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Extended displacement discontinuity method for analysis of penny-shaped cracks in three-dimensional thermal piezoelectric semiconductors

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ABSTRACT

In this paper, the extended displacement discontinuity (EDD) boundary element method is developed to analyze a penny-shaped crack in the isotropic plane of a three-dimensional (3D) transversely isotropic thermal piezoelectric semiconductor (PSC). The generalized Almansi's theorem and the operator theory are used to obtain the general solutions under generalized loading. The fundamental solutions for extended displacement discontinuities (EDDs) applied on the penny-shaped crack surface, which include the displacement, electric potential, carrier density, and temperature discontinuities, are derived. By using the EDD boundary element method, the EDD under mechanical, electrical and heat loading near the edge of a penny-shaped crack is calculated. The stress and heat flux intensity factors of the crack are obtained. The influence of uniform and non-uniform heat loadings on the fracture of 3D transversely isotropic thermal PSCs is investigated.

1. Introduction

Piezoelectric semiconductors (PSCs) are materials that have piezoelectric and semiconductor properties. They have been used extensively in smart structures, electromechanical devices and systems, such as the multifunctional sensors, acoustic phonon spectroscopy, and implantable nanogenerators, because of their excellent force, electrical properties and a variety of energy conversion capabilities (Wang, 2007; Jenkins et al., 2015; Mante et al., 2015; Li and Wang, 2017). In 1960, Hutson discovered PSCs (Hutson, 1960). Shortly afterwards, Hutson and White showed that mechanical fields and mobile charges can interact with each other, and the interaction was called the acousto-electric effect (Hutson and White, 1962). Since then, many devices have been developed for the discovery of the properties of ZnO nanowires stemming from the piezoelectric-semiconducting coupling (Wang et al., 2006). Zhang et al. (2012) and Liu et al. (2015) reviewed the fundamental theories of piezotronics and piezo-phototronics, respectively. Wen et al. (2015) reviewed new development and progress in the piezotronics field.

PSCs are very sensitive to internal defects such as cracks and cavities (Bykhovski et al., 1996; Ancona et al., 2012), and the defects can reduce the reliability of devices (Del and Joh, 2009). Hence, analysis of cracks in PSCs is important for intelligent device design and performance. Generally speaking, there are analytical (e.g., Zhao et al., 1998) and numerical (e.g., Lai et al., 2017; Wang et al., 2017) solutions for crack problems. For piezoelectric media, Zhao et al. (1997a, 1997b) derived the analytical solution for an isolated crack in a three-dimensional piezoelectric solid. Because of the mathematical complexity, advanced numerical methods are required for piezoelectric solids. The extended finite element method (XFEM) (Bui and Zhang, 2012; Bui, 2015; Liu et al., 2013; Sharma et al., 2013; Yu et al., 2015; Wang et al., 2016), the boundary element method (BEM) (Pan, 1999; Lei et al., 2014, 2015), the distributed dislocation method (Sharma et al., 2016, 2017), and the extended displacement discontinuity (EDD) method (Fan et al., 2014a,b) were developed to simulate piezoelectric solids. In recent years, research on the fracture of PSCs has attracted wide attentions (Sladek and Sladek, 2014; Zhao et al., 2016a; Fan et al., 2016). Yang (2005) studied an anti-plane semi-infinite crack in a PSC, and obtained an explicit solution for the electromechanical field near the crack tip. Hu et al. (2007) analyzed a finite Mode III crack in a PSC of 6 mm crystals and showed how the fracture behavior affected the semiconducting properties. Sladek and Sladek (2014) studied an in-plane crack problem in finite domains under mechanical and electric loading in PSCs with static and transient boundary conditions. Using the meshless local Petrov-Galerkin method, they showed the influence of the electric conductivity on intensity factors of cracks in homogeneous conducting piezoelectric solids. Sladek et al. (2015) also investigated the influence of electric conductivity on intensity factors of

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cracks in functionally graded conducting piezoelectric materials. Recently, Fan et al. (2016) proposed a piezoelectric-conductor iterative method (PCIM) for fracture analysis of PSCs under combined mechanical loading, electric strength field and electric current. For three-dimensional (3D) cases, Zhao et al. (2016b) extended the displacement boundary integral equation method to analyze the singularity of near-border fields of arbitrarily shape of planar cracks in the isotropic plane of a 3D transversely isotropic PSC. Using the EDD method, Zhao et al. (2016) studied penny-shaped cracks in 3D PSCs.

