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COUPLING OF ASYMPTOTIC SOLUTIONS WITH FINITE ELEMENTS AT INTERFACE CONFIGURATIONS IN PIEZOELECTRIC COMPOSITES

Matthias Scherzer and Meinhard Kuna

Freiberg University of Mining and Technology, Institute of Mechanics and Machine Components
Lampadiusstraße 4, D-09596 Freiberg, Germany

ABSTRACT

The present work is directed to the analysis of interface corner and crack configurations which occur in smart composite materials. It delivers a new technique for solving the corresponding piezoelectric boundary value problems by asymptotic eigenfunction expansions in connection with the conventional finite element method. This approach represents the extension to coupled electromechanical material behaviour of a method which was introduced for geometrical and physical linear and non-linear solid mechanics formerly [9, 10]. The proposed approach has the advantage that the asymptotic stiffness matrix does not depend on the distance to the tip and that oscillating terms of the asymptotics can be circumvented numerically but are still fully contained. Therefore, results can be achieved with much better accuracy than by means of regular finite elements.

KEYWORDS

Piezoelectric materials, fracture, asymptotic analyses, numerical methods

INTRODUCTION

Piezoelectric, ferroelectric and dielectric ceramics or polymers are widely applied in Micro Electro Mechanical Systems (MEMS) to supply the essential sensing and/or actuating functionality [5]. As a consequence of their integration into MEMS, problems of fracture and fatigue play an important role for the optimum design and reliable service performance of MEMS. Fracture mechanics analyses and safety concepts have to be applied to crack-like defects in piezoelectric bulk materials or in interface structures and lead to the corresponding asymptotic solutions at interface crack and corner tips with the associated coefficients of the eigenfunctions as fracture parameters.
First theoretical studies [3, 7, 14] about interface crack tips in piezoelectrics show that difficult singular oscillatory solutions can occur. According to its prior importance for many micromechanical applications, models of interface crack problems in dissimilar piezoelectric materials has been published recently with a fast-growing rate (see for instance [8, 15] and other and the references therein). Most of the authors use the Lekhnitzkij and Stroh formalisms or the Fourier transform technique in connection with dual boundary value problems including Cauchy-type-integrals for linear statements within infinite bodies. In this context it is interesting to note that the usual expecting singular oscillatory behaviour can change to solutions without oscillations for modified electric boundary conditions [4, 7, 14]. By means of the analytic solution in [2] it is shown that an interface crack tip between a piezoelectric

and a conductor produces three non-oscillating singular terms of the form $\xi^{(-0.5-\nu)}\tilde{\mu}_1(\theta)$, $\xi^{-0.5}\tilde{\mu}_2(\theta)$ and $\xi^{(-0.5+\nu)}\tilde{\mu}_3(\theta)$, whereby ξ is the distance to the tip, θ represents the polar angle and ν is defined through $\nu = 0.5 - h$ with $0 < h < 0.5$. This way, energetic possible solutions may have a singular behaviour which is stronger than -0.5.

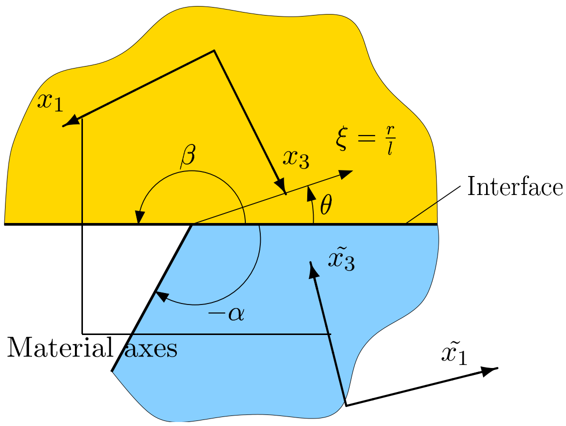

Figure 1: Interface corner configuration

The preponderant majority of the existing solutions at interface crack tips between piezoelectric materials represent linear boundary value problems for infinite bodies although real electromechanical materials show non-linear behaviour, too [6, 12]. But in general, the linear solution procedures mentioned above are not extensible to non-linear problems. Thus, there is a need to develop solution techniques filling this gap. The extension of the methods elaborated in [9, 10] to piezoelectric materials seems to be very hopeful in this sense. In the following, the approach of [9, 10] is applied to linear piezoelectric problems including interface cracks within finite body domains.

