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Mathematical modeling of electro-elastic dislocations in piezoelectric materials

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In this work, based on the theory of linear incompatible piezoelectricity with eigendistortion and eigenelectric field, the concept of electro-elastic dislocations is presented. Both field variables, the displacement vector $\boldsymbol{u}$ and the electrostatic potential φ, possess a jump discontinuity at the dislocation surface. Electro-elastic dislocations are described not only by the dislocation density tensor but also by a new introduced field, the so-called electric dislocation density vector. In addition to electro-elastic dislocations, inhomogeneities, body forces and body charges are also considered. Within this framework, material balance laws that correspond to the symmetries of translation, scaling and rotation are derived. All fundamental fields of configurational mechanics like the Eshelby stress tensor, the electro-elastic Peach-Koehler force, the Cherepanov force, the Eshelby force among others, which take place in the broken (translational, scaling and rotational) conservation laws anymore are given.

1 Introduction

Dislocations in piezoelectric materials can strongly influence the performance and properties of electronic devices. In this work, we use the terminology of an *electro-elastic dislocation* to refer to a dislocation in a piezoelectric material, that is characterized by the jump of the displacement vector and the jump of the electric potential along the dislocation surface. Studying dislocations in piezoelectric materials, Barnett and Lothe [1] were the first to mention that the jump in the electric potential corresponds to an electric dipole layer along the cut plane. Using the concept of the electric dislocation density vector, Agiasofitou and Lazar [2] have proven that an electric dislocation loop represents an electric dipole layer.

The derivation of material balance laws corresponding to the symmetries of translations, scaling and rotation is essential, since these laws provide all primary quantities such as the configurational forces, configurational work and configurational vector moments which are respectively represented by the $\boldsymbol{J}$-, M- and $\boldsymbol{L}$-integrals, which are powerful tools in the study of problems of piezoelectric materials suffering by dislocations. It is well-known that the $\boldsymbol{J}$-integral of dislocations is equivalent to the Peach-Koehler force. In the framework of three-dimensional incompatible linear elasticity, Agiasofitou and Lazar [3] have given the physical interpretation of the M- and $\boldsymbol{L}$-integrals of dislocations. The M-integral of two straight dislocations represents the interaction energy (depending on the distance and on the angle) between the two dislocations and the $\boldsymbol{L}$-integral represents the configurational vector moment or rotational moment (torque) caused by the interaction of the two dislocations. Furthermore, Lazar and Agiasofitou [4] showed that the M-integral (per unit length) of a single dislocation represents the total energy of the dislocation which is the sum of the self energy (per unit length) of the dislocation and the dislocation core energy (per unit length). The latter can be identified with the work produced by the Peach-Koehler force and equals twice the corresponding pre-logarithmic energy factor. Moreover, through the comparison of the $\boldsymbol{J}$-, M- and $\boldsymbol{L}$-integrals of body charges and point charges in electrostatics and the $\boldsymbol{J}$-, M- and $\boldsymbol{L}$-integrals of body forces and point forces in elasticity in [5], a deeper insight has been achieved showing that the $\boldsymbol{J}$-, M- and $\boldsymbol{L}$-integrals are fundamental concepts which can be applied in any field theory.

2 The concept of electro-elastic dislocations

The theory of linear incompatible piezoelectricity with eigendistortion and eigenelectric field is considered. The notion of the eigenelectric field vector concerning problems of dislocations in piezoelectric materials has been used by Nowacki [6] but described as "external" source field. The first one who used the terminology of the eigenelectric field in dislocations is Wang [7]. Based on this notion, we proceed to define an additional defect measure, the electric dislocation density vector, necessary for the description of the jump of the electrostatic potential.

The total distortion tensor β^{T}_{ij}, which is defined as the spatial gradient of the displacement vector u_i, is decomposed into elastic and plastic parts

$$\beta^{\mathrm{T}}_{ij} := u_{i,j} = \beta_{ij} + \beta^*_{ij}\,, \tag{1}$$

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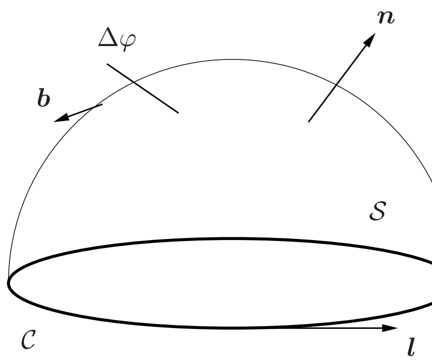

Fig. 1: Electro-elastic dislocation loop.

