figure 1. 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. The piezoelectric material is subjected to far field antiplane mechanical and in plane electric loads. In this configuration, the piezoelectric boundary value problem is simplified considerably because only the out-of-plane displacement and in-plane electric fields exist [1, 4, 6]. The constitutive relations for the piezoelectric material are [2, 5]:

$$\tau_{zi} = c_{44}\gamma_{zi} - e_{15}E_i \;\; ; \;\; D_i = e_{15}\gamma_{zi} + \in_{11} E_i \tag{1}$$

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 (constant electric field), piezoelectric constant, and dielectric permittivity (constant strain) of piezoelectric material, respectively.

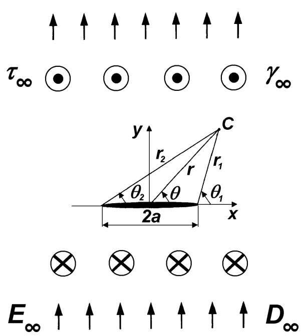

Figure 1. Geometry of the problem

Taking in consideration that the boundary conditions are: on the surfaces of the crack ($|x| < a$, $y = 0$): $\tau_{zy} = 0$, $D_y = 0$, and 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 uniform quantities, the governing equations can be expressed as:

$$\nabla^2 w = 0 \;\; ; \;\; \nabla^2 \varphi = 0 \tag{2}$$

where $w(x,y)$ is mechanical displacement. The solution can be found by letting w and φ be the complex analytic functions such that $w = W(Z)$, $\varphi = \varphi(Z)$, where $Z = x + iy$ is a complex variable.

Due to complex variable solution, a crack on the x-axis is constructed using the following mapping function [5, 6]:

$$\xi = a^{-1}(Z + \sqrt{Z^2 - a^2}) \tag{3}$$

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 dislocation subjected to a line force and a line charge, and the potential functions W and φ has 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 [3, 4, 6], and the forces acting on a screw dislocation are given with:

$$F_x = b_z\tau_{zy}^T + \Delta\varphi D_y^T + p_z^S\gamma_{zx}^T + q_z^S E_x^T \;\; ; \;\; F_y = -b_z\tau_{zx}^T - \Delta\varphi D_x^T + p_z^S\gamma_{zy}^T + q_z^S E_y^T \tag{4}$$

where b_z, $\Delta\varphi$, p_z, and q_z are the Burgers vector, electric potential jump, line force, and line charge, respectively [3, 6].

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 specific forces on a screw dislocation located in arbitrary position near a crack, are determined [6]. For the numerical analysis, these equations are translated into MatLab simulation code in m-type script. Basic values of piezoelectric PZT-5H ceramic material parameters are: $a = 1\cdot10^{-8}$ m, $b_z = 1\cdot10^{-9}$ m, $\Delta\varphi = 1$ V,

$p_z = 10$ N/m, $q_z = 1 \cdot 10^{-8}$ C/m, $c_{44} = 2{,}3 \cdot 10^{10}$ N/m^2, $e_{15} = 17$ C/m^2, $\in_{11} = 150 \cdot 10^{-10}$ C/Vm, $\gamma_\infty = 9{,}5 \cdot 10^{-5}$, $E_\infty = 2 \cdot 10^5$ V/m. In analysis are taken three ratios: $r = 0{,}5a$, $r = a$, and $r = 2a$.