LINEAR PIEZOELECTRICITY AND ASYMPTOTIC ANALYSIS

In order to solve the complicated boundary value problem of interface configurations in connection with their difficult asymptotic features and to develop associated stable numerical methods for its handling, it is necessary to dispose of the complete eigenfunction expansions at interface corner and interface crack tips. We will restrict our analysis to the simplest approach for the constitutive laws in both material domains of the interface configuration. The main assumptions are:

1. Neglegtion of magnetic and time effects
2. Introducing the thermomechanical-electric coupling by the electric energy term in the first law of thermodynamics
3. Linearization of the ferroelectric hysteresis loop
4. Transversal isotropic piezoelectric behaviour

The governing relations describing this coupled electromechanical field problem are the equations of stress equilibrium, the compatibility equations and Gauss' law of electrostatics

$$\sigma_{ij,i} = 0, \quad S_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}), \quad D_{i,i} = 0, \quad \text{(i,j=1,2,3)} \tag{1}$$

as well as the equations of the linear piezoelectric material behaviour:

$$\begin{aligned}
\sigma_{11} &= c_{11}S_{11} + c_{12}S_{22} + c_{13}S_{33} - e_{31}E_3,\ \sigma_{21} = (c_{11} - c_{12})S_{21} \\
\sigma_{22} &= c_{12}S_{11} + c_{11}S_{22} + c_{13}S_{33} - e_{31}E_3,\ \sigma_{13} = 2c_{44}S_{13} - e_{15}E_1 \\
\sigma_{33} &= c_{13}S_{11} + c_{13}S_{22} + c_{33}S_{33} - e_{33}E_3,\ \sigma_{32} = 2c_{44}S_{32} - e_{15}E_2 \\
&D_1 = 2e_{15}S_{13} + \kappa_{11}E_1,\ D_2 = 2e_{15}S_{32} + \kappa_{11}E_2 \\
&D_3 = e_{31}S_{11} + e_{31}S_{22} + e_{33}S_{33} + \kappa_{33}E_3.
\end{aligned} \tag{2}$$

In (1) and (2) σ_{ij}, S_{ij}, u_i, E_i and D_i denote the stress and deformation tensor, the mechanical displacement vector, the negativ gradient of the electrical potential ϕ and the dielectric displacements, respectively. The material parameters c_{ij} (elastic), e_{ij} (piezoelectric) and κ_{ij} (dielectric) characterize transversly isotropic piezoelectrics with pooling-axis along the third direction of the chosen material co-ordinate system in (2). These material equations are written with regard to the material axes of each dissimilar material domain as shown in Figure 1 (x_1–x_3, $\tilde{x_1}$–$\tilde{x_3}$). The axes x_2 and $\tilde{x_2}$ are directed perpendicular to the plane of Figure 1.

Further simplifications lead to two-dimensional statements with the assumptions of plane strain:

$$S_{22} = S_{32} = S_{12} = E_2 = 0 \; (x_2 - \text{direction normal to the plane}) \tag{3}$$

and reduce the system (1) and (2) to

$$\left\{ \begin{array}{c} S_{11} \\ S_{33} \\ S_{13} \end{array} \right\} = \begin{pmatrix} a_{11} & a_{13} & 0 \\ a_{13} & a_{33} & 0 \\ 0 & 0 & \frac{d_{33}}{2} \end{pmatrix} \left\{ \begin{array}{c} \sigma_{11} \\ \sigma_{33} \\ \sigma_{13} \end{array} \right\} + \begin{pmatrix} 0 & b_{13} \\ 0 & b_{33} \\ \frac{b_{31}}{2} & 0 \end{pmatrix} \left\{ \begin{array}{c} D_1 \\ D_3 \end{array} \right\} \tag{4}$$

$$\left\{ \begin{array}{c} E_1 \\ E_3 \end{array} \right\} = - \begin{pmatrix} 0 & 0 & b_{31} \\ b_{13} & b_{33} & 0 \end{pmatrix} \left\{ \begin{array}{c} \sigma_{11} \\ \sigma_{33} \\ \sigma_{13} \end{array} \right\} + \begin{pmatrix} \delta_{11} & 0 \\ 0 & \delta_{33} \end{pmatrix} \left\{ \begin{array}{c} D_1 \\ D_3 \end{array} \right\} \tag{5}$$