where β_{ij} is the *elastic distortion tensor* and β^*_{ij} is the *eigendistortion* or *plastic distortion tensor*. The subscript comma denotes partial differentiation with respect to the spatial coordinates x_j. Moreover, the *Maxwell-Faraday electric field vector* E_i^M, which is defined as the negative gradient of the *electrostatic potential* φ, is decomposed into the *electric field strength vector* E_i and the *eigenelectric field vector* E^*_i as follows

$$E_i^M := -\varphi_{,i} = E_i - E^*_i \, . \tag{2}$$

We consider a variational problem with the Lagrangian density $\mathcal{L}$ depending on the field variables $\boldsymbol{u}$ and φ for prescribed body forces and body charges as well as for prescribed eigendistortion and eigenelectric field, which is defined by

$$\mathcal{L} = \mathcal{L}(u_i, u_{i,j}, \varphi, \varphi_{,i}) = -\mathcal{H}(\beta_{ij}, E_i) - \mathcal{V}(u_i, \varphi) \tag{3}$$

with $\mathcal{H}$ being the *electric enthalpy density*

$$\mathcal{H}(\beta_{ij}, E_i) = \frac{1}{2}\,\sigma_{ij}\beta_{ij} - \frac{1}{2}\,D_i E_i \, , \tag{4}$$

where σ_{ij} is the *Cauchy stress tensor* and D_i is the *electric displacement vector* and $\mathcal{V}$ being the *electro-elastic potential* of the *body force density* f_i and the *body charge density* q

$$\mathcal{V}(u_i, \varphi) = -f_i u_i + q\varphi \, . \tag{5}$$

For a linear piezoelectric material, the electric enthalpy density is given by [8]

$$\mathcal{H} = \frac{1}{2}\,C_{ijkl}\beta_{ij}\beta_{kl} - e_{ijk}E_i\beta_{jk} - \frac{1}{2}\,\varepsilon_{ij}E_iE_j \, , \tag{6}$$

where C_{ijkl} is the *tensor of the elastic moduli* measured in a constant electric field, e_{ijk} is the *tensor of the piezoelectric moduli* and ε_{ij} is the *tensor of the dielectric moduli* measured at constant strain possessing the symmetries

$$C_{ijkl} = C_{klij} = C_{ijlk} = C_{jikl} \, , \quad e_{kij} = e_{kji} \, , \quad \varepsilon_{ij} = \varepsilon_{ji} \, . \tag{7}$$

The Euler-Lagrange equations associated to the Lagrangian density (3) provide the *force equilibrium condition*

$$\sigma_{ij,j} + f_i = 0 \tag{8}$$

and the *Gauss law of electrostatics*

$$D_{j,j} = q \, , \tag{9}$$

accompanied by the following constitutive relations

$$\sigma_{ij} = \frac{\partial \mathcal{H}}{\partial \beta_{ij}} = C_{ijkl}\beta_{kl} - e_{lij}E_l \, , \tag{10}$$

$$D_j = -\frac{\partial \mathcal{H}}{\partial E_j} = e_{jkl}\beta_{kl} + \varepsilon_{jl}E_l \, . \tag{11}$$

An *electro-elastic dislocation* is a line defect $\mathcal{C}$, which is the boundary of the dislocation surface $\mathcal{S}$ where both fields, the displacement vector $\boldsymbol{u}$ and the electrostatic potential φ possess a jump. The jump of the displacement vector is the Burgers vector $\boldsymbol{b}$, and the jump of the electrostatic potential $\Delta\varphi$ corresponds to the potential discontinuity of an electric dipole layer along the surface $\mathcal{S}$ as it has been shown in [2] (see also Figure 1).

The *dislocation density tensor* is defined by

$$\alpha_{ij} = -\epsilon_{jkl}\beta^*_{il,k} \quad \text{or} \quad \alpha_{ij} = \epsilon_{jkl}\beta_{il,k} \,. \tag{12}$$

The Burgers vector b_i is given by

$$b_i = \int_\sigma \alpha_{ij}\,\mathrm{d}S_j = -\oint_\gamma \beta^*_{ij}\,\mathrm{d}l_j = \oint_\gamma \beta_{ij}\,\mathrm{d}l_j \,, \tag{13}$$

where γ is the Burgers circuit, σ is the Burgers surface bounded by γ, $\mathrm{d}S_j$ is the area element and $\mathrm{d}l_j$ is the corresponding line element. The *electric dislocation density vector* is given by

$$A_j = -\epsilon_{jkl}E^*_{l,k} \quad \text{or} \quad A_j = -\epsilon_{jkl}E_{l,k} \,. \tag{14}$$

Analogous to Eq. (13), the jump of the electrostatic potential $\Delta\varphi$ can be written as the surface integral of the electric dislocation density vector

$$\Delta\varphi = \int_\sigma A_j\,\mathrm{d}S_j = -\oint_\gamma E^*_j\,\mathrm{d}l_j = -\oint_\gamma E_j\,\mathrm{d}l_j \,. \tag{15}$$

It can be seen that the above definitions of the electro-elastic dislocation and of the electric dislocation density vector are not restricted to piezoelectric materials.

