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Perfectly Matched Layers for Elastic Waves in Piezoelectric Solids

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The material constants of perfectly matched layers (PMLs) for elastic waves in piezoelectric solids in orthogonal coordinates, such as the cylindrical and spherical coordinates, in the frequency domain were derived from the differential form. Using the coordinate transformation laws of tensors, the quotient rule, and complex coordinate stretching, we obtained the material parameters of PMLs in the real coordinate. Our results on stress and piezoelectric stress constants are different from the parameters determined by the analytic continuation because we include or exclude the transformation of the contravariant components in the differential form or the analytic continuation, respectively. The presented results are extensions of our results for anisotropic solids without piezoelectricity.

1. Introduction

Perfectly matched layers (PMLs) for elastic and electromagnetic waves are widely used in the finite-difference time-domain (FD-TD) method and the finite element method (FEM). A PML is an absorbing boundary condition for truncating the computational domain of open regions without reflection of oblique incident waves. In 1994, Berenger invented a PML for electromagnetic waves in the FD-TD method by a splitting field method.[1] The extension of PMLs to elastic waves in isotropic solids in the Cartesian coordinate first appeared in 1996.[2,3] In the cylindrical and spherical coordinates, PMLs were presented by a splitting field method in isotropic solids in 1999[4] and by analytic continuation or complex coordinate stretching[5,6] in anisotropic solids in 2002.[7] Recently, the validity and usefulness of PMLs derived from the analytic continuation in piezoelectric solids was demonstrated.[8–10]

We recommend that readers who are unfamiliar with PMLs consult Taflove and Hagness[11] about PMLs in electromagnetic waves, Kucukcoban and Kallivokas,[12] and Basu and Chopra[13] about the FEM implementation of PMLs in transient and time-harmonic elastodynamics, respectively.

From the differential form, we have derived PMLs for elastic waves in the Cartesian,[14] cylindrical, and spherical coordinates[15] and demonstrated the validity of our PML con-

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stants.[14,16] Our derivation revealed that the contravariant components of stress tensors and the particle displacement vectors in the analytic continuation are not transformed into real space.[14] Therefore, the discrepancy in the stiffness constants derived from the two methods, one is based on the differential form[14,16] and the other use analytic continuation,[7] exists.

In this paper, we examine the derivation of PMLs of elastic wave propagation in piezoelectric solids from the differential form. PML material parameters in the orthogonal coordinate systems such as the Cartesian, cylindrical, and spherical coordinates are presented. A discrepancy in piezoelectric stress constants exists in addition to the stiffness constants appeared in nonpiezoelectric solids in the Cartesian[14] and cylindrical coordinates.[15] The different transformation rules for the contravariant components cause this discrepancy.

2. Differential Form of the Quasi-Static Electromagnetic Fields

Using a quasi-static approximation of electromagnetic fields in piezoelectric solids with omission of rotational electric fields and representing irrotational electric fields as $\mathbf{E} = -d\phi$, we consider the electric potentials ϕ, the irrotational electric fields $\mathbf{E}$, electrical displacements $\mathbf{D}$, and the Gauss law in the piezoelectric solids for computing elastic fields that couple with electromagnetic fields. Here, d is the exterior differential operator.

The electric potentials are scalars, whose tensor type is contravariant and covariant of rank 0. Two vector fields $\mathbf{E}$ and $\mathbf{D}$ in the differental forms in a coordinate (x^0, x^1, x^2) are given as follows:

$$\mathbf{E} = E_{x\alpha} dx^{\alpha}, \quad (1)$$

$$\mathbf{D} = \frac{1}{2} D_{x\alpha\beta} dx^{\alpha} \wedge dx^{\beta}. \quad (2)$$