$$\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{13}}{\partial x_3} = 0, \; \frac{\partial \sigma_{13}}{\partial x_1} + \frac{\partial \sigma_{33}}{\partial x_3} = 0, \; \frac{\partial D_1}{\partial x_1} + \frac{\partial D_3}{\partial x_3} = 0 \tag{6}$$

$$\frac{\partial^2 S_{11}}{\partial x_3^2} + \frac{\partial^2 S_{33}}{\partial x_1^2} = 2\frac{\partial^2 S_{13}}{\partial x_1 \partial x_3}, \; \frac{\partial E_1}{\partial x_3} - \frac{\partial E_3}{\partial x_1} = 0, \tag{7}$$

whereby the coefficients a_{11}, ..., b_{13}, ..., δ_{11} and δ_{33} ($b_{13} \neq b_{31}$) can be determined from the material parameters introduced above. In each material co-ordinate system the solution can be written in form of the potentials $U(x_1, x_3)$ and $\chi(x_1, x_3)$ [13]:

$$\begin{aligned} \sigma_{11} &= U(x_1,x_3)_{,33}, \; \sigma_{33} = U(x_1,x_3)_{,11}, \; \sigma_{13} = -U(x_1,x_3)_{,13} \\ D_1 &= \chi(x_1,x_3)_{,3}, \; D_3 = -\chi(x_1,x_3)_{,1}. \end{aligned} \tag{8}$$

Finally, we end up in a linear partial differential equation of sixth order for $U(x_1, x_3)$. The general solution of this equation and therewith also the solution of the whole problem - because $\chi(x_1, x_3)$ follows from $U(x_1, x_3)$ by integration - has the form

$$U(x_1, x_3) = \sum_k \sum_{i=1}^{6} d_i(\lambda_k)(x_1 + \tau_i x_3)^{\lambda_k + 2}. \tag{9}$$

The complex variables $d_i(\lambda_k)$ are free coefficients to be determined from the overall solution and τ_i stands for the roots of the characteristic polynom (sixth order with real coefficients) of the partial differential equation. The numbers λ_j, which are in general complex ones, represent the roots of the solvability condition of the interface corner configuration together with the associated boundary and transition conditions. There exists the corresponding conjugate complex root $\overline{\tau_i}$ for each complex τ_i. Because $U(x_1, x_3)$ is a real function, terms of the form

$$\begin{aligned} & e_i p^{(\lambda_k + 2)} \cos\left[(\lambda_k + 2)(\kappa + \tfrac{\pi}{2})\right] + f_i p^{(\lambda_k + 2)} \sin\left[(\lambda_k + 2)(\kappa + \tfrac{\pi}{2})\right] \\ & \text{with } \; p = \sqrt{(x_1)^2 + 2\tau_i^r x_1 x_3 + (x_3)^2[(\tau_i^i)^2 + (\tau_i^r)^2]}, \quad \kappa = \arctan\left((x_1 + \tau_i^r x_3)/(\tau_i^i x_3)\right) \\ & \text{and } \; \tau_i = \tau_i^r + \sqrt{-1}\tau_i^i, \; d_i(\lambda_k) = e_i(\lambda_k) + \sqrt{-1} f_i(\lambda_k) \end{aligned} \tag{10}$$

occur for τ_i and $\overline{\tau_i}$ in (9). The solution representation (10) is valid for each material domain of the interface configuration which has its own material parameters, axes, τ_i and $d_i(\lambda_k)$. The construction of the associated eigenfunction expansion results in the following steps:

1. Transformation of the solutions (9) into the same polar co-ordinate system (ξ, θ) for both material regions ($0 \leq \theta \leq \beta$ and $0 \geq \theta \geq -\alpha$) of the interface corner configuration
2. Establishing the transcendental solvability condition according to the boundary and transition conditions

$$\Rightarrow \; Det(\lambda, ...) = 0 \tag{11}$$

The boundary and transition conditions have the usual form:

- Vanishing normal and tangent stresses $(\sigma_{\theta\theta}, \sigma_{\xi\theta})$ and vanishing normal dielectric displacements (D_θ) at $\theta = \beta, \; \theta = -\alpha$

- Continuity of normal and tangent stresses, both displacement components (u_ξ, u_θ), electric potential (ϕ, $E_1 = -\frac{\partial \phi}{\partial x_1}$, $E_3 = -\frac{\partial \phi}{\partial x_3}$) and normal dielectric displacements at $\theta = 0$
Other boundary conditions can be applied by the given solution technique, too. The only requirements are that they must result from physical reasons and have to give correctly formulated problems.