3 Configurational fields: forces, work and vector moments

Based on the calculus of variations (see, e.g., [9, 10]), we consider an arbitrary infinitesimal functional derivative δH of the electric enthalpy

$$H = \int_V \mathcal{H}\,\mathrm{d}V \,, \tag{16}$$

where V is the volume of the three-dimensional body. The material balance laws which correspond to translation, scaling and rotation groups of transformations for a piezoelectric material with electro-elastic dislocations are derived. For the detailed derivation, the reader is addressed to [2].

3.1 Configurational forces and J-integral

We specify the functional derivative to be translational

$$\delta = (\delta x_k)\partial_k \,, \tag{17}$$

where (δx_k) is an infinitesimal translation in the x_k-direction and $\partial_k = \partial/\partial x_k$.

The *global translational balance law for incompatible piezoelectricity* reads as

$$\begin{aligned}\int_V \partial_j \big[\mathcal{H}\delta_{jk} - \sigma_{ij}\beta_{ik} + D_jE_k\big]\mathrm{d}V \\ = \int_V \Big\{\epsilon_{kjl}\sigma_{ij}\alpha_{il} + \epsilon_{kjl}D_jA_l + f_i\beta_{ik} + qE_k \\ + \frac{1}{2}\,\beta_{ij}[\partial_k C_{ijmn}]\beta_{mn} - E_j[\partial_k e_{jmn}]\beta_{mn} - \frac{1}{2}\,E_i[\partial_k\varepsilon_{ij}]E_j\Big\}\mathrm{d}V \,.\end{aligned} \tag{18}$$

The quantity in the divergence in the first integral of Eq. (18) is the so-called *Eshelby stress tensor of piezoelectricity*

$$P_{kj} = \mathcal{H}\delta_{jk} - \sigma_{ij}\beta_{ik} + D_jE_k \,. \tag{19}$$

The integral on the right-hand side of Eq. (18) contains terms breaking the translational symmetry and defines a sum of the so-called *configurational* or *material force densities*

$$\begin{aligned}f^{\text{conf}}_k &= \epsilon_{kjl}\sigma_{ij}\alpha_{il} + \epsilon_{kjl}D_jA_l + f_i\beta_{ik} + qE_k + \frac{1}{2}\,\beta_{ij}[\partial_k C_{ijmn}]\beta_{mn} - E_j[\partial_k e_{jmn}]\beta_{mn} - \frac{1}{2}\,E_i[\partial_k\varepsilon_{ij}]E_j \\ &= f^{\text{eePK}}_k + f^{\text{C}}_k + f^{\text{L}}_k + f^{\text{inh}}_k \,.\end{aligned} \tag{20}$$

These *configurational* or *material force densities* have different physical origin and interpretation as follows:

- *The electro-elastic Peach-Koehler force density*

$$f_k^{\mathrm{eePK}} = \epsilon_{kjl}\left(\sigma_{ij}\alpha_{il} + D_j A_l\right) , \tag{21}$$

which is the configurational force density on an electro-elastic dislocation with dislocation density tensor α_{il} and electric dislocation density vector A_l in presence of a stress σ_{ij} and an electric displacement D_j, respectively.

- *The Cherepanov force density*

$$f_k^{\mathrm{C}} = f_i\beta_{ik} , \tag{22}$$

which is the configurational force density on a body force density f_i in presence of an elastic distortion β_{ik}. This means that the existence of a body force density causes the existence of a configurational force density, namely the Cherepanov force density.

- *The electrostatic part of the Lorentz force density*

$$f_k^{\mathrm{L}} = qE_k , \tag{23}$$

which is the electric configurational force density on a body charge density q in presence of an electric field E_k.

- *The piezoelectric inhomogeneity force density* or *Eshelby force density for piezoelectric materials*

$$f_k^{\mathrm{inh}} = \frac{1}{2}\,\beta_{ij}[\partial_k C_{ijmn}]\beta_{mn} - E_j[\partial_k e_{jmn}]\beta_{mn} - \frac{1}{2}\,E_i[\partial_k \varepsilon_{ij}]E_j , \tag{24}$$

which appears due to the gradient of the constitutive tensors when the piezoelectric material is non-homogeneous.