Here, $dx^i (i = 0, 1, 2)$ is a covariant basis vector, and $\wedge$ represents the exterior product. Note that the summation convention is used. Changing the coordinate gives the relations of tensor components: for $\mathbf{E} = E_{X\alpha} dX^{\alpha} = E_{x\beta} dx^{\beta}$ and $\mathbf{D} = D_{X\alpha_1\alpha_2} dX^{\alpha_1} \wedge dX^{\alpha_2} = D_{x\beta_1\beta_2} dx^{\beta_1} \wedge dx^{\beta_2}$, the relations of the components are $E_{X\alpha} = E_{x\beta} \partial x^{\beta} / \partial X^{\alpha}$ and $D_{X\alpha_1\alpha_2} = D_{x\beta_1\beta_2} \partial x^{\beta_1} / \partial X^{\alpha_1} \partial x^{\beta_2} / \partial X^{\alpha_2}$, respectively. Using the complex coordinate stretching[5–7] given by

$$X^i = \int^{x^i} \tilde{s}_i(\tau) d\tau = \int^{x^i} \tilde{s}_{i\mathrm{R}}(\tau) + \mathrm{j} \tilde{s}_{i\mathrm{I}}(\tau) d\tau$$

with the two real functions $\tilde{s}_{i\mathrm{R}}(\tau)$ and $\tilde{s}_{i\mathrm{I}}(\tau)$, we have the relations

$$E_{X\alpha} = \frac{E_{x\alpha}}{\tilde{s}_{\alpha}(x^{\alpha})}, \quad (3)$$

$$D_{X\alpha_1\alpha_2} = \frac{D_{x\alpha_1\alpha_2}}{\tilde{s}_{\alpha_1}(x^{\alpha_1}) \tilde{s}_{\alpha_2}(x^{\alpha_2})}. \quad (4)$$

Here, j is the imaginary unit.

3. Material Constants of PMLs for Elastic Waves in Piezoelectric Solids

In complex coordinate stretching, we consider that the real coordinate (x^0, x^1, x^2) is any orthogonal coordinate system: for example, (x^0, x^1, x^2) identifies (x, y, z), (r, θ, z), or (r, θ, ϕ) for the Cartesian, cylindrical, or the spherical coordinates, respectively.

3.1 Constitutive equations in a complex coordinate

Assuming that the same constitutive equations in the real coordinate (x^0, x^1, x^2) exist in the complex coordinate (X^0, X^1, X^2), we have

$$\mathbf{P}^{\mathrm{c}} = \rho \mathbf{v}^{\mathrm{c}}, \tag{5}$$

$$T_{ij}^{\mathrm{c}} = C_{ijkl} F_{kl}^{\mathrm{c}} - \underline{e_{ijk}} E_k^{\mathrm{c}}, \tag{6}$$

$$D_i^{\mathrm{c}} = e_{ikl} F_{kl}^{\mathrm{c}} + \epsilon_{ik}^{\mathrm{S}} E_k^{\mathrm{c}}. \tag{7}$$

Here, the superscript c denotes the value in the complex coordinate. $\mathbf{P}$, $\mathbf{v}$, T_{ij}, and F_{kl} are the vector of the density of momentum, a particle velocity vector, the ij-component of a stress tensor ($i, j = X^0, X^1, X^2$), and the kl-component ($k, l = X^0, X^1, X^2$) of a displacement gradient tensor, respectively. The mass density ρ, the stiffness C_{ijkl} ($i, j, k, l = X^0, X^1, X^2$), the piezoelectric stress constants $\underline{e_{ijk}}$, e_{ikl}, and the permittivity at the constant strain $\epsilon_{ik}^{\mathrm{S}}$ are the values corresponding to the original material parameters of a PML in the real coordinate.

3.2 Rules of transformation from tensors in the complex coordinate into the tensors in the real coordinate

Using Eqs. (3) and (4), and replacing the base differentials with the unit vectors, we obtain

$$E_i^{\mathrm{c}} = \frac{1}{s_i} E_i \ \text{(no summation)}, \tag{8}$$

$$D_i^{\mathrm{c}} = \frac{s_i}{s_0 s_1 s_2} D_i \ \text{(no summation)}. \tag{9}$$

Here, $s_i = (h_i^{\mathrm{c}}/h_i^{\mathrm{r}})\tilde{s}_i$ where h_i^{r} and h_i^{c} are the scale factors of the general orthogonal coordinate systems (x^0, x^1, x^2) and (X^0, X^1, X^2), respectively. Note that the scale factors h_i are given as follows: $h_0 = 1, h_1 = r, h_2 = 1$ in the cylindrical coordinate (r, θ, z); $h_0 = 1, h_1 = r, h_2 = r \sin\theta$ in the spherical coordinate (r, θ, ϕ); and $h_0 = h_1 = h_2 = 1$ in the Cartesian coordinate (x, y, z).