3. Numerical determination of λ: $\Rightarrow \lambda_k, k = 1, ..., \infty$ in (11)
4. For complex roots $\lambda_k = \nu_k + \mathrm{i}\mu_k$ the conjugate complex root $\overline{\lambda_k} = \nu_k - \mathrm{i}\mu_k$ exists:
$\Rightarrow$ terms of the quality $\xi^{\nu_k} \cos(\mu_k ln(\xi))$, $\xi^{\nu_k} \sin(\mu_k ln(\xi))$ occur
5. Determination of the associated eigenvectors and eigenfunctions (and removing of the energetic "useless" functions) to get the expansions

$$U(\xi,\theta) = \sum_{k=1}^{\infty} C_k \xi^{(\lambda_k+2)} f_k^{(U)}(\theta,\lambda_k), \quad \sigma_{\xi\xi}(\xi,\theta) = \sum_{k=1}^{\infty} C_k \xi^{\lambda_k} f_{k\xi\xi}^{(\sigma)}(\theta,\lambda_k), ... \tag{12}$$

with the unknown coefficients C_k

For solving whole boundary value problems of components having interface corner configurations, the sole knowledge of the eigenfunctions introduced above is insufficient. The asymptotic eigenfunction expansion in the neighbourhood of the interface corner tip must be connected to the solution in the remaining part of the structure. Doing this, finite element nodes of a regular net can be established at a distance of $\xi = \xi_0$ from the corner together with the degrees of freedom $u_i(\xi_0, \theta_j)$ for the displacements and the electric potential ϕ (Figure 2).

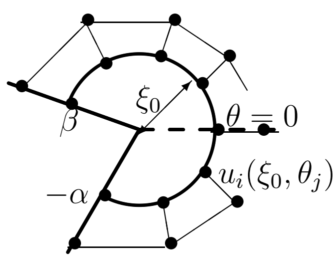

Figure 2: Neighbourhood of an interface corner together with the finite element nodes

The main idea of the presented approach (which was developed in [9, 10] for pure mechanical behaviour) consists in a replacement of the corner neighbourhood ($\xi < \xi_0$) effect to the surrounding body ($\xi > \xi_0$) by introducing a special stiffness matrix at $\xi = \xi_0$ which can be assembled in a conventional way together with the other element stiffness matrices to the global stiffness matrix. The description of this procedure cannot be given here because of the limited space. It is referred to [9, 10, 11] for more details. The main essentials of the proposed approach result in the facts that the asymptotic stiffness matrix does not depend on ξ_0 and the oscillating terms are circumvented numerically but still fully contained.

This makes it possible from the numerical point of view to "live" with the oscillatory asymptotic solutions at the interface crack tip if not any physical arguments forbid this behaviour from other reasons. To avoid the oscillations it is necessary to introduce the corresponding kinematical assumptions in the interface crack tip region.
Since the coefficients of the eigenfunctions C_k describe the electromechanical fields in the interface corner region completely they can be applied as fracture parameters and used to formulate failure criteria.

FIRST TEST EXAMPLES

The asymptotic stiffness matrix was calculated by the help of modern computer algebra systems and implemented as a user defined element within the commercial finite element code ABAQUS [1]. Results of test computations will be explained. An interface crack specimen (Figure 3) of two different piezoelectric materials (extension: 100*200 dimensionless units, crack in the middle of the specimen with a length of 50, plane strain (3) conditions) is strained homogenously at the upper specimen end and clamped right opposite. The electric potential is given at the right specimen side ($x_1 = 50$, $-100 \leq x_3 \leq 100$) with zero values. For this specimen the material parameters are introduced by:

Upper half (PZT-4):

