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EFFECTIVE THERMAL EXPANSION AND PYROELECTRIC CONSTANTS FOR CRACKED PIEZOELECTRIC SOLIDS

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ABSTRACT:The Effective thermal expansion and pyroelectric constants of 2D cracked piezoelectric materials are obtained through use of the extended Stroh formalism and analytical solution of a crack embedded in a 2D thermopiezoelectric sheet. In the analysis, the self-consistent and Mori-Tanaka methods are used to take account of weakening effect among cracks.

I. INTRODUCTION

The determination of effective thermal expansion and pyroelectric coefficients of piezoelectric composites has drawn the attention of many researchers in the field of mechanics and material engineering. In this context, Dunn[1] evaluated the effective properties of two-phase composites using dilute, self-consistent, Mori-Tanaka and differential micromechanical models. Benveniste[2] showed that the effective thermal-stress constants and pyroelectric coefficients are related to the corresponding isothermal electroelastic moduli in two-phase media. For multiphase media, Benveniste[3] showed that the effective thermal-stress constants and pyroelectric coefficients follow from a knowledge of the influence functions related to an electromechanical loading of the composite aggregate. Chen[4] further obtained some formulae for the prediction of overall thermoelectroelastic moduli of multiphase fibrous composites with the self-consistent and Mori-Tanaka methods. More recently, Yu and Qin[5,6] obtained an analytical solution for a crack in an infinite plane piezoelectric solid under coupling mechanical, electric and thermal loading. In their papers the effective electroelastic moduli of a cracked material were derived by means of dilute, self-consistent, generalized self-consistent and Mori-Tanaka methods. They, however, presented no formulation about the estimations of effective thermal expansion and pyroelectric coefficients in those papers. The purpose of this work is just to fill the gap. The study shows that the prediction of effective thermal expansion and pyroelectric constants required a knowledge of both the effective conductivity and electroelastic moduli for crack problem, which seems more complex than those for two-phase composites in which the pyroelectric constants are only related to the corresponding isothermal electroelastic moduli[2]. In some sense this paper constitutes a continuation of our previous analysis[5,6]. In this paper some algebraic formulae are provided to predict the overall thermal expansion and pyroelectric constants of 2D cracked materials with dilute, self-consistent and Mori-Tanaka methods. The formulae are derived by way of an analytical solution for a crack in an infinite thermopiezoelectric medium[5]. The orientation and the lengths of the microcrack in the medium may be randomly distributed.

II. THE CRACKED THERMOPIEZOELECTRICITY

Using the notation employed in Ref.[5], The constitutive relations for plane thermopiezoelectric solids can be written in the form

$$\begin{Bmatrix}\sigma_{11}\\ \sigma_{33}\\ \sigma_{13}\\ D_1\\ D_3\end{Bmatrix}=\begin{bmatrix}c_{11} & c_{13} & 0 & 0 & e_{31}\\ c_{13} & c_{33} & 0 & 0 & e_{33}\\ 0 & 0 & c_{44} & e_{15} & 0\\ 0 & 0 & e_{15} & -\kappa_{11} & 0\\ e_{31} & e_{33} & 0 & 0 & -\kappa_{33}\end{bmatrix}\begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ 2\varepsilon_{12}\\ -E_1\\ -E_3\end{Bmatrix}-\begin{Bmatrix}\gamma_{11}\\ \gamma_{33}\\ 0\\ 0\\ \rho_3\end{Bmatrix}\theta \tag{1}$$

or inversely

$$\begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{33}\\ 2\varepsilon_{13}\\ -E_1\\ -E_3\end{Bmatrix}=\begin{bmatrix}s_{11} & s_{13} & 0 & 0 & g_{31}\\ s_{13} & s_{33} & 0 & 0 & g_{33}\\ 0 & 0 & s_{44} & g_{15} & 0\\ 0 & 0 & g_{15} & \beta_{11} & 0\\ g_{31} & g_{33} & 0 & 0 & \beta_{33}\end{bmatrix}\begin{Bmatrix}\sigma_{11}\\ \sigma_{33}\\ \sigma_{13}\\ D_1\\ D_3\end{Bmatrix}+\begin{Bmatrix}\alpha_{11}\\ \alpha_{33}\\ 0\\ 0\\ \lambda_3\end{Bmatrix}\theta \tag{2}$$