3. RESULTS AND CONCLUSION

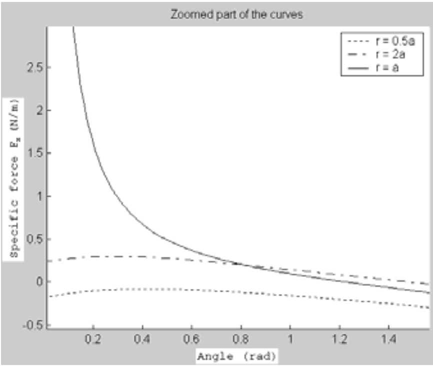

Figure 2. Specific force in x-direction vs. dislocation angle

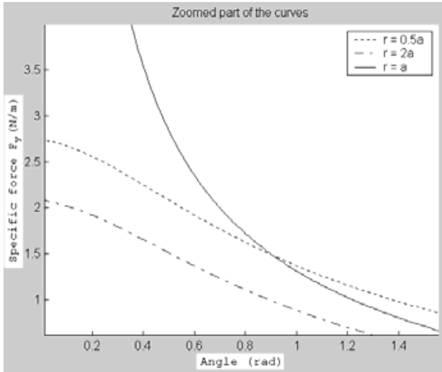

Figure 3. Specific force in y-direction vs. dislocation angle

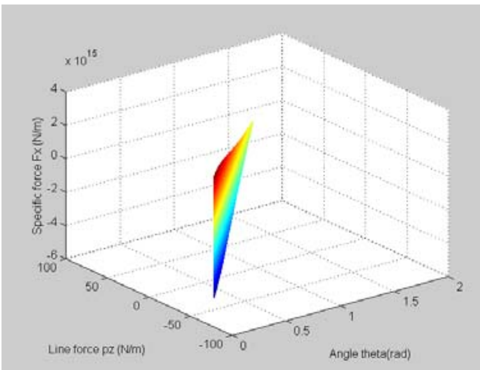

Figure 4. Line and specific x-axe force vs. dislocation angle

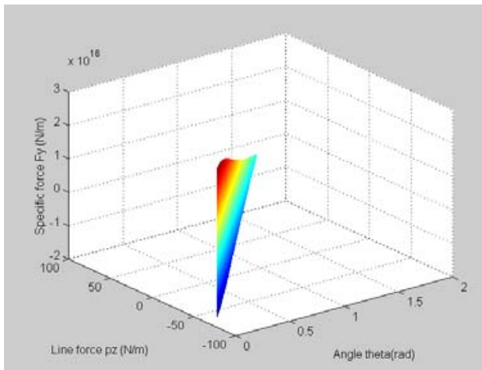

Figure 5. Line and specific y-axe force vs. dislocation angle

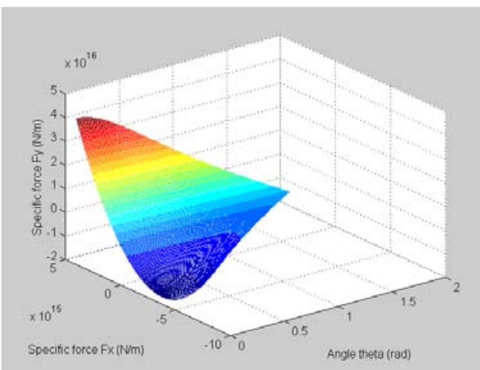

Figure 6. Specific forces vs. dislocation angle

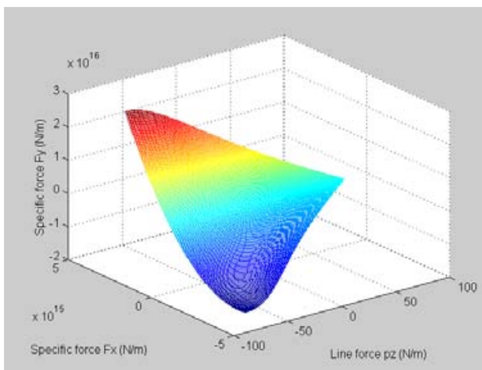

Figure 7. Specific forces vs. line force

The numerical results for PZT-5H material is graphically presented. Specific force F_x in *x*-direction versus dislocation angle θ for ratios: $r = 0{,}5a$, $r = a$, and $r = 2a$, is presented in Figure 2. Figure 3. shows the specific force F_y in *y*-direction versus dislocation angle θ for ratios: $r = 0{,}5a$, $r = a$, and $r = 2a$. It is evident that lower angles of dislocation produce higher forces in *x* and *y*-direction, which leads to break the material. This is possible in nano-structures, one deal with atomic-size structures and nuclear forces takes over any other force. Line force p_z and specific forces F_x and F_y on screw dislocation in dependence on dislocation angle θ, are shown in Figure 4. and 5. Figure 6. and 7. shows specific forces F_x and F_y versus dislocation angle θ and line force p_z.

Fracture mechanics has very important role in safety analysis of final products. Degradation of materials due to both normal aging processes and operating stresses cause fracture and mechanical failure. Critical stress will arise around defects in production process more likely than at some other position. In this work is analyzed a simple continuum model of a single screw dislocation near a 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 for piezoelectric PZT-5H ceramic material is obtained in MatLab and they are presented in 2D and 3D graphs. The results of this investigation can be very useful for producers and users of PZT materials.

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