

HOMOGENIZATION-BASED COMPUTATIONAL DESIGN AND TWO-SCALE PERFORMANCE OPTIMIZATION OF ELECTROACTIVE STRUCTURES

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HOMOGENIZATION-BASED COMPUTATIONAL DESIGN AND
TWO-SCALE PERFORMANCE OPTIMIZATION OF ELEC-
TROACTIVE STRUCTURES

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September 2024

We certify that we have read this thesis and that in our opinion it is fully adequate,
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ABSTRACT

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Macroscopic materials and structures with enhanced characteristics have been extensively studied in the context of solid mechanics. The advantages of microstructured materials with active constituents have been reported in the literature. In view of tunable microstructures, further intriguing traits of such materials can be achieved through imposing external stimuli. The ultimate goal of the present study is to establish a homogenization-based computational design framework to actively control the time-varying macroscopic stress response and behavior of structures with piezoelectric constituents. This is accomplished by temporally adapting the macroscopic electric field enforced on a microstructure and controlling the time-variation of the macroscopic electric potential imposed on a macroscopic solid. This periodic microstructure is optimized in a non-restrictive design space that embodies not only the topology, but also anisotropic material orientation and the unit cell geometry. In order to enrich the optimization space to capture the intriguing time-varying mechanical aspects, additional optimization variables, namely performance variables, are developed. Extensive numerical investigations are conducted to test the limits of this framework based on the discreteness of the microstructure and the accurateness of attaining the targeted mechanical behavior. The overall computational work is implemented through a parallel C++-based in-house FE program.

Keywords: Computational design, homogenization, two-scale performance, electroactive solids.

ÖZET

ELEKTROAKTİF YAPILARIN TÜRDEŞLEME TEMELLİ HEŞAPLAMALI TAŞARIMI VE İKİ ÖLÇEKLİ DAVRANIŞ ENİYİLEMESİ

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Geliştirilmiş özelliklere sahip makroskopik malzemeler ve yapılar, katı mekaniği bağlamında kapsamlı bir şekilde incelenmiştir. Aktif bileşenlere sahip mikroyapılı malzemelerin avantajları kaynaklarda bildirilmiştir. Ayarlanabilir mikroyapılar göz önüne alındığında, bu tür malzemelerin daha ilginç özellikleri dış uyaranlar dayatılarak elde edilebilir. Bu çalışmanın nihai amacı, piezoelektrik bileşenlere sahip yapıların zamanla değişen makroskopik gerilme tepkisini ve davranışını aktif olarak kontrol etmek için türdeşleme temelli hesaplamalı tasarım sistemi oluşturmaktır. Bu sistem, mikroyapının üzerine uygulanan makroskopik elektrik alanının zamanla uyarlanması ve makroskopik katının üzerine uygulanan makroskopik elektrik potansiyelinin zamana göre değişiminin kontrol edilmesi ile gerçekleştirilir. Bahsedilen periyodik mikroyapının, sadece topolojisi değil, aynı zamanda anizotropik malzeme yönelimini ve birim hücre geometrisini de içeren kapsamlı bir tasarım uzayında eniyilemesi sağlanmıştır. Zamanla değişen mekanik özellikleri yakalamak için eniyileme uzayını zenginleştirmek amacıyla, davranış değişkenleri olarak adlandırılan ek eniyileme değişkenleri geliştirilmiştir. Mikroyapının ayrıklı yapısı ve hedeflenen mekanik davranışın elde edilme doğruluğu temel alınarak, bu sistemin sınırlarını denetlemek için geniş kapsamlı sayısal soruşturmalar yürütülmüştür. Bahsedilen bütün hesaplar, bu çalışmaya ait paralel hesaplama içeren C++ tabanlı sonlu elemanlar (SE) programı ile gerçekleştirilmiştir.

Anahtar sözcükler: Hesaplamalı tasarım, türdeşleme, iki ölçekli davranış, elektroaktif yapılar.

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Chapter 1

Introduction

1.1 Scope

Macroscopic materials and structures with enhanced characteristics have been a focus in solid mechanics. Designing microstructured materials have been extensively studied in the literature. When such materials additionally respond to external stimuli, further intriguing traits may be exploited for tuning the mechanical behavior. The ultimate goal of this study is to establish a homogenization-based computational design framework to actively control the time-varying macroscopic behavior and stress response of structures with piezoelectric constituents. This is achieved by temporally adapting a macroscopic electric field imposed on a microstructure. This microstructure is optimized in a non-restrictive design space that incorporates not only the topology, but also anisotropic material orientation and the unit cell geometry. Earlier studies which build a foundation for this goal from both theoretical and computational standpoints are summarized next.

1.2 Smart Materials

The core idea of this study is to attain a desired target stress response or structural behavior by adapting an external stimulus. To this end, an approach is to utilize a smart composite that is composed of smart and passive constituents. When electric, magnetic or optical excitation [1–6] is supplied to smart materials, its overall behavior maybe controlled. Moreover, the multifunctional and programmable behavior of such smart materials is considerably enhanced by the multiphase nature of composites [7, 8]. By virtue of their intrinsic capability to convert between mechanical and electrical energy [2, 9–12], piezoelectric materials particularly qualify as the active smart constituent within the scope of this work. In the view of their unique characteristic, piezoelectric materials have achieved significant attention as precision actuators, pressure sensors and transducers in electronic devices, energy harvesting and storage devices, MEMS/NEMS, scaffolds in biomedical engineering etc. [13–17]. Recent advancements in additive manufacturing technology has facilitated the physical implementation and multiscale designs of piezoelectric composites—see [18] for recent trends in additive manufacturing of piezoelectric materials and composites.