and simply, in matrix form

$$\mathbf{\Pi}=\mathbf{EZ}-\gamma\theta, \tag{3}$$

$$\mathbf{Z}=\mathbf{F\Pi}+\alpha\theta \tag{4}$$

where **E** and **F** are elastic stiffness and compliance tensors, in which g_{ij} and e_{ij} are the piezoelectric constant tensors, β_{ij} and κ_{ij} the dielectric permitivity coefficient tensors, α_{ij} and γ_{ij} are thermal expansion and thermal-stress constant tensors, λ_3 and ρ_3 are pyroelectric constants, $\Pi=\{\sigma_{11}\ \sigma_{33}\ \sigma_{13}\ D_1\ D_3\}^T=\{\sigma_1\ \sigma_3\ \sigma_5\ D_1\ D_3\}^T$, $Z=\{Z_{11}\ Z_{22}\ 2Z_{12}\ Z_{31}\ Z_{32}\}^T=\{\varepsilon_1\ \varepsilon_3\ 2\varepsilon_5\ -E_1\ E_3\}^T$, $\gamma=E\alpha$, θ is temperature change, σ_{ij} and D_i are the components of stress tensor and the components of electric displacement vector, ε_{ij} and E_i are the components elastic strain tensor and electric field vector.

The effective material properties of the cracked body are defined as

$$\overline{\mathbf{\Pi}}=\mathbf{E}^*\overline{\mathbf{Z}}-\gamma^*\overline{\theta} \quad \text{or} \quad \overline{\mathbf{Z}}=\mathbf{F}^*\overline{\mathbf{\Pi}}+\alpha^*\overline{\theta} \tag{5}$$

where overbar denotes the area average of a quantity over a representative area element(RAE) Ω, and the superscript "*" stands for the effective value.

To obtain the relations between the thermal and electroelastic moduli of a cracked medium, an auxiliary uniform temperature problem is considered in which following boundary conditions are prescribed:

$$\theta(S)=\theta^0, \quad \Pi(S)=0 \tag{6}$$

or

$$\theta(S)=\theta^0, \quad \mathbf{U}(S)=0 \tag{7}$$

where "S" stands for the external surface, the superscript "0" denotes constant, $\mathbf{U}=\{u_1\ u_2\ \phi\}^T$, u_i and ϕ are, respectively, the elastic displacements and the electric potential.

When the boundary conditions (6) are applied, it follows from the energy theorem that[7]

$$\overline{\Pi}=0, \quad \overline{\theta}=\theta^0, \quad \overline{\mathbf{Z}}=\alpha^*\theta^0, \quad \mathbf{Z}^{(1)}=\mathbf{F}^{(1)}\Pi+\alpha^{(1)}\theta \tag{8}$$

where superscript "(1)" denotes the moduli associated with the uncracked material. Likewise for the boundary conditions (7) the corresponding fields are defined as

$$\overline{\mathbf{Z}} = 0, \ \overline{\theta} = \theta^0, \ \overline{\Pi} = -\gamma^* \theta^0, \ \Pi^{(1)} = \mathbf{E}^{(1)}\mathbf{Z} - \gamma^{(1)}\theta \tag{9}$$

In the case of cracked body, the average strain and stress are defined on the basis of integral average are[5]

$$\overline{\mathbf{Z}} = \frac{1}{\Omega}\int_\Omega \mathbf{Z}^{(1)} d\Omega + \overline{\mathbf{Z}}^c, \quad \overline{\Pi} = \frac{1}{\Omega}\int_\Omega \Pi d\Omega = \overline{\Pi}^{(1)} \tag{10}$$

with

$$\overline{Z}_{ij}^c = \frac{1}{2\Omega}\sum_{k=1}^{M}\int_{l_k}\{[1 + H(i-3)]\Delta U_i' n_j' + \Delta U_j' n_i'\} dl \tag{11}$$

where M is the crack number within the area Ω, ΔU_i is the jump of elastic displacement(or electric potential) across the crack surfaces, l_k the length of k-th crack, the symbol $(\ )'$ stands for the related variable being measured in a coordinate system local to the kth crack, $\mathbf{n}' = \{0,\ 1\}^T$ is the normal local to the crack surface, and $H(x)$ is the Heaviside step function.

We obtain through use of (8) and (9)

$$\alpha^* \theta^0 = \alpha^{(1)}\theta^0 + \overline{\mathbf{Z}}^c, \ \gamma^* \theta^0 = \gamma^{(1)}\theta^0 - \mathbf{E}^{(1)}\overline{\mathbf{Z}}^c \tag{12}$$

From (10) to (12) it is immediately seen that the determination of the effective thermal expansion and pyroelectric constants requires a knowledge of the jump $\Delta\mathbf{U}$ across the cracks in a RAE when (6)[or (7)] is prescribed. For a microcrack-weakened medium an exact solution of $\Delta\mathbf{U}$ is not feasible and approximate methods are usually devised to determine $\Delta\mathbf{U}$ and thus the effective properties. The approximation of $\overline{\mathbf{Z}}^c$ through use of the dilute, self-consistent and Mori-Tanaka schemes is the subject of the subsequent section.

