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Stable perfectly-matched-layer boundary conditions for finite-difference time-domain simulation of acoustic waves in piezoelectric crystals

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ABSTRACT

Perfectly-matched-layer (PML) boundary conditions are derived for finite-difference time-domain analysis of acoustic waves within piezoelectric crystals. The robustness and effectiveness of the derived boundary conditions are demonstrated by simulating acoustic wave propagation in the bismuth germanate material system—a system in which simple absorbing boundary conditions cause instabilities. An investigation into the stability and effectiveness of the PML is then presented in terms of the PML thickness and absorption profile. A range of optimised absorption profiles were determined by finding the maximum permissible absorption within the stability limit of the system. In the optimised case, the form of the absorption profile had little influence on the effectiveness of the PML. However, in the unoptimised case the linearly increasing absorption profile was found to be the most effective.

1. Introduction

The finite-difference time-domain (FDTD) method, introduced by Yee [1] in 1966 for simulating Maxwell's equations, was first applied to the acoustic wave equations of motion in piezoelectric crystals by Smith et al. in 2002 [2]. Since the solutions of both these systems involve propagating waves, the method of truncating an otherwise infinite simulation domain around some region of interest (ROI) is critical in stopping reflections off these artificial boundaries interfering with the physics being investigated. In 2006, Chagla et al. [3] added absorbing boundary conditions to the acoustic wave problem by adding an absorbing layer with a quadratically increasing damping coefficient to dissipate the energy from any oscillations which reach the boundaries. Although this method worked well in some cases, Chagla et al. showed that it does not remain stable for all material systems.

Since it was first introduced by Berenger in 1994 [4], the perfectly-matched layer (PML) has been used extensively in FDTD simulations of electromagnetic waves. It may be viewed as an analytic continuation of spatial variables onto the complex plane such that any oscillating solution that enters the PML will be transformed into an oscillating component with an exponentially decaying envelope [5]. Despite the ongoing interest in development of the PML [6–9] in electromagnetic simulations as well as its application in both elastodynamics [10] and fluid dynamics [11], the PML has not been applied to the simulation of acoustic waves in piezoelectric crystals.

In this work, we derive PML boundary conditions for the acoustic wave equations of motion within a piezoelectric crystal by applying a complex coordinate stretching of spatial variables in the frequency domain. The boundary conditions are then transformed back to the time domain and discretised using the same interlaced mesh used by Smith et al. such that both the

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ROI and PMLs may be solved using the same FDTD algorithm, thereby avoiding any increase in computational complexity in the simulation.

The robustness and effectiveness of our PML implementation is demonstrated in the following section, and is shown to be stable for a bismuth germanate material system in which absorbing boundary conditions fail [3]. This is followed by a discussion of the stability criteria for the discretised PML and a quantitative analysis of their effectiveness with respect to their operating parameters as well as optimisation of those parameters.

2. Derivation of PML boundaries for the acoustic wave equations of motion

The equation of motion for an acoustic wave in a piezoelectric crystal is

$$\rho \ddot{u}_i = \frac{\partial \sigma_{ij}}{\partial x_j} \quad \text{for } i, j = 1, 2, 3, \tag{1}$$

where $\mathbf{u}$ is the displacement of a particle in three orthogonal directions x_1, x_2 and x_3, and

$$\sigma_i = C_{ij}\epsilon_j + e^{\mathrm{T}}_{ik}\frac{\partial \phi}{\partial x_k} \quad \text{for } i, j = 1, 2, \ldots, 6;\ k = 1, 2, 3, \tag{2}$$

is Hooke's law for piezoelectric crystals, where $\boldsymbol{\sigma}$ is the stress, C is the elastic constant tensor, e^{T} is the transpose of the piezoelectric constant tensor, ϕ is the induced piezoelectric potential inside the crystal structure and $\boldsymbol{\epsilon}$ is the strain inside the crystal which is defined as

$$\epsilon_i = \frac{\partial u_i}{\partial x_i} \quad \text{for } i = 1, 2, 3, \tag{3}$$

$$\epsilon_4 = \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}, \tag{4}$$

$$\epsilon_5 = \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}, \tag{5}$$

$$\epsilon_6 = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}. \tag{6}$$

Note that the subscript of $\boldsymbol{\sigma}$ has changed from tensor notation in (1) to matrix notation in (2), as in Ref. [12], so that both the wave equation and Hooke's law may be expressed using the Einstein summation convention.

The computational effort required for the simulation is greatly reduced by assuming that the acoustic waves are of Rayleigh wave type, and therefore have no variation in the direction aligned parallel to the propagating wave front. Taking this direction to be along the x_2-axis, all terms containing $\frac{\partial}{\partial x_2}$ may be set to zero. This reduces the number of independent terms on the RHS of (1) to two, or in the summation notation $j = 1, 3$, and in (2) the number of independent equations reduces from six to five as σ_2 is not used, so in the summation convention $i = 1, 3, 4, 5, 6$. The summations for the equations of motion and Hooke's law remain the same throughout the rest of this work so will no longer be shown. While the variation in the x_2 direction is assumed to be zero the displacement in this direction, u_2, is not zero and therefore cannot be discounted. The problem may be simplified further if the solution is restricted to one particular crystal class such that many of the terms in (2) become zero due to symmetries within the crystal's unit cell. In the following derivation however, all terms within (2) have been included to make PMLs applicable to all crystal classes and therefore to be material independent.

Since the acoustic velocity inside a crystal is slow compared to the piezoelectric response, the induced charge displacement from the acoustic wave, ρ, is assumed to be adiabatic and takes the form

$$\rho = -\nabla_i \cdot e_{ij}\epsilon_j \quad \text{for } i = 1, 3;\ j = 1, 3, 4, 5, 6, \tag{7}$$

therefore allowing ϕ to be found by solving Poisson's equation

$$\nabla \cdot \varepsilon \nabla \phi = -\rho. \tag{8}$$

In order to implement PML boundary conditions we split the second-order time differential by introducing an auxiliary field, $\mathbf{v}$, such that (1) becomes

$$\rho \frac{\partial u_i}{\partial t} = \frac{\partial v_{ij}}{\partial x_j}, \tag{9}$$

where the time differential of $\mathbf{v}$ is defined as

$$\frac{\partial v_i}{\partial t} = \sigma_i = C_{ij}\epsilon_j + e^{\mathrm{T}}_{ik}\frac{\partial \phi}{\partial x_k}. \tag{10}$$

Transforming to the frequency domain, such that $\mathbf{u}(t) \to \mathbf{U}(\omega)$ and $\mathbf{v}(t) \to \mathbf{V}(\omega)$, we obtain