1.3 Piezocomposites in Computational Design

Enforcing direct size scale separation to model the behavior of composite structures requires simultaneously resolving field variations at both macroscopic and microscopic scales. In order to address arising theoretical and numerical challenges, averaging and homogenization strategies were built on a two-scale treatment to efficiently correlate the microstructure with the macroscopic response. Specifically, the framework offered by homogenization through asymptotic analysis [19–24] was first adapted for the analysis of emerging piezocomposites in pioneering works [25, 26] – see also [11] for an approach in the context of dynamical effects that are beyond the scope of this study. Although closed-form expressions of macroscopic moduli including elasticity, piezoelectric and dielectric

tensors can be analytically expressed for basic material distributions [27–29], it is advantageous to invoke numerical methods such as the finite element method (FEM) for more complicated distributions [30] – see also [31] for an early application of FEM in laminated piezoelectric plate theory. Combining an active piezoelectric material with a passive matrix has proven its effectiveness on enhancing overall performance characteristics of piezocomposites—see [32] for the advantages of 1-3 piezocomposite with negative Poisson ratio. The identification of a suitable microstructure that leads to an enhanced performance may be rigorously cast within an inverse design problem where homogenization cooperates with topology optimization [33]. This approach was initiated in [34] for low- and high-frequency applications, followed by [35] for designing an optimal porous matrix for piezocomposites with an early example of a 3D-printed microstructure and [36] for resonator applications.

In topology optimization, the individual phases of the microstructure are typically distinguished through the well-known material pseudo-density model, solid isotropic material with penalization (SIMP). It is noted that the non-centrosymmetric nature of piezocomposites intrinsically invokes handling anisotropic constituents [10]—see [36] for PEMP (piezoelectric material with penalization) and [37] PEMP-P (piezoelectric material with penalization and polarization) models as possible modifications of SIMP in this context. The significance of the optimization of the material orientation for such anisotropic constituents has been highlighted extensively in the literature—see [38] for thermal conductivity, [39] for orthotropic materials in general, [40] for fiber orientation and [41] as a tensor variable. The incorporation of material orientation delivers more flexible design space. This flexibility may be further improved by relaxing the unit cell geometry through optimization—see [42] for unit cell design within the context of linear elasticity and [43] for surface texture design within the context of active lubrication. As a minor goal of this study, material orientation and unit cell geometry optimization capabilities will be developed for piezoelectric microstructure design.

The problem of macroscopic structural behavior optimization may be correlated with piezoelectric actuator or sensor design. This problem has been

discussed in different ways—see [44] for multiscale design of piezoelectric actuators, [45] for an optimal electrode design and [46] for multi-material macroscopic treatment. The major goal of this study is to propose a computational framework which can address time-dependent objectives by utilizing the electric field indirectly as an additional optimization variable. Building upon recent tunable microstructure design studies [42, 43, 47], this will be achieved through the simultaneous optimization of a macroscopic electric potential variation and the microstructure which interacts with the induced electric field.

1.4 Content

Boundary value problem (BVP) for linear piezoelectric solids is discussed in Chapter 2 by deriving governing equations for infinitesimal deformations and electrostatics, while compactly presenting the constitutive relations based on the IEEE standard [48]. After this macroscopic presentation of the problem, the homogenization methodology is introduced to extract the cell problems and the closed-forms of the macroscopic constitutive tensors through a two-scale treatment within the same chapter. The generic optimization framework, namely homogenization-based computational design, is highlighted by exploiting the variational structure of FEM in Chapter 3, where compact sensitivity expressions with respect to design variables are formulated. The novel parametrization of unit cell geometry and material orientation for piezoelectric microstructures will also be developed in this chapter. Furthermore, the macroscopic performance variables will be proposed in a generic sense to fully characterize the macroscopic behavior of the solid based on time-varying stress response and structural behavior. Chapter 4 will then present the main features of the overall approach. Here, the relevant optimization parameters and their significance are systemically investigated via comparative numerical studies. Chapter 5 concludes the discussion of the proposed computational design framework for piezoelectric composites and its potential applications from a macroscopic standpoint.

Chapter 2

Linear Theory of Piezoelectricity

In this chapter, the governing theoretical basis for linear piezoelectricity is derived by compactly summarizing the relevant mechanical and electrical aspects of the subject. Even though the governing equations and the constitutive relations of piezoelectric solids within a linear macroscopic setting have been secured under IEEE standard in [48], derivations of the corresponding mathematical relations have also been reported in the literature within a more comprehensive theoretical framework [9, 10, 12, 49]. Eventually, the ultimate goal will be to formulate the macroscopic BVP for a linear piezoelectric medium subject to suitable boundary conditions (BCs) and a set of problem specific assumptions.

2.1 Infinitesimal Deformations

”Small” or ”infinitesimal” deformation assumption states that within the theoretical framework of continuum mechanics, two distinct configurations of a solid medium (i.e. *referential* and *spatial*) are indistinguishable. The quantities associated with this sole configuration may be uniquely expressed by applying Taylor

series expansion and omitting higher-order contributions. This so-called linearization process substantially simplifies the mathematical representation of deformation measures as well as the stress field and the electric displacement.

As a preliminary to the theoretical development, the selection of an orthonormal basis set $\{\mathbf{e}_i\}$ is essential and convenient to define the kinematic and kinetic quantities in a Euclidean space described by a Cartesian coordinate system $\mathbb{R}^n$, where n represents the corresponding dimension and $i \in \{1, 2, \dots, n\}$. Hence, let $\mathbf{x}$ be the position vector of a material point P on a solid body $\mathfrak{B}$. Displacement vector field $\mathbf{u}$ mathematically represents the infinitesimal mechanical displacement of P . Displacement gradient tensor defined as $\mathbf{H} := \nabla \mathbf{u}$. The infinitesimal strain tensor $\boldsymbol{\epsilon}$ is equal to $\mathbf{H}^{sym} = \frac{1}{2}(\mathbf{H} + \mathbf{H}^T)$ whereas $\mathbf{H}^{skw}$ describes the infinitesimal rigid body rotation tensor $\boldsymbol{\omega}$ at P . The linear momentum balance (LMB) for indistinguishable configurations reads

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = \rho \ddot{\mathbf{u}} \quad \text{in } \mathfrak{B}, \quad (2.1)$$

where $\boldsymbol{\sigma}$, ρ , $\mathbf{f}$ and $\ddot{\mathbf{u}}$ respectively represent the infinitesimal stress tensor, the density, the body force density and the acceleration of the solid body. Note that $\ddot{\mathbf{u}}$ involves only partial time derivatives in view of the linearized formulation. Additionally, the angular momentum balance (AMB) must be satisfied. As a result of this, the 2nd-order infinitesimal stress tensor is symmetric (i.e. $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$).