III. MICROMECHANICS APPROXIMATIONS

We start by developing the dilute approximation and then extend it to the self-consistent and Mori-Tanaka methods.

The dilute and self-consistent methods: The key assumption made in the dilute approximation is that the interaction among the cracks in a RAE can be ignored. Thus the strain $\overline{\mathbf{Z}}^c$ is obtained from the solution $\Delta\mathbf{U}$ of the auxiliary problem for a single crack embedded in an infinite matrix.

Consider the kth crack with half-length a in an infinite thermopiezoelectric sheet uniformly loaded with far field. Let (X_1, X_2) and (x_1, x_2) be the global and local coordinate systems. The jumps of displacements and electric potential(DEP) across the crack take the form[5]:

$$\Delta\mathbf{U}'(x_1) = -\mathbf{b}'\theta^0(a^2 - x_1^2)^{1/2} \qquad |x_1| < a \tag{13}$$

where $\mathbf{b}'$ was defined elsewhere[5].

The orientations and lengths of microcracks in the medium can be viewed as random variables and represented by a probability density function $p(a,\omega)$, which must satisfy the following normalising condition

$$\int_{a_{\min}}^{a_{\max}}\int_0^{\pi} p(a,\omega)\, da\, d\omega = 1 \tag{14}$$

where ω is the angle between X_1-axis and crack line under consideration.

Thus the overall effective thermal expansion and pyroelectric coefficients of the cracked sheet are

$$\alpha^*_{ij} = \alpha^{(1)}_{ij} + Z^c_{ij} / \theta^0 \tag{15}$$

where

$$Z^c_{ij} = -\frac{\pi M \theta^0}{4\Omega} \int_{a_{\min}}^{a_{\max}} a^2 \int_0^{\pi} p(a,\omega) \Psi_{ki} \Psi_{lj} \{[1 + H(k-3)] b'_k \, \delta_{2l} + b'_l \, \delta_{2k}\} da d\omega \tag{16}$$

$$\Psi = \begin{bmatrix} \cos\omega & \sin\omega & 0 \\ -\sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{17}$$

In particular, in the case of all microcrack with the same half-length a and uniform distribution in the orientation space, i.e.,

$$p(a,\omega) = 1/\pi \tag{18}$$

the microcrack-induced strain Z^c_{ij} are

$$Z^c_{ij} = -\frac{\varepsilon\theta^0}{4} \int_0^{\pi} \Psi_{ki} \Psi_{lj} \{[1 + H(k-3)] b'_k \, \delta_{2l} + b'_l \, \delta_{2k}\} d\omega \tag{19}$$

where $\varepsilon = Ma^2/\Omega$ stands for the crack density[5]

Substituting (19) into (12), the dilute method yields

$$\alpha^*_{ij} = \alpha^{(1)}_{ij} - \frac{\varepsilon}{4} \int_0^{\pi} \Psi_{ki} \Psi_{lj} \{[1 + H(k-3)] b'_k \, \delta_{2l} + b'_l \, \delta_{2k}\} d\omega \tag{20}$$

$$\gamma^*_{ij} = \gamma^{(1)}_{ij} + \frac{\varepsilon}{4} E_{im} \int_0^{\pi} \Psi_{km} \Psi_{lj} \{[1 + H(k-3)] b'_k \, \delta_{2l} + b'_l \, \delta_{2k}\} d\omega \tag{21}$$

Let us now extend the above analysis to the self-consistent method. By the method, we mean that the effect of microcrack interaction is taken into account approximately by embedding each crack directly in the effective medium. Therefore the algebraic equations resulting for effective moduli are formed through replacing $b^{(1)}_i$ in (20) and (21)[here we omit the superscript "(1)" for simplicity] by as-yet-unknown constants b^*_i. It can be seen from the expression of $\mathbf{b}$[5] that the effective thermal expansion and pyroelectric coefficients are related to the corresponding conductivity and isothermal electroelastic moduli, which is different from the conclusion obtained by Benveniste[2] in treating two-phase media. They showed in their papers that the effective thermal expansion and pyroelectric coefficients are only related to the corresponding isothermal electroelastic moduli.