In our previous paper,[15] the following relations were reported:

$$T_{ij}^{\mathrm{c}} = \frac{s_i s_j}{s_0 s_1 s_2} T_{ij} \ \text{(no summation)}, \tag{10}$$

$$F^{c}_{ij} = \frac{s_i}{s_j} F_{ij} \quad \text{(no summation).} \tag{11}$$

3.3 Derivation of PML constants

The quotient rule and Eqs. (6)- (11) yield PML material constants: the permittivity and piezoelectric stress constants are

$$\underline{e^{\mathrm{PML}}_{ijk}} = \frac{s_o s_1 s_2}{s_i s_j s_k} \underline{e_{ijk}} \quad \text{(no summation),} \tag{12}$$

$$e^{\mathrm{PML}}_{ikl} = \frac{s_0 s_1 s_2 s_k}{s_i s_l} e_{ikl} \quad \text{(no summation),} \tag{13}$$

$$\epsilon^{\mathrm{PML}}_{ik} = \frac{s_0 s_1 s_2}{s_i s_k} \epsilon_{ik} \quad \text{(no summation).} \tag{14}$$

Here, $s_0 = \tilde{s}_0$, $s_1 = (R/r)\tilde{s}_1$, $s_2 = \tilde{s}_2$ in the cylindrical coordinate system (r, θ, z) with its complex coordinate (R, Θ, Z); $s_0 = \tilde{s}_0$, $s_1 = (R/r)\tilde{s}_1$, $s_2 = [(R \sin\Theta)/(r \sin\theta)]\tilde{s}_2$ in the spherical coordinate system (r, θ, ϕ) with its complex coordinate (R, Θ, Φ); and $s_i = \tilde{s}_i$ in the Cartesian coordinate system. In addition, the stiffness is

$$C^{\mathrm{PML}}_{ijkl} = \frac{s_0 s_1 s_2 s_k}{s_i s_j s_l} C_{ijkl} \quad \text{(no summation).} \tag{15}$$

Note that this result of the stiffness and mass density ρ^{PML} shown below were presented in our previous paper.[15)]

$$\rho^{\mathrm{PML}} = s_0 s_1 s_2 \rho. \tag{16}$$

Equations (12)-(16) show that the PML parameters for elastic waves in solids in any orthogonal coordinate system such as the cylindrical and spherical coordinates must be calculated by the same procedure as that used for the parameters in the Cartesian coordinates.

4. Derivation of Piezoelectric PML Constants in the Cylindrical and Spherical Coordinates from the Analytic Continuation

We present procedures of deriving material constants in the Cartesian, cylindrical, and spherical coordinates from the analytic continuation.

4.1 Transformation rules derived from the analytic continuation

The transformation rules of the stress tensors, the displacement gradient, and the mass density in the Cartesian, cylindrical, and spherical coordinates have been derived by the analytic continuation and reported[7, 15)] as follows:

$$T^{c}_{ij} = \frac{s_j}{s_0 s_1 s_2} T^{\mathrm{PMLA}}_{ij} \quad \text{(no summation),} \tag{17}$$

$$F^{\mathrm{c}}_{kl} = \frac{1}{s_l} F^{\mathrm{PMLA}}_{kl} \quad \text{(no summation)}, \tag{18}$$

$$\rho^{\mathrm{PMLA}} = s_0 s_1 s_2 \rho. \tag{19}$$

Here, the superscript PMLA denotes the value translated by the rules with the analytic continuation into the real coordinate. Note that the transformation rules derived from the analytic continuation for the generalized orthogonal coordinate system were not reported.

In this subsection, we present a derivation of the transformation rules of the electric field and electrical displacement from $\mathbf{E}^{\mathrm{c}} = -\nabla\phi^{\mathrm{c}}$ and $\nabla \cdot \mathbf{D}^{\mathrm{c}} = 0$ in the complex coordinate.