2.2 Electrostatics

Electrostatics in vacuum is governed by two equations [49,50]: (i) the electric field (or, electric field intensity) $\mathbf{E}$ of a continuous total charge density ρ_e in a specified volume V can be expressed locally as $\mathbf{E} = -\nabla \phi$ (*first equation of electrostatics*) where ϕ describes the electrostatic potential, and (ii) utilizing the local form of Gauss's theorem in V suggests $\nabla \cdot \mathbf{E} = \frac{\rho_e}{\epsilon_0}$ (*second equation of electrostatics*) where ϵ_0 is the electric permittivity of free space. Without mentioning appropriate BCs, substituting the first equation into the second delivers Poisson's equation

$$\nabla^2 \phi = -\frac{\rho_e}{\epsilon_0} \quad \text{in } V. \quad (2.2)$$

Outside of V , where $\rho_e = 0$, (2.2) reduces to Laplace's equation.

The governing equations of electrostatics in vacuum must be altered to address a dielectric medium. Since the first equation of electrostatics is independent of the medium, no modifications are required. Due to the polarization phenomenon in dielectrics, the total charge density expression in the second equation of electrostatics may be expressed as

$$\rho_e = \rho_f + \rho_b , \quad (2.3)$$

in which ρ_b represents the bound charge density and can be associated with the polarization vector $\mathbf{P}$ via $\rho_b = -\nabla \cdot \mathbf{P}$, whereas the free charge density is denoted by ρ_f . The second equation of electrostatics can now be expressed as

$$\nabla \cdot \mathbf{D} = \rho_f , \quad (2.4)$$

where the electric displacement field (or, the electric flux density) $\mathbf{D}$ satisfies the relation $\mathbf{D} = \mathbf{P} + \epsilon_0 \mathbf{E}$ and simplifies to $\mathbf{D} = \epsilon_0 \mathbf{E}$ in vacuum.

2.3 Linear Piezoelectricity

The phenomenon called piezoelectricity (after the Greek word *piezein* for "press"), discovered by Pierre and Jacques Curie in 1880, describes how the conversion of mechanical energy into electrical energy (or vice versa) occurs in crystals lacking a center of symmetry [10]. The *direct piezoelectric* effect is known as the generation of polarization through strain, whereas the *inverse piezoelectric* effect emphasizes the appearance of strain by an applied electric field [10]. According to IEEE, in the presence of dynamic mechanical effects, electrostatics are not purely static, but only quasistatic¹, and linearity argument in piezoelectricity is maintained by enforcing infinitesimal deformation and field assumptions on the governing equations. This simply suggests that the electro-mechanical coupling

¹The phase velocities of acoustic waves are approximately five orders of magnitude less than the velocities of electromagnetic waves, which motivates the quasielectrostatic approximation [48].

may be represented by a single constant, called the piezoelectric constant, at the constitutive level [48]. Based on these fundamental concepts of piezoelectricity, BVP of a linear piezoelectric medium and suitable BCs are discussed next.

For the sake of further theoretical developments regarding both microscopic and macroscopic scales, for the rest of the study, relevant macroscopic quantities are denoted by a convention $\{\bullet\}$. Let $\bar{\mathbf{u}}$ and $\bar{\phi}$ be denoted respectively as the displacement vector and the scalar potential. According to IEEE, (2.1) and (2.4) are revisited by employing the quasistatic assumption (i.e. $\ddot{\mathbf{u}} = \mathbf{0}$) and formulating linear piezoelectric materials as insulators (i.e. $\bar{\rho}_e = 0$) [48]:

$$\nabla_{\mathbf{x}} \cdot \bar{\boldsymbol{\sigma}} + \bar{\mathbf{f}} = \mathbf{0} \ , \quad \nabla_{\mathbf{x}} \cdot \bar{\mathbf{D}} = 0 \quad \text{in } \mathfrak{B} \ . \quad (2.5)$$

Here, in order to emphasize that the balance equations pertain to the macroscopic scale, the divergence operator is denoted with a subscript $\mathbf{x}$. The constitutive relations which link kinetics with kinematics can be expressed as

$$\bar{\boldsymbol{\sigma}} = \bar{\mathcal{C}}\bar{\boldsymbol{\epsilon}} - \bar{\mathcal{Q}}^T \bar{\mathbf{E}} \quad , \quad \bar{\mathbf{D}} = \bar{\mathcal{Q}}\bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}} \bar{\mathbf{E}} \ . \quad (2.6)$$

Here, the transposition of a 3rd-order tensor is defined as $\bar{\mathcal{Q}}_{ijk}^T = \bar{\mathcal{Q}}_{kij}$ in index notation. It is noted that the symmetry of $\bar{\boldsymbol{\sigma}}$ requires the minor symmetry of the 4th-order elasticity tensor $\bar{\mathcal{C}}$ (i.e. $\bar{\mathcal{C}}_{ijkl} = \bar{\mathcal{C}}_{jikl}$) and the symmetry of the 3rd-order piezoelectric tensor $\bar{\mathcal{Q}}$ (i.e. $\bar{\mathcal{Q}}_{ijk} = \bar{\mathcal{Q}}_{ikj}$). The major symmetry of the elasticity tensor and the symmetry of the dielectric tensor $\bar{\boldsymbol{\epsilon}}$ can be deduced from the total free energy [12]:

$$\begin{aligned} \bar{\mathcal{C}}_{ijkl} &= \bar{\mathcal{C}}_{jikl} = \bar{\mathcal{C}}_{ijlk} = \bar{\mathcal{C}}_{klij} \ , \\ \bar{\mathcal{Q}}_{ijk} &= \bar{\mathcal{Q}}_{ikj} \ , \\ \bar{\boldsymbol{\epsilon}}_{ij} &= \bar{\boldsymbol{\epsilon}}_{ji} \ . \end{aligned} \quad (2.7)$$

For an isotropic material, the elasticity tensor may be expressed as $\bar{\mathcal{C}}_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$ and the dielectric tensor as $\bar{\boldsymbol{\epsilon}}_{ij} = \epsilon_r \epsilon_0 \delta_{ij}$ where λ and μ are the so-called Lamé parameters, ϵ_r denotes the relative permittivity and δ_{ij} is the Kronecker delta. Only zero-tensors can satisfy isotropic symmetry conditions for indifferent linear 3rd-order tensors [51]. Therefore, $\bar{\mathcal{Q}} = \mathbf{0}$ must hold for isotropic materials. For anisotropic materials, the constitutive tensors depend

on the material symmetries and the microstructure, which are elaborated in the following chapters.