$c_{11} = 1.39 * 10^{11} \frac{N}{m^2}$, $c_{33} = 1.13 * 10^{11} \frac{N}{m^2}$, $c_{12} = 7.78 * 10^{10} \frac{N}{m^2}$, $c_{13} = 7.43 * 10^{10} \frac{N}{m^2}$, $c_{44} = 2.56 * 10^{10} \frac{N}{m^2}$
$\kappa_{11} = 6.0 * 10^{-9} \frac{C}{Vm}$, $\kappa_{33} = 5.470 * 10^{-9} \frac{C}{Vm}$, $e_{15} = 13.44 \frac{C}{m^2}$, $e_{31} = -6.98 \frac{C}{m^2}$, $e_{33} = 13.84 \frac{C}{m^2}$

Lower half (hypothetical):

$$c_{11} = 2.39 * 10^{11} \frac{N}{m^2},\ c_{33} = 1.13 * 10^{10} \frac{N}{m^2},\ c_{12} = 4.78 * 10^{10} \frac{N}{m^2},\ c_{13} = 5.43 * 10^{10} \frac{N}{m^2},\ c_{44} = 2.56 * 10^{9} \frac{N}{m^2}$$
$$\kappa_{11} = 4.0 * 10^{-9} \frac{C}{Vm},\ \kappa_{33} = 2.470 * 10^{-9} \frac{C}{Vm},\ e_{15} = 12.0 \frac{C}{m^2},\ e_{31} = -4.98 \frac{C}{m^2},\ e_{33} = 14.0 \frac{C}{m^2}$$

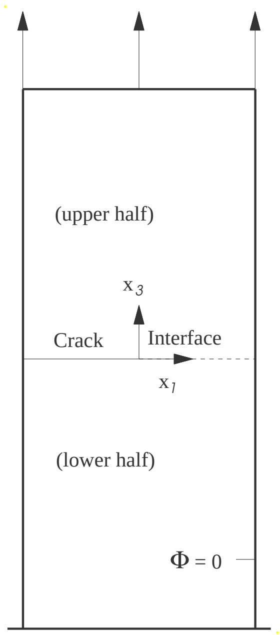

Figure 3: Piezoelectric specimen under tension

Both material domains have the same pooling directions (x_3). The homogenous boundary and transition conditions given above lead to the roots λ_k of the solvability condition (11) resulting in:

1. $-0.5 \pm \sqrt{-1} * 0.11733,\ 0.5 \pm \sqrt{-1} * 0.11733,\ 1.5 \pm \sqrt{-1} * 0.11733,\ ...$
2. $-0.5,\ 0.5,\ 1.5,\ 3.5,\ 4.5,\ 5.5,\ ...$
3. $0.0,\ 1.0,\ 2.0,\ 3.0,\ 4.0,\ 5.0,\ ...$

Each pair of the conjugate complex roots (1.) produces two linear independent eigenvectors from the free constants $d_i(\lambda_k)$ while the second part of the roots (2.) have single eigenvectors and the third part (3.) generates three linear independent eigenvectors for each concrete value.
In Figure 4 the stress components σ_{33}, σ_{13} and the electric field E_3 are shown around the crack tip within a zoom radius $\xi_z = 1.0$. The crack comes from the left (negative x_1-axis) and the interface lies on the horizontal straight line (positve x_1-axis) on the ligament in front of the crack. The solutions of usual finite element computations ("without asymptotics") are compared with solutions following from the technique introduced above ("with asymptotics", $\xi_0 = 0.01$).

The results confirm the fact observed at pure mechanical analyses [9, 10] that the regular finite element method cannot give the correct solution at interface crack tips in general. The regular finite element representation of σ_{33} is familar to the asymptotic behaviour at a crack tip inside a homogenous isotropic material and cannot "feel" interface tip effects. Furthermore, the stress component σ_{13} of the same solution ("without asymptotics") fulfils the given boundary conditions on the crack surfaces very bad only. The differences between the solutions with and without asymptotics can also be seen on the representations of the electric variable E_3. The poor performance of regular finite elements in the vicinity of an interface crack tip may be explained by means of the fact that the polynomial shape functions cannot reproduce both the radial $\xi^{\nu_k}-$ asymptotics and the oscillating behaviour of the form $\cos(\mu_k ln(\xi))$ even if the element size is extremely diminished. Regular finite elements produce an asymptotic behaviour at interface crack tips which is severe different from that of the actual eigenfunctions.