The irrotational electric fields in the complex coordinate are represented as $\mathbf{E}^{\mathrm{c}} = -\nabla\phi^{\mathrm{c}}$:

$$\mathbf{E}^{\mathrm{c}} = -\Big(\hat{X}^0 \frac{1}{h^{\mathrm{c}}_0}\frac{\partial}{\partial X^0} + \hat{X}^1 \frac{1}{h^{\mathrm{c}}_1}\frac{\partial}{\partial X^1} + \hat{X}^2 \frac{1}{h^{\mathrm{c}}_2}\frac{\partial}{\partial X^2}\Big)\phi^{\mathrm{c}}. \tag{20}$$

Using $\partial/\partial X^i = (1/\tilde{s}_i)(\partial/\partial x^i)$ and $h^{\mathrm{r}}_i s_i = h^{\mathrm{c}}_i \tilde{s}_i$, we obtain

$$\mathbf{E}^{\mathrm{c}} = -\Big(\hat{X}^0 \frac{1}{h^{\mathrm{r}}_0 s_0}\frac{\partial}{\partial x^0} + \hat{X}^1 \frac{1}{h^{\mathrm{r}}_1 s_1}\frac{\partial}{\partial x^1} + \hat{X}^2 \frac{1}{h^{\mathrm{r}}_2 s_2}\frac{\partial}{\partial x^2}\Big)\phi^{\mathrm{c}}. \tag{21}$$

Note that this equation is in the real coordinate.

On the other hand, in the real coordinate, the same equation $\mathbf{E}^{\mathrm{PLMA}} = -\nabla\phi^{\mathrm{PMLA}}$ is given by

$$\mathbf{E}^{\mathrm{PMLA}} = -\Big(\hat{x}^0 \frac{1}{h^{\mathrm{r}}_0}\frac{\partial}{\partial x^0} + \hat{x}^1 \frac{1}{h^{\mathrm{r}}_1}\frac{\partial}{\partial x^1} + \hat{x}^2 \frac{1}{h^{\mathrm{r}}_2}\frac{\partial}{\partial x^2}\Big)\phi^{\mathrm{PMLA}}. \tag{22}$$

Using the assumptions of identifying of the unit vectors, $\hat{X}^i = \hat{x}^i$ in the analytic continuation, and recalling that $\phi^{\mathrm{c}} = \phi^{\mathrm{PMLA}}$ because of the transformation rule of scalar functions, we determine the relation of the electric fields as

$$E^{\mathrm{c}}_i = \frac{E^{\mathrm{PMLA}}_i}{s_i} \quad \text{(no summation)}. \tag{23}$$

The Gauss law in the complex coordinate (X^0, X^1, X^2) is given by $\nabla \cdot \mathbf{D}^{\mathrm{c}} = 0$:

$$\frac{1}{h^{\mathrm{c}}_0 h^{\mathrm{c}}_1 h^{\mathrm{c}}_2}\Big(\frac{\partial}{\partial X^0}(D^{\mathrm{c}}_0 h^{\mathrm{c}}_1 h^{\mathrm{c}}_2) + \frac{\partial}{\partial X^1}(D^{\mathrm{c}}_1 h^{\mathrm{c}}_2 h^{\mathrm{c}}_0) + \frac{\partial}{\partial X^2}(D^{\mathrm{c}}_2 h^{\mathrm{c}}_0 h^{\mathrm{c}}_1)\Big) = 0. \tag{24}$$

Multiplying Eq. (24) by $s_0 s_1 s_2$, and using $\frac{\partial}{\partial X^i} = \frac{1}{\tilde{s}_i}\frac{\partial}{\partial x^i}$, we obtain

$$\frac{1}{h^{\mathrm{r}}_0 h^{\mathrm{r}}_1 h^{\mathrm{r}}_2}\Big(\tilde{s}_1\tilde{s}_2 \frac{\partial}{\partial x^0}(D^{\mathrm{c}}_0 h^{\mathrm{c}}_1 h^{\mathrm{c}}_2) + \tilde{s}_2\tilde{s}_0 \frac{\partial}{\partial x^1}(D^{\mathrm{c}}_1 h^{\mathrm{c}}_2 h^{\mathrm{c}}_0) + \tilde{s}_0\tilde{s}_1 \frac{\partial}{\partial x^2}(D^{\mathrm{c}}_2 h^{\mathrm{c}}_0 h^{\mathrm{c}}_1)\Big) = 0. \tag{25}$$