Finally, relevant BCs must be imposed to formulate a well-defined BVP. Thus, let $\partial\mathcal{B}$ denote the boundary of the solid body. The super-script $\{M, E\}$ will depict respectively the mechanical and the electrical parts of the boundary and the sub-script $\{e, n\}$ will distinguish the essential and natural BCs. Mechanical and electrical parts of the boundary may now be decomposed as $\partial\mathcal{B} \equiv \partial\mathcal{B}_e^M \cup \partial\mathcal{B}_n^M \equiv \partial\mathcal{B}_e^E \cup \partial\mathcal{B}_n^E$ and $\partial\mathcal{B}_e^M \cap \partial\mathcal{B}_n^M \equiv \partial\mathcal{B}_e^E \cap \partial\mathcal{B}_n^E \equiv \emptyset$, on which the BCs are expressed as follows:

$$\begin{aligned} \bar{\mathbf{u}} &= \bar{\mathbf{u}}^* & \text{on } \partial\mathcal{B}_e^M & \text{ and } \bar{\boldsymbol{\sigma}}\bar{\mathbf{n}} = \bar{\mathbf{t}} & \text{on } \partial\mathcal{B}_n^M, \\ \bar{\phi} &= \bar{\phi}^* & \text{on } \partial\mathcal{B}_e^E & \text{ and } \bar{\mathbf{D}} \cdot \bar{\mathbf{n}} = -\bar{q} & \text{on } \partial\mathcal{B}_n^E. \end{aligned} \quad (2.8)$$

Here, $\bar{\mathbf{n}}$, $\bar{\mathbf{t}}$ and $\bar{q}$ respectively represent the outward unit normal vector, the surface traction and the electric surface charge. It must be highlighted that introducing $\bar{q}$ and simultaneously ignoring electromagnetic field on the outside of $\partial\mathcal{B}$ is a restrictive but valid assumption, which may be employed in dielectric-vacuum interfaces [9]. Therefore, $\bar{q} = 0$ and $\bar{\mathbf{f}} = \mathbf{0}$ are assumed for the rest of the thesis. This BVP formulation also forms a basis for piezomagnetic solids by adjusting the relevant material constants and the fields without having to introduce Maxwell's equations.

2.4 Homogenization Theory

In this section, the homogenization framework for piezoelectric solids is applied to outline the relation between the microstructure and material constants at a constitutive level. As mentioned previously, without loss of generality, this framework can also be utilized for piezomagnetic solids. The ultimate goal of this section is to extract the closed forms of macroscopic material constitutive tensors (effective properties) with respect to the microscopic quantities based on the classical two-scale treatment (i.e. asymptotic expansion) to acquire cell (or local) problems for a periodic microstructure $\mathcal{Y}$ [23, 24].

Due to the nature of the problem, the solid body $\mathfrak{B}$ admits material inhomogeneities at a fine scale. The heterogeneity distribution is represented with a macroscopic position vector $\mathbf{x}$ and its microscale counterpart $\mathbf{y} = \mathbf{x}/\varepsilon$, in which $\varepsilon \rightarrow 0$ enforces the scale separation. Rapidly fluctuating primary fields may now be denoted as

$$\begin{aligned} \mathbf{u}^{(\varepsilon)} &= \mathbf{u}(\mathbf{x}, \mathbf{y}) = \mathbf{u}^{(0)}(\mathbf{x}, \mathbf{y}) + \varepsilon \mathbf{u}^{(1)}(\mathbf{x}, \mathbf{y}) + \varepsilon^2 \mathbf{u}^{(2)}(\mathbf{x}, \mathbf{y}) + \mathcal{O}(\varepsilon^3) \quad , \\ \phi^{(\varepsilon)} &= \phi(\mathbf{x}, \mathbf{y}) = \phi^{(0)}(\mathbf{x}, \mathbf{y}) + \varepsilon \phi^{(1)}(\mathbf{x}, \mathbf{y}) + \varepsilon^2 \phi^{(2)}(\mathbf{x}, \mathbf{y}) + \mathcal{O}(\varepsilon^3) \quad . \end{aligned} \quad (2.9)$$

The differential forms can be expanded by the use of the chain rule

$$\nabla_{\mathbf{x}^{(\varepsilon)}} \cdot [\bullet] = \nabla_{\mathbf{x}} \cdot [\bullet] + \frac{1}{\varepsilon} \nabla_{\mathbf{y}} \cdot [\bullet] \quad , \quad \nabla_{\mathbf{x}^{(\varepsilon)}} [\bullet] = \nabla_{\mathbf{x}} [\bullet] + \frac{1}{\varepsilon} \nabla_{\mathbf{y}} [\bullet] \quad . \quad (2.10)$$

By utilizing (2.10), the displacement gradient and the electric field can be expanded

$$\begin{aligned} \mathbf{H}^{(\varepsilon)} &= \frac{1}{\varepsilon} \nabla_{\mathbf{y}} \mathbf{u}^{(0)} + \underbrace{\nabla_{\mathbf{x}} \mathbf{u}^{(0)} + \nabla_{\mathbf{y}} \mathbf{u}^{(1)}}_{=: \mathbf{H}^{(0)}} + \varepsilon (\nabla_{\mathbf{x}} \mathbf{u}^{(1)} + \nabla_{\mathbf{y}} \mathbf{u}^{(2)}) + \varepsilon^2 \nabla_{\mathbf{x}} \mathbf{u}^{(2)} + \mathcal{O}(\varepsilon^2) \quad , \\ \mathbf{E}^{(\varepsilon)} &= -\frac{1}{\varepsilon} \nabla_{\mathbf{y}} \phi^{(0)} - \underbrace{\nabla_{\mathbf{x}} \phi^{(0)} + \nabla_{\mathbf{y}} \phi^{(1)}}_{=: \mathbf{E}^{(0)}} - \varepsilon (\nabla_{\mathbf{x}} \phi^{(1)} + \nabla_{\mathbf{y}} \phi^{(2)}) - \varepsilon^2 \nabla_{\mathbf{x}} \phi^{(2)} + \mathcal{O}(\varepsilon^2) \quad . \end{aligned} \quad (2.11)$$