The global translational balance law for incompatible piezoelectricity (18) with the definitions (19) and (20) is alternatively written as

$$J_k = \int_V \partial_j P_{kj}\,\mathrm{d}V = \int_V f_k^{\mathrm{conf}}\,\mathrm{d}V , \tag{25}$$

representing the vectorial $\boldsymbol{J}$*-integral for incompatible piezoelectricity* for a non-homogeneous piezoelectric medium with electro-elastic dislocations in presence of body forces and body charges. It possesses contributions due to electro-elastic dislocations, body forces, body charges and inhomogeneities.

3.2 Configurational work and M-integral

Let us consider scaling transformations here, specifying the functional derivative to be dilatational

$$\delta = x_k\partial_k . \tag{26}$$

The *global balance law for scaling transformations in incompatible piezoelectricity* reads as

$$\int_V \partial_j\Big[x_k P_{kj} - \frac{d-2}{2}\left(u_k\sigma_{kj} + \varphi D_j\right)\Big]\mathrm{d}V = \int_V \Big\{x_k f_k^{\mathrm{conf}} + \frac{d-2}{2}\Big(f_i u_i - q\varphi - \beta^*_{ij}\sigma_{ij} - E^*_j D_j\Big)\Big\}\mathrm{d}V , \tag{27}$$

where $d = \delta_{kk}$ is the space dimension. The quantity in the divergence in the first integral of Eq. (27) is the *dilatation* or *scaling flux vector for incompatible piezoelectricity*

$$Y_j = x_k P_{kj} - \frac{d-2}{2}\left(u_k\sigma_{kj} + \varphi D_j\right) . \tag{28}$$

The integral on the right-hand side of Eq. (27) contains terms breaking the dilatation or scaling symmetry and form the *total configurational* or *material work density*

$$w^{\mathrm{tot}} = w^{\mathrm{conf}} + w^{\mathrm{intr}}, \tag{29}$$

containing the following two terms:

- the *configurational work density* produced by the configurational force density (20)

$$w^{\mathrm{conf}} = x_k f_k^{\mathrm{conf}} , \tag{30}$$

- the *intrinsic* or *field work density* produced by the body force density, body charge density, eigendistortion and eigenelectric fields

$$w^{\text{intr}} = \frac{d-2}{2}\Big(f_i u_i - q\varphi - \beta^*_{ij}\sigma_{ij} - E^*_j D_j\Big)\,. \tag{31}$$

The factor

$$d_u = d_\varphi = -\frac{d-2}{2} \tag{32}$$

is the *scaling* or *canonical dimension* and it is the same for both fields, the displacement vector u_k and the electrostatic potential φ.

The global balance law for scaling transformations in incompatible piezoelectricity (27) via the definitions (28) and (29) provides the *M-integral for incompatible piezoelectricity*

$$M = \int_V \partial_j Y_j \,\mathrm{d}V = \int_V w^{\text{tot}}\,\mathrm{d}V \tag{33}$$

for a non-homogeneous piezoelectric medium with electro-elastic dislocations in presence of body forces and body charges. The M-integral (33) represents the total configurational or material work.

It is of great importance the fact that the global balance law for scaling transformations (27) depends on the space dimension. In the case of study of two-dimensional problems, the second parts of the appearing integrals vanish and the contribution of the eigenfields (plastic fields) is lost. A fact that has caused many misunderstandings in the past about the M-integral and its physical interpretation having as a result less applications (see related discussion in [2]). A dislocation is a line defect in a three-dimensional crystal, hence $d = 3$. Therefore, for studying dislocations as well as other three-dimensional problems in Engineering Science, the appropriate formula of the M-integral is the one with $d = 3$. Therefore, for the problem under study, the scaling flux vector and the M-integral are given by the following formulas

$$Y_j = x_k P_{kj} - \frac{1}{2}\big(u_k\sigma_{kj} + \varphi D_j\big) \tag{34}$$

and

$$M = \int_V \partial_j\Big[x_k P_{kj} - \frac{1}{2}\big(u_k\sigma_{kj} + \varphi D_j\big)\Big]\mathrm{d}V = \int_V \Big\{x_k f^{\text{conf}}_k + \frac{1}{2}\Big(f_i u_i - q\varphi - \beta^*_{ij}\sigma_{ij} - E^*_j D_j\Big)\Big\}\,\mathrm{d}V\,. \tag{35}$$

3.3 Configurational vector moments and *L*-integral

We specify here the functional derivative to be rotational

$$\delta = (\delta x_k)\epsilon_{kji} x_j \partial_i\,, \tag{36}$$

where (δx_k) denotes the x_k-direction of the axis of rotation.