Recalling that $h^{\mathrm{r}}_i s_i = h^{\mathrm{c}}_i \tilde{s}_i$ and $\tilde{s}_i$ is interchangeable with the partial derivative $\partial/\partial x^j$ for $i \neq j$, we obtain

$$\frac{1}{h^{\mathrm{r}}_0 h^{\mathrm{r}}_1 h^{\mathrm{r}}_2}\Big(\frac{\partial}{\partial x^0}(D^{\mathrm{c}}_0 s_1 s_2 h^{\mathrm{r}}_1 h^{\mathrm{r}}_2) + \frac{\partial}{\partial x^1}(D^{\mathrm{c}}_1 s_2 s_0 h^{\mathrm{r}}_2 h^{\mathrm{r}}_0) + \frac{\partial}{\partial x^2}(D^{\mathrm{c}}_2 s_0 s_1 h^{\mathrm{r}}_0 h^{\mathrm{r}}_1)\Big) = 0. \tag{26}$$

For identifying Eq. (26) as the Gauss law in the real coordinate, $\nabla \cdot \mathbf{D}^{\mathrm{PMLA}} = 0$, we determine the electrical displacement in the real coordinate as

$$D_i^{\mathrm{PMLA}} = \frac{s_0 s_1 s_2}{s_i} D_i^{\mathrm{c}} \quad \text{(no summation).} \tag{27}$$

Note that the relations of the electric fields [Eq. (23)] and the electrical displacements [Eq. (27)] between the real coordinate and the complex coordinate are the same as those of Eqs. (8) and (9), although the relations of stress tensors and displacement gradients [Eqs. (17) and (18), respectively] are different from those of Eqs. (10) and (11).

4.2 PML constants derived by the analytic continuation

Using Eqs. (17), (18), (23), and (27), the quotient rule, and the constitutive equations [Eqs. (6) and (7)], we obtain the material constants of the PML in the real coordinate:

$$C_{ijkl}^{\mathrm{PMLA}} = \frac{s_0 s_1 s_2}{s_j s_l} C_{ijkl} \quad \text{(no summation),} \tag{28}$$

$$\underline{e_{ijk}^{\mathrm{PML}}} = \frac{s_o s_1 s_2}{s_j s_k} \underline{e_{ijk}} \quad \text{(no summation),} \tag{29}$$

$$e_{ikl}^{\mathrm{PML}} = \frac{s_0 s_1 s_2}{s_i s_l} e_{ikl} \quad \text{(no summation),} \tag{30}$$

$$\epsilon_{ik}^{\mathrm{PML}} = \frac{s_0 s_1 s_2}{s_i s_k} \epsilon_{ik} \quad \text{(no summation).} \tag{31}$$

Note that Eq. (28) is reported in Refs. 7 and 12.

5. Comparison with PML Material Constants Derived From Differential Forms and the Analytic Continuation

The mass density and the permittivity constants obtained using the analytic continuation [Eqs.(19) and (31), respectively] are identical to those obtained using the differential forms [Eqs. (16) and (14)]. However, the stiffness and the piezoelectric stress constants [Eqs. (28), (29), and (30)] are different from our results [Eqs. (15), (12), and (13)] because in the analytic continuation, the manipulation of the coordinate transformation corresponding to the part of the stress tensor and the particle displacement vector, the tensor type of the omitted parts is contravariant of rank 1, is excluded.[14,15)]

Note that the transpose symmetry relations of piezoelectric stress constants hold for the constants derived from the analytic continuation [Eqs. (29) and (30)], but for those derived using the differential forms [Eqs. (12) and (13)], the relation does not hold. In addition, the symmetry of the stress tensor in the real coordinate holds for the constants derived from differential forms [Eqs. (12) and (15)], but does not hold for those derived from the analytic continuation [Eqs. (28) and (29)], although the symmetry of the stress tensor in the complex coordinate is assumed.

6. Conclusions

PMLs in the orthogonal coordinates for elastic waves in piezoelectric solids were derived from differential forms. To the best of our knowledge, PML parameters for piezoelectric solids in the non-Cartesian coordinate systems such as the cylindrical and spherical coordinates are presented here for the first time. Our results show that the PML parameters for elastic waves in piezoelectric solids are determined by the same procedure as that used for the parameteres in the Cartesian coordinates. This rule is an extension of our previous results[15] for anisotropic solids without piezoelectricity.

In this paper, we focused on the procedure of deriving PML constants in the generalized orthogonal coordinate systems. Demonstration of the validity and usefulness of the PML constants in FEM and FD-TD analyses of elastic waves in solids in the frequency range is one of our future topics.

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