$\mathbf{H}^{(\varepsilon)}$ and $\mathbf{E}^{(\varepsilon)}$ must be bounded when $\varepsilon \rightarrow 0$, which can be ensured by admitting $\nabla_{\mathbf{y}} \mathbf{u}^{(0)} = \mathbf{0}$ and $\nabla_{\mathbf{y}} \phi^{(0)} = \mathbf{0}$. Thus, it can be observed that $\mathbf{u}^{(0)}(\mathbf{x}, \mathbf{y}) = \mathbf{u}^{(0)}(\mathbf{x})$ and $\phi^{(0)}(\mathbf{x}, \mathbf{y}) = \phi^{(0)}(\mathbf{x})$ must hold. These observations can alternatively be induced by the expansion of the balance laws [23, 24]. In order to establish the connection between the macroscopic and microscopic quantities, *cell average* $\langle \bullet \rangle = |\mathcal{Y}|^{-1} \int_{\mathcal{Y}} \bullet dv$ notation on $\mathcal{Y}$ -periodic microstructure should be introduced and applied to $\mathbf{H}^{(0)}$ and $\mathbf{E}^{(0)}$:

$$\overline{\mathbf{H}} := \nabla_{\mathbf{x}} \mathbf{u}^{(0)} = \langle \mathbf{H}^{(0)} \rangle \quad , \quad \overline{\mathbf{E}} := -\nabla_{\mathbf{x}} \phi^{(0)} = \langle \mathbf{E}^{(0)} \rangle \quad . \quad (2.12)$$

These equalities can be easily obtained by applying *generalized Stokes' theorem* and making use of $\mathcal{Y}$ -periodicity. One can similarly derive expressions for $\overline{\boldsymbol{\varepsilon}}$, $\overline{\boldsymbol{\sigma}}$ and $\overline{\mathbf{D}}$. It is highlighted that all relevant microscopic constitutive tensors are solely $\mathbf{y}$ -dependent and $\mathcal{Y}$ -periodic.

In order to derive cell problems and expressions of effective material properties, one has to expand balance laws and enforce the scale separation under

boundedness argument for terms of the order of ε^{-1} and ε^0 . Before introducing expanded governing equations, separation of variables technique should be applied to relevant primary fields:

$$\begin{aligned} u_i^{(1)}(\mathbf{x}, \mathbf{y}) &= {}^{MM}\chi_i^{mn} \frac{\partial u_m^{(0)}}{\partial x_n} + {}^{ME}\chi_i^m \frac{\partial \phi^{(0)}}{\partial x_m} , \\ \phi^{(1)}(\mathbf{x}, \mathbf{y}) &= {}^{EM}\chi^{mn} \frac{\partial u_m^{(0)}}{\partial x_n} + {}^{EE}\chi^m \frac{\partial \phi^{(0)}}{\partial x_m} . \end{aligned} \quad (2.13)$$

Here, in index notation, the so-called *first-order corrector* $\mathcal{Y}$ -periodic $\{\bullet\}\chi(\mathbf{y})$ fields parameterize and estimate *fluctuation* fields $\{\mathbf{u}^{(1)}, \phi^{(1)}\}$, where super-scripts $\{M, E\}$ differentiate the relevant variables by abbreviating and highlighting the mechanical and electrical contributions separately. After substituting (2.13) into the kinetic quantities, expanding the balance laws with respect to (2.5) and extracting resultant ε^{-1} contributions, cell problems are derived through the following set of coupled well-posed² differential equations (cf. [11, 25, 26]):

$${}^{MM}\Lambda_{kl}^{mn} = \frac{\partial {}^{MM}\chi_k^{mn}}{\partial y_l} , \quad {}^{ME}\Lambda_{kj}^m = \frac{\partial {}^{ME}\chi_k^m}{\partial y_j} , \quad (2.14a)$$

$${}^{EM}\Lambda_j^{mn} = \frac{\partial {}^{EM}\chi^{mn}}{\partial y_j} , \quad {}^{EE}\Lambda_k^m = \frac{\partial {}^{EE}\chi^m}{\partial y_k} , \quad (2.14b)$$

$${}^{MM}\Gamma_{kl}^{mn} = \delta_{mk}\delta_{nl} + {}^{MM}\Lambda_{kl}^{mn} , \quad {}^{EE}\Gamma_k^m = \delta_{mk} + {}^{EE}\Lambda_k^m , \quad (2.14c)$$

$$\frac{\partial}{\partial y_j} (\mathcal{C}_{ijkl} {}^{MM}\Gamma_{kl}^{mn} + \mathcal{Q}_{kij} {}^{EM}\Lambda_k^{mn}) = 0 , \quad \frac{\partial}{\partial y_j} (\mathcal{C}_{ijkl} {}^{ME}\Lambda_{kl}^m + \mathcal{Q}_{kij} {}^{EE}\Gamma_k^m) = 0 , \quad (2.14d)$$

$$\frac{\partial}{\partial y_i} (\mathcal{Q}_{ijk} {}^{MM}\Gamma_{jk}^{mn} - \mathcal{E}_{ij} {}^{EM}\Lambda_j^{mn}) = 0 , \quad \frac{\partial}{\partial y_i} (\mathcal{Q}_{ijk} {}^{ME}\Lambda_{jk}^m - \mathcal{E}_{ij} {}^{EE}\Gamma_j^m) = 0 . \quad (2.14e)$$

(2.14d) is induced from the mechanical equilibrium, whereas (2.14e) can be derived from the electrostatic equilibrium. Note that coupling exists between the pairs of equations of (2.14d)₁-(2.14e)₁ and (2.14d)₂-(2.14e)₂. Periodic boundary conditions are imposed for $\{\bullet\}\chi(\mathbf{y})$ fields and can be uniquely determined up to

²In addition to boundedness, other relevant criteria (i.e. uniqueness and existence) will be mentioned later in this chapter to define well-posed cell problems.