Semiconductor devices, such as high temperature sensors, are usually accompanied by heat flux or thermal loading during the manufacture and service (Morkoç et al., 1994; Oszwaldowski and Berus, 2007). Thermal effects must be considered in analyzing semiconductor structures. Mindlin (1961) first proposed the theory of thermo-piezoelectricity. Since then, the fracture behavior of piezoelectric solids under thermal loading has been investigated in a number of studies. Yu and Qin (1996a, b) studied the fracture and damage behaviors of a cracked piezoelectric solid under coupled thermal, mechanical and electrical loads. Recently, thermal crack problems in piezoelectricity have been extensively investigated, including static thermal fracture problems (Niraula and Noda, 2002; Shang and Kuna, 2003; Ding et al., 2000; Wang and Noda, 2004; Zhong and Zhang, 2013; Yang et al., 2014; Zhang and Wang, 2015; Li and Lee, 2015) and transient thermal fracture problems (Wang and Mai, 2002; Dai and Wang, 2005; Ishihara and Noda, 2005; Sladek et al., 2007, 2010; Ueda, 2008; Liu et al., 2014). Sladek et al. (2014) studied the effect of the initial electron density on the intensity factors and energy release rate under a transient thermal load in PSCs. Zhao et al. (2017) investigated the stress and heat flux intensity factors at the crack tip and the effect of temperature on the fracture behavior under a static load. Motivated by this issue, this work investigated the penny-shaped crack problem in a 3D PSC under thermal and mechanical loads. Section 2 presents the basic equations for thermal PSCs subjected to a thermal load. In Section 3, general solutions for EDDs are derived. Section 4 presents the fundamental solutions for uniform displacement discontinuities applied on penny-shaped cracks. In Section 5, the EDD boundary element method is developed to analyze a crack on which distributed extended loadings are applied. Numerical results are presented in Section 6, and some conclusions drawn from the present study are given in Section 7.

2. Basic equations

In the absence of body forces, electric charge, electric and body heat sources, the governing equations for 3D n-type PSCs can be written as follows

$$\frac{\partial\sigma_{xx}}{\partial x}+\frac{\partial\tau_{xy}}{\partial y}+\frac{\partial\tau_{zx}}{\partial z}=0,\quad \frac{\partial\tau_{xy}}{\partial x}+\frac{\partial\sigma_{yy}}{\partial y}+\frac{\partial\tau_{yz}}{\partial z}=0,\quad \frac{\partial\tau_{zx}}{\partial x}+\frac{\partial\tau_{yz}}{\partial y}+\frac{\partial\sigma_{zz}}{\partial z}=0,\tag{1a}$$

$$\frac{\partial D_x}{\partial x}+\frac{\partial D_y}{\partial y}+\frac{\partial D_z}{\partial z}=q(N_D^+-n_0-\Delta n),\tag{1b}$$

$$\frac{\partial J_x}{\partial x}+\frac{\partial J_y}{\partial y}+\frac{\partial J_z}{\partial z}=0,\tag{1c}$$

$$\frac{\partial h_x}{\partial x}+\frac{\partial h_y}{\partial y}+\frac{\partial h_z}{\partial z}=0,\tag{1d}$$

where σ_{ij}, D_i, and J_i are the stress tensor, the electric displacement vector, and the electric current, respectively, h_i is the heat flux, and $i,j=x,y,z$. N_D^+ is the known donor density and it can be assumed to be uniform. $(n_0+\Delta n)$ is the entire electron density where $n_0=N_D^+$, Δn is the deviation of the electron density from n_0, and $n=n_0+\Delta n$. q denotes the electric charge of an electron. The charge equation (1b) can then be written as

$$\frac{\partial D_x}{\partial x}+\frac{\partial D_y}{\partial y}+\frac{\partial D_z}{\partial z}=-q\Delta n.\tag{1e}$$