The *global rotational balance law for incompatible piezoelectricity* reads as

$$\int_V \epsilon_{kji}\partial_l\big[x_j P_{il} + u_j\sigma_{il}\big]\mathrm{d}V = \int_V \epsilon_{kji}\Big[x_j f^{\text{conf}}_i - u_j f_i + \beta^*_{jl}\sigma_{il} + \beta_{jl}\sigma_{il} + \beta_{lj}\sigma_{li} - E_j D_i\Big]\mathrm{d}V\,. \tag{37}$$

In the integral on the left-hand side of Eq. (37) appears the divergence of the *angular momentum tensor for incompatible piezoelectricity*

$$M_{kl} = \epsilon_{kji}\big[x_j P_{il} + u_j\sigma_{il}\big] = M^{(\mathrm{o})}_{kl} + M^{(\mathrm{i})}_{kl} \tag{38}$$

consisting of two parts:

- the *orbital angular momentum tensor* given in terms of the Eshelby stress tensor (19)

$$M^{(\mathrm{o})}_{kl} = \epsilon_{kji} x_j P_{il}\,, \tag{39}$$

- the *intrinsic* or *spin angular momentum tensor* given in terms of the displacement vector and the Cauchy stress tensor

$$M^{(\mathrm{i})}_{kl} = \epsilon_{kji} u_j \sigma_{il}\,. \tag{40}$$

The integrand of the integral on the right-hand side of Eq. (37) is the *total configurational* or *material vector moment density*

$$m_k^{\text{tot}} = m_k^{\text{conf}} + m_k^{\text{intr}} + m_k^{\text{anis}} \tag{41}$$

containing terms breaking the rotational symmetry, which are:

- the *configurational vector moment density* produced by the configurational force density f_i^{conf} given in Eq. (20)

$$m_k^{\text{conf}} = \epsilon_{kji} x_j f_i^{\text{conf}} , \tag{42}$$

- the *intrinsic* or *field vector moment density* due to the body force density vector and the eigendistortion tensor

$$m_k^{\text{intr}} = -\epsilon_{kji} (u_j f_i - \beta^*_{jl} \sigma_{il}) , \tag{43}$$

- the *configurational vector moment density* due to the material anisotropy

$$m_k^{\text{anis}} = \epsilon_{kji} (\beta_{jl} \sigma_{il} + \beta_{lj} \sigma_{li} - E_j D_i) . \tag{44}$$

The global rotational balance law for incompatible piezoelectricity (37) with the definitions (38) and (41), is written as

$$L_k = \int_V \partial_j M_{kj} \, \mathrm{d}V = \int_V m_k^{\text{tot}} \, \mathrm{d}V , \tag{45}$$

representing the *vectorial* $\boldsymbol{L}$*-integral for incompatible piezoelectricity* for a non-homogeneous piezoelectric medium with electro-elastic dislocations in presence of body forces and body charges.

It is important to notice that in piezoelectricity, even if the material is dislocation-free, homogeneous and body forces and body charges are absent, the *"isotropy condition"* is not fulfilled

$$m_k^{\text{anis}} = \epsilon_{kji} \big[\beta_{jl} \sigma_{il} + \beta_{lj} \sigma_{li} - E_j D_i \big] \neq 0 , \tag{46}$$

due to the anisotropic character of the constitutive relations (10) and (11). Hence, the $\boldsymbol{L}$-integral cannot be zero or a conserved integral (see also [2]).

4 Conclusion

In the presenting mathematical modeling of electro-elastic dislocations in piezoelectric materials, two eigenfields are considered: the eigendistortion tensor and the eigenelectric field vector. The $curl$ of these two eigenfields defines two "dislocation densities": the dislocation density tensor and the electric dislocation density vector, respectively. The last serves as an additional defect measure necessary for the description of the jump of the electrostatic potential at the dislocation surface. This framework enables to capture the "full" force with elastic and electric contributions acting on an electro-elastic dislocation, that is the so-called electro-elastic Peach-Kohler force. The $\boldsymbol{J}$-, M- and $\boldsymbol{L}$-integrals of piezoelectric materials with electro-elastic dislocations in presence of body forces, body charges and inhomogeneities have been derived. The vectorial $\boldsymbol{J}$-integral represents the total configurational or material force, the M-integral represents the total configurational or material work and the vectorial $\boldsymbol{L}$-integral represents the total configurational or material vector moment. The explicit expressions of the above integrals for straight dislocations as well as for dislocation loops are given in [2].

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