an additive constant [23, 24]. In order to resolve this arbitrariness, $\{\bullet\}\chi(\mathbf{y}) = \mathbf{0}$ is enforced at the corners of $\mathcal{Y}$. Having solved the system of equations, taking the cell average of remaining ε^0 contributions leads to the macroscopic balance equations (2.5) where $\bar{\boldsymbol{\sigma}} := \langle \boldsymbol{\sigma}^{(0)} \rangle$ and $\bar{\mathbf{D}} := \langle \mathbf{D}^{(0)} \rangle$ are expressed based on (2.6) with the following explicit formulations of the homogenized constitutive tensors:

$$\bar{\mathcal{C}}_{ijmn} = \langle \mathcal{C}_{ijkl}^{MM} \Gamma_{kl}^{mn} + \mathcal{Q}_{kij}^{EM} \Lambda_k^{mn} \rangle, \quad \bar{\mathcal{Q}}_{mij}^* = \langle \mathcal{C}_{ijkl}^{ME} \Lambda_{kl}^m + \mathcal{Q}_{kij}^{EE} \Gamma_k^m \rangle, \quad (2.15a)$$

$$\bar{\mathcal{Q}}_{imn} = \langle \mathcal{Q}_{ijk}^{MM} \Gamma_{jk}^{mn} - \mathcal{E}_{ij}^{EM} \Lambda_j^{mn} \rangle, \quad \bar{\mathcal{E}}_{im} = \langle \mathcal{E}_{ij}^{EE} \Gamma_j^m - \mathcal{Q}_{ijk}^{ME} \Lambda_{jk}^m \rangle. \quad (2.15b)$$

Here, the microscopic contributions to the macroscopic constitutive tensors are obtained through the solution of the cell problems (2.14d) and (2.14e). Moreover, the symmetry of $^{MM}\Lambda_{\bullet}^{mn}$ and $^{EM}\Lambda_{\bullet}^{mn}$ with respect to m and n is ensured by the structure of (2.14d) and (2.14e). Thus, $\bar{\mathcal{C}}$ clearly displays the minor symmetry and $\bar{\mathcal{Q}}$ is symmetric. The relation between $\bar{\mathcal{Q}}$ and $\bar{\mathcal{Q}}^*$ and the remaining symmetry considerations in (2.7) of the derived macroscopic quantities will be addressed shortly.

Chapter 3

Optimization Framework

In this chapter, the numerical optimization framework is outlined. Because the derived differential equations are not amenable to an analytical treatment, FEM will be utilized to solve the equations. Furthermore, the interaction between FEM and the optimization scheme will be established. In particular, the computation of design and performance variable sensitivities will be discussed. Finally, the objective and constraint functions which are relevant to the two-scale performance assessment are described. The overall computational work is implemented through an C++-based in-house FE program.

3.1 Variational Formulation of Cell Problems

An approximate solution of (2.14d) and (2.14e) can numerically be captured with FEM. Therefore, the strong forms of the coupled differential equations are

transformed into weak forms as

$$\langle \frac{\partial^M \eta_i}{\partial y_j} (\mathcal{C}_{ijkl}^{MM} \Gamma_{kl}^{mn} + \mathcal{Q}_{kij}^{EM} \Lambda_k^{mn}) \rangle = 0, \quad \langle \frac{\partial^E \eta_i}{\partial y_j} (\mathcal{C}_{ijkl}^{ME} \Lambda_{kl}^m + \mathcal{Q}_{kij}^{EE} \Gamma_k^m) \rangle = 0, \quad (3.1a)$$

$$\langle \frac{\partial^M \omega}{\partial y_i} (\mathcal{Q}_{ijk}^{MM} \Gamma_{jk}^{mn} - \mathcal{E}_{ij}^{EM} \Lambda_j^{mn}) \rangle = 0, \quad \langle \frac{\partial^E \omega}{\partial y_i} (\mathcal{Q}_{ijk}^{ME} \Lambda_{jk}^m - \mathcal{E}_{ij}^{EE} \Gamma_j^m) \rangle = 0, \quad (3.1b)$$

where $\{\bullet\}_{\eta_i}$ and $\{\bullet\}_{\omega}$ are $\mathcal{Y}$ -periodic test functions. Note that transition to the weak forms is based on first formulating weighted-residual forms, then invoking generalized Stokes' theorem, and finally enforcing or weakening relevant BCs. Since the minuscule superscripts emphasize the parametrization of the right hand-sides, the dimensions of the test functions are selected as the dimensions of the primary fields. After deriving the weak forms, Bubnov-Galerkin FEM formulation of the cell problems can be obtained by introducing FE discretization of the test functions and the corrector fields on $\mathcal{Y}$ (i.e. $\bigcup_{e=1}^{N_e} \mathcal{Y}^e \equiv \mathcal{Y}$ and $\mathcal{Y}^i \cap \mathcal{Y}^{i \neq j} \equiv \emptyset$ where $i, j \in \{1, 2, \dots, N_e\}$ and N_e is the number of finite elements $\mathcal{Y}^e$):

$$\int_{\mathcal{Y}} \{\bullet\} dv \equiv \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \{\bullet\} dv \quad , \quad (3.2a)$$

$$^M \eta_i^e = \sum_I^{n_e} (^M \eta_i^e)^I N^I(\mathbf{y}) \quad , \quad ^E \eta_i^e = \sum_I^{n_e} (^E \eta_i^e)^I N^I(\mathbf{y}) \quad , \quad (3.2b)$$

$$^M \omega^e = \sum_I^{n_e} (^M \omega^e)^I N^I(\mathbf{y}) \quad , \quad ^E \omega^e = \sum_I^{n_e} (^E \omega^e)^I N^I(\mathbf{y}) \quad , \quad (3.2c)$$

$$^{MM} \chi_i^{mn^e} = \sum_J^{n_e} (^{MM} \chi_i^{mn^e})^J N^J(\mathbf{y}) \quad , \quad ^{ME} \chi_i^{m^e} = \sum_J^{n_e} (^{ME} \chi_i^{m^e})^J N^J(\mathbf{y}) \quad , \quad (3.2d)$$

$$^{EM} \chi^{mn^e} = \sum_J^{n_e} (^{EM} \chi^{mn^e})^J N^J(\mathbf{y}) \quad , \quad ^{EE} \chi^{m^e} = \sum_J^{n_e} (^{EE} \chi^{m^e})^J N^J(\mathbf{y}) \quad . \quad (3.2e)$$