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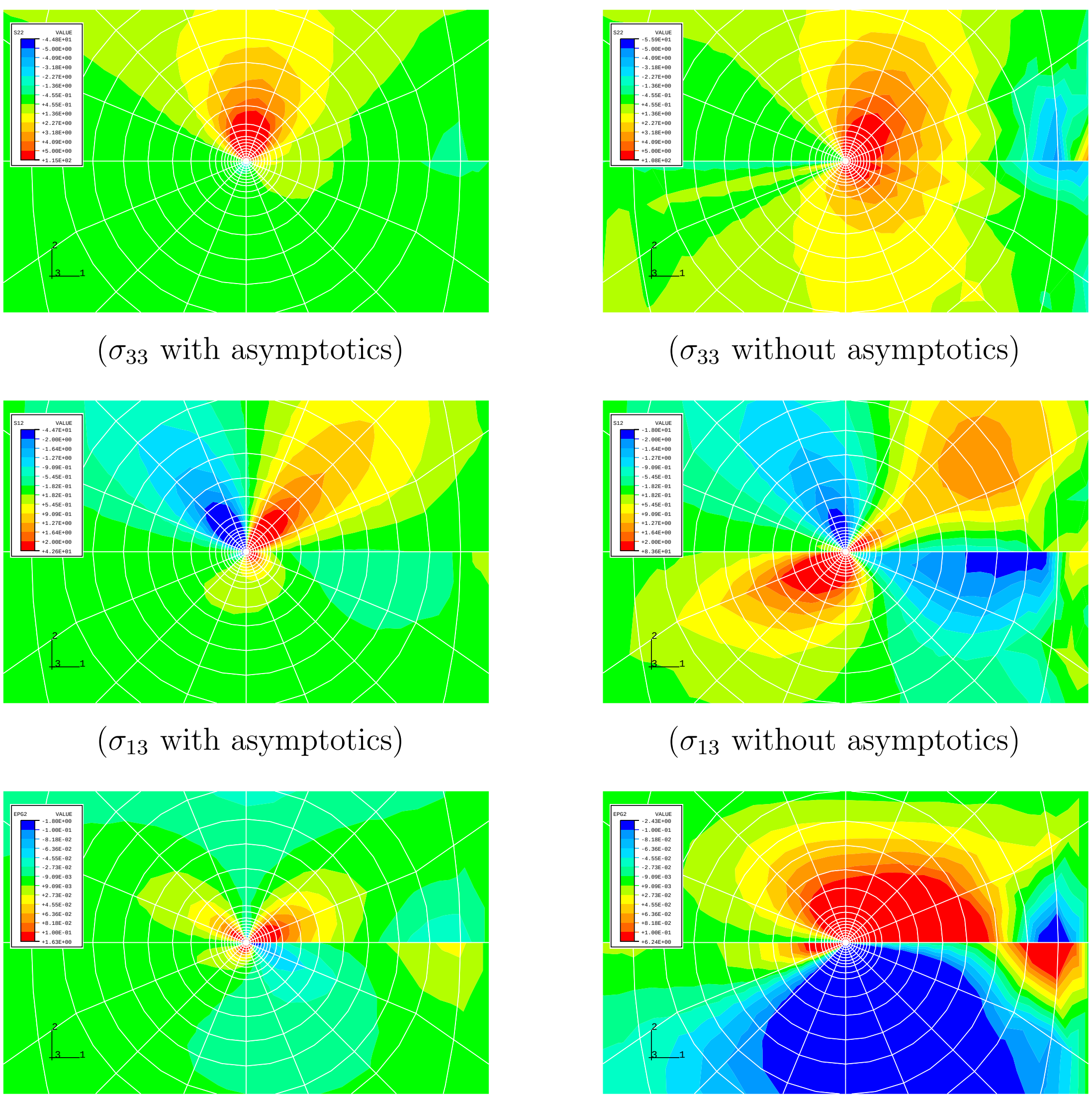

(σ_{33} with asymptotics) (σ_{33} without asymptotics)

(σ_{13} with asymptotics) (σ_{13} without asymptotics)

(E_3 with asymptotics) (E_3 without asymptotics)

Figure 4: Piezoelectric solutions at an interface crack tip under tension