<u>Mori-Tanaka method:</u> The key assumption in the Mori-Tanaka method[8] is that $\overline{\mathbf{Z}}^c$ is given by the solution for a single crack embedded in an infinite matrix subjected to an applied temperature field whose strain tensor equals to the as-yet-unknown average field in the matrix. By the assumption one sees[5]

$$\overline{Z}_{11} = (\overline{Z}_{11} + \widetilde{Z}_{11})(1 - I_{11}), \qquad \overline{Z}_{22} = (\overline{Z}_{22} + \widetilde{Z}_{22})(1 - I_{22}),$$
$$\overline{Z}_{32} = (\overline{Z}_{32} + \widetilde{Z}_{32})(1 - I_{32}) \tag{22}$$

where $\overline{Z}_{ij} = \alpha^*_{ij}\theta^0$, $\widetilde{Z}_{ij}$ are the perturbed strain due to the presence of the cracks, and I_{ij} are given by

$$I_{ij} = \frac{\varepsilon}{4\alpha_{ij}^{(1)}} \int_0^{\pi} \Psi_{ki} \Psi_{lj} \{[1 + H(k-3)] b'_k \delta_{2l} + b'_l \delta_{2k}\} d\omega \quad (i,\, j \text{ not summed}) \tag{23}$$

where $\alpha_{32}^{(1)} = \lambda_3^{(1)}$.

Solving (22) for $\tilde{Z}_{ij}$, we have

$$\begin{aligned} \tilde{Z}_{11} &= I_{11}\alpha_{11}^{*}\theta^0 / (1 - I_{11}), \quad \tilde{Z}_{22} = I_{11}\alpha_{33}^{*}\theta^0 / (1 - I_{22}), \\ \tilde{Z}_{32} &= I_{32}\lambda_3^{*}\theta^0 / (1 - I_{32}) \end{aligned} \tag{24}$$

through use of $\bar{Z}_{ij}^{c} = -\tilde{Z}_{ij}$.

The substitution of (24) into $(12)_2$, we have

$$\boldsymbol{\alpha}^{*} = (\mathbf{e}^{*} - \mathbf{p}\mathbf{e}^{(1)})^{-1}\mathbf{e}^{(1)}\boldsymbol{\alpha}^{(1)} \tag{25}$$

in which the superscript "-1" stands for the matrix inverse, c_{ij}^{*}, e_{ij}^{*}, κ_{ij}^{*} can be evaluated by way of the method given in our previous paper[5], $\boldsymbol{\alpha}^{(1)} = \{\alpha_{11}^{(1)},\, \alpha_{33}^{(1)},\, \lambda_3^{(1)}\}^T$, and

$$\mathbf{p} = diag[I_{11}/(1 - I_{11}),\, I_{22}/(1 - I_{22}),\, I_{32}/(1 - I_{32})],$$

$$\mathbf{e}^{(1)} = \begin{bmatrix} c_{11}^{(1)} & c_{13}^{(1)} & e_{31}^{(1)} \\ c_{13}^{(1)} & c_{33}^{(1)} & e_{33}^{(1)} \\ e_{31}^{(1)} & e_{33}^{(1)} & -\kappa_{33}^{(1)} \end{bmatrix}, \quad \begin{bmatrix} c_{11}^{*} & c_{13}^{*} & e_{31}^{*} \\ c_{13}^{*} & c_{33}^{*} & e_{33}^{*} \\ e_{31}^{*} & e_{33}^{*} & -\kappa_{33}^{*} \end{bmatrix}$$

It can be seen from (25) that the Mori-Tanaka theory provide explicit expressions for effective thermal expansion and pyroelectric coefficients of cracked thermopiezoelectric material, except the requirement for the knowledge of effective elastoelectric moduli and effective conductivity.

IV. CONCLUSION

The analytical solution for coupled thermoelectroelastic fields in a piezoelectric sheet containing a crack[5] has been implemented in three micromechanics models to determine the effective thermal expansion and pyroelectric coefficients of a microcrack-weakened piezoelectric material. The study shows that both the dilute and Mori-Tanaka methods return explicit expressions for α_{11}^{*}, α_{33}^{*} and λ_3^{*}. The self-consistent method, on the other hand, returns an implicit algebraic equation group for the α_{11}^{*}, α_{33}^{*} and λ_3^{*}. The study also shows that the effective thermal expansion and pyroelectric coefficients are related to both the corresponding conductivity and isothermal electroelastic moduli in the case of cracked piezoelectric materials, which is different from the conclusion obtained by Benveniste[2] in treating two-phase media. They showed in their paper that the thermal expansion and pyroelectric coefficients were only related to the corresponding isothermal electroelastic moduli.

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