Here, $(\{\bullet\})^e$ notation represents the nodal values of mathematical entities on the corresponding element e whereas $\{\bullet\}^e$ is the actual element function. Furthermore, n_e represents the number of element nodes and $N^I(\mathbf{y})$ is the corresponding shape function. Ultimately, substituting the FE discretization into the weak form results in a system of linear equations with identical stiffness matrices but distinct right-hand sides. This system may be expressed by introducing the stiffness

matrix entries

$${}^{MM}K_{ik}^{IJ} = \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_j} c_{ijkl} \frac{\partial N^J(\mathbf{y})}{\partial y_l} dv, \quad {}^{ME}K_i^{IJ} = \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_j} \mathcal{Q}_{kij} \frac{\partial N^J(\mathbf{y})}{\partial y_k} dv, \quad (3.3a)$$

$${}^{EM}K_k^{IJ} = \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_i} \mathcal{Q}_{ijk} \frac{\partial N^J(\mathbf{y})}{\partial y_j} dv, \quad {}^{EE}K^{IJ} = - \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_i} \mathcal{E}_{ij} \frac{\partial N^J(\mathbf{y})}{\partial y_j} dv, \quad (3.3b)$$

and right-hand side entries

$$({}^{MM}B_i^{mn})^I = - \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_j} c_{ijmn} dv, \quad ({}^{ME}B_i^m)^I = - \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_j} \mathcal{Q}_{mij} dv, \quad (3.4a)$$

$$({}^{EM}B^{mn})^I = - \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_i} \mathcal{Q}_{imn} dv, \quad ({}^{EE}B^m)^I = \sum_{e=1}^{N_e} \int_{\mathcal{Y}^e} \frac{\partial N^I(\mathbf{y})}{\partial y_i} \mathcal{E}_{im} dv, \quad (3.4b)$$

which lead to the compact representation

$$\begin{bmatrix} {}^{MM}K_{ik}^{IJ} & {}^{ME}K_i^{IJ} \\ {}^{EM}K_k^{IJ} & {}^{EE}K^{IJ} \end{bmatrix} \begin{bmatrix} ({}^{MM}\chi_k^{mn^e})^J & ({}^{ME}\chi_k^{m^e})^J \\ ({}^{EM}\chi^{mn^e})^J & ({}^{EE}\chi^{m^e})^J \end{bmatrix} = \begin{bmatrix} ({}^{MM}B_i^{mn})^I & ({}^{ME}B_i^m)^I \\ ({}^{EM}B^{mn})^I & ({}^{EE}B^m)^I \end{bmatrix}. \quad (3.5)$$

It is straight forward to show that the resultant global stiffness matrix is real symmetric indefinite (i.e. neither positive nor negative definite¹) with the help of (2.7). Periodic boundary conditions are enforced to solve the system. In order to achieve an efficient computational framework, the global stiffness matrix is factorized once and multiple back substitutions are conducted, which eliminates the computational overload occurring during the factorization step. Element level integrals are numerically computed with Gauss quadrature by utilizing the isoparametric settings. Hence, let $\boldsymbol{\xi}$ be the position vector of the so-called master (or parent) element $\mathcal{Y}^\square$ and $\mathbf{y} = \boldsymbol{\varphi}(\boldsymbol{\xi})$ be a map between physical and parent coordinates:

$$\mathbf{y}^e = \sum_I^{n_e} (\mathbf{y}^e)^I N^I(\mathbf{y}) \quad \text{and} \quad \mathbf{F}^\square := \frac{\partial \mathbf{y}^e}{\partial \boldsymbol{\xi}} = \sum_I^{n_e} (\mathbf{y}^e)^I \frac{\partial \hat{N}^I(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}. \quad (3.6)$$

¹If a matrix is said to be positive/negative definite, then, all of its eigenvalues are positive/negative respectively.

Note that $N^I(\mathbf{y}) = N^I(\boldsymbol{\varphi}(\boldsymbol{\xi})) = \hat{N}^I(\boldsymbol{\xi})$ defines the pullback of the shape functions and that, the discretization of the position vector and primary fields are identical. The standard operation of the change of coordinates

$$\int_{\mathcal{Y}^e} g(\mathbf{y}) dv = \int_{\mathcal{Y}^\square} \hat{g}(\boldsymbol{\xi}) J dv^\square \quad , \quad (3.7)$$

holds for each element where $J = \det(\mathbf{F}^\square)$ is the Jacobian (or Jacobian determinant) that is presently assumed to be a constant over the domain (see Figure 3.1a and 3.1b for a representative mesh structure and master element). Consequently, element level integrals can be mapped onto the master element and Gauss quadrature can be applied in parametric coordinates. The resulting integrals can then be assembled into the global stiffness matrix and right-hand side vectors:

$$Q_i^I = \frac{\partial \hat{N}^I(\boldsymbol{\xi})}{\partial \xi_j} F_{ji}^{\square^{-1}} \quad , \quad (3.8a)$$

$${}^{MM}K_{ik}^{IJ} = \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_j^I \mathcal{C}_{ijkl} Q_l^J J, \quad {}^{ME}K_i^{IJ} = \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_j^I \mathcal{Q}_{kij} Q_k^J J, \quad (3.8b)$$

$${}^{EM}K_k^{IJ} = \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_i^I \mathcal{Q}_{ijk} Q_j^J J, \quad {}^{EE}K^{IJ} = - \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_i^I \mathcal{E}_{ij} Q_j^J J, \quad (3.8c)$$

$$({}^{MM}B_i^{mn})^I = - \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_j^I \mathcal{C}_{ijmn} J, \quad ({}^{ME}B_i^m)^I = - \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_j^I \mathcal{Q}_{mij} J, \quad (3.8d)$$

$$({}^{EM}B^{mn})^I = - \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_i^I \mathcal{Q}_{imn} J, \quad ({}^{EE}B^m)^I = \sum_{e=1}^{N_e} \sum_{g=1}^{G_p} w_g Q_i^I \mathcal{E}_{im} J \quad . \quad (3.8e)$$

Here, G_p represents the total number of Gauss points (i.e. roots of Legendre polynomials) and w_i denotes the corresponding weight constants. Variables depending on $\boldsymbol{\xi}$ must be computed at the quadrature points to calculate the relevant integrals. A uniform linear mesh with *isoparametric linear Lagrange elements* ($\mathcal{L}^1$) having $G_p = 2$ in each physical dimension is selected in the implementation of the cell problems (Figure 3.1).