By following Hutson and White (1962), Sladek et al. (2014) and Zhao et al. (2016b), the linear constitutive equations for a 3D n-type PSC can be written as

$$\begin{aligned}
\sigma_{xx}&=c_{11}\frac{\partial u}{\partial x}+c_{12}\frac{\partial v}{\partial y}+c_{13}\frac{\partial w}{\partial z}+e_{31}\frac{\partial\phi}{\partial z}-\lambda_{11}\theta,\\
\sigma_{yy}&=c_{12}\frac{\partial u}{\partial x}+c_{11}\frac{\partial v}{\partial y}+c_{13}\frac{\partial w}{\partial z}+e_{31}\frac{\partial\phi}{\partial z}-\lambda_{11}\theta,\\
\sigma_{zz}&=c_{13}\frac{\partial u}{\partial x}+c_{13}\frac{\partial v}{\partial y}+c_{33}\frac{\partial w}{\partial z}+e_{33}\frac{\partial\phi}{\partial z}-\lambda_{33}\theta,\\
\tau_{yz}&=c_{44}\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)+e_{15}\frac{\partial\phi}{\partial y},\\
\tau_{zx}&=c_{44}\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)+e_{15}\frac{\partial\phi}{\partial x},\\
\tau_{xy}&=c_{66}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right),
\end{aligned}\tag{2a}$$

$$\begin{aligned}
D_x&=e_{15}\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)-\varepsilon_{11}\frac{\partial\phi}{\partial x},\\
D_y&=e_{15}\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)-\varepsilon_{11}\frac{\partial\phi}{\partial y},\\
D_z&=e_{31}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)+e_{33}\frac{\partial w}{\partial z}-\varepsilon_{33}\frac{\partial\phi}{\partial z}+p_3\theta,
\end{aligned}\tag{2b}$$

$$\begin{aligned}
J_x&=-qn_0\mu_{11}\frac{\partial\phi}{\partial x}+qd_{11}\frac{\partial\Delta n}{\partial x},\\
J_y&=-qn_0\mu_{11}\frac{\partial\phi}{\partial y}+qd_{11}\frac{\partial\Delta n}{\partial y},\\
J_z&=-qn_0\mu_{33}\frac{\partial\phi}{\partial z}+qd_{33}\frac{\partial\Delta n}{\partial z},
\end{aligned}\tag{2c}$$

$$h_x=-\beta_{11}\frac{\partial\theta}{\partial x},\quad h_y=-\beta_{11}\frac{\partial\theta}{\partial y},\quad h_z=-\beta_{33}\frac{\partial\theta}{\partial z},\tag{2d}$$

where $u(v,w)$, ϕ, and θ are the mechanical displacements, the electric potential, and the temperature change, respectively, which are known as extended displacements. c_{ij}, e_{ij}, ε_{ij}, d_{ij}, μ_{ij}, and p_3 are the elastic, piezoelectric, dielectric, carrier diffusion constant, electron mobility, and pyroelectric material coefficients. β_{ij} denotes the heat conduction coefficients. The stress-temperature modulus λ_{ij} can be expressed through the stiffness coefficients and the coefficients of linear thermal expansion α_{kl} by (Sladek et al., 2014)

$$\lambda_{ij}=c_{ijkl}\alpha_{kl},\tag{3}$$

where c_{ijkl} is the elasticity tensor, α_{kl} can be obtained by $\alpha_{kl}=\alpha_{11}\delta_{k1}\delta_{l1}+\alpha_{22}\delta_{k2}\delta_{l2}+\alpha_{33}\delta_{31}\delta_{l3}$, and δ_{ij} represents the Kronecker delta.

Substituting Eqs. (2a-2d) into Eqs. (1a-1e), the governing equations become

$$\left(c_{11}\frac{\partial^2}{\partial x^2}+c_{66}\frac{\partial^2}{\partial y^2}+c_{44}\frac{\partial^2}{\partial z^2}\right)u+(c_{12}+c_{66})\frac{\partial^2 v}{\partial x\partial y}+(c_{13}+c_{44})\frac{\partial^2 w}{\partial x\partial z}+(e_{31}+e_{15})\frac{\partial^2\phi}{\partial x\partial z}-\lambda_{11}\frac{\partial\theta}{\partial x}=0,\tag{4a}$$

$$(c_{12}+c_{66})\frac{\partial^2 u}{\partial x\partial y}+\left(c_{66}\frac{\partial^2}{\partial x^2}+c_{11}\frac{\partial^2}{\partial y^2}+c_{44}\frac{\partial^2}{\partial z^2}\right)v+(c_{13}+c_{44})\frac{\partial^2 w}{\partial y\partial z}+(e_{31}+e_{15})\frac{\partial^2\phi}{\partial y\partial z}-\lambda_{11}\frac{\partial\theta}{\partial y}=0,\tag{4b}$$