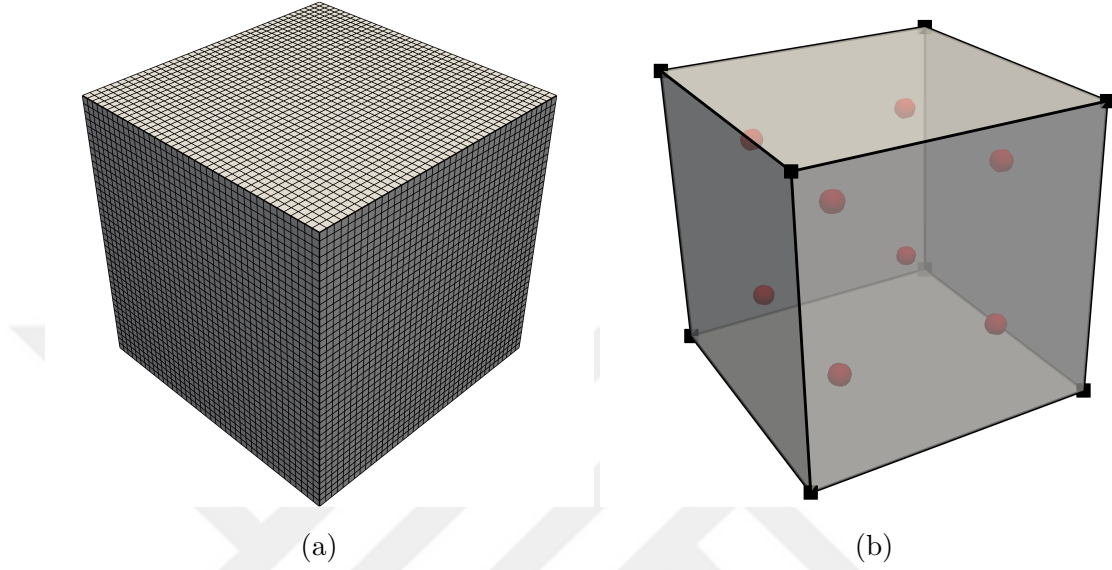


Figure 3.1: A representative uniform linear rectangular mesh (a) and the corresponding master element (b) with Gauss points depicted as red spheres are illustrated.

3.2 Computational Design

Within the optimization framework, after deriving the solutions of unknown fields, effective properties and their sensitivities are calculated for each optimization iteration. Therefore, in this section, material and geometry design variables as well as the relevant sensitivities are covered based on a homogenization framework.

3.2.1 Generic Material Design Variable

Within a microstructure-dependent design problem, the determination of the set of microscopic material design variables is central to achieving desired effective

properties. The material design variables include material distribution and material orientation design variables. Clearly, (2.15a) and (2.15b) display both explicit and implicit dependence on these variables, the former through the microscopic constitutive tensors and the latter through the microscopic corrector fields. Thus, generic variable ζ is selected to describe parameterized functional relation of macroscopic quantities (i.e. $\bar{\mathcal{C}}[\zeta]$, $\bar{\mathcal{Q}}[\zeta]$ and $\bar{\mathcal{E}}[\zeta]$) with respect to the microscopic material variables admitting that ζ parameterizes the microscopic constitutive tensors through notation $\mathcal{C}(\mathbf{y}) = \mathcal{C}[\zeta]$, $\mathcal{Q}(\mathbf{y}) = \mathcal{Q}[\zeta]$ and $\mathcal{E}(\mathbf{y}) = \mathcal{E}[\zeta]$. Therefore, the sensitivity of the macroscopic constituents with respect to the relevant design variables is calculated via cooperating with these expressions $\frac{\partial \bar{\mathcal{C}}[\zeta]}{\partial \zeta}$, $\frac{\partial \bar{\mathcal{Q}}[\zeta]}{\partial \zeta}$ and $\frac{\partial \bar{\mathcal{E}}[\zeta]}{\partial \zeta}$.

Most of the time, sensitivity analysis is conducted via adjoint, finite difference or semi-analytical methods (e.g. see [34]). Suggested methodologies have high computational cost due to the calculation of sensitivity of the corrector field gradients for high number of design variables and DOFs. To this end, compact variational formulation is derived for the sensitivities of the design variables which ultimately decreases the overall computational cost (e.g. see [42, 43, 52]). Before introducing the relevant microscopic material variables, *quadratic forms* of the effective properties are formulated. Upon interchanging $\{\bullet\}_{\eta_i}$ and $\{\bullet\}_{\omega}$ with admissible $\{\bullet\}_{\chi}$ fields in (3.1a) and (3.1b) implies the paired relations:

$$\begin{aligned} \langle {}^{MM}\Lambda_{ij}^{pq} \mathcal{C}_{ijkl} {}^{MM}\Gamma_{kl}^{mn} + {}^{MM}\Lambda_{ij}^{pq} \mathcal{Q}_{kij} {}^{EM}\Lambda_k^{mn} \rangle &= 0 \quad , \\ \langle {}^{EM}\Lambda_i^{pq} \mathcal{Q}_{ijk} {}^{MM}\Gamma_{jk}^{mn} - {}^{EM}\Lambda_i^{pq} \mathcal{E}_{ij} {}^{EM}\Lambda_j^{mn} \rangle &= 0 \quad ; \end{aligned} \quad (3.9a)$$

$$\begin{aligned} \langle {}^{MM}\Lambda_{ij}^{pq} \mathcal{C}_{ijkl} {}^{ME}\Lambda_{kl}^m + {}^{MM}\Lambda_{ij}^{pq} \mathcal{Q}_{kij} {}^{EE}\Gamma_k^m \rangle &= 0 \quad , \\ \langle {}^{EM}\Lambda_i^{pq} \mathcal{Q}_{ijk} {}^{ME}\Lambda_{jk}^m - {}^{EM}\Lambda_i^{pq} \mathcal{E}_{ij} {}^{EE}\Gamma_j^m \rangle &= 0 \quad ; \end{aligned} \quad (3.9b)$$

$$\begin{aligned} \langle {}^{ME}\Lambda_{ij}^p \mathcal{C}_{ijkl} {}^{MM}\Gamma_{kl}^{mn} + {}^{ME}\Lambda_{ij}^p \mathcal{Q}_{kij} {}^{EM}\Lambda_k^{mn} \rangle &= 0 \quad , \\ \langle {}^{EE}\Lambda_i^p \mathcal{Q}_{ijk} {}^{MM}\Gamma_{jk}^{mn} - {}^{EE}\Lambda_i^p \mathcal{E}_{ij} {}^{EM}\Lambda_j^{mn} \rangle &= 0 \quad ; \end{aligned} \quad (3.9c)$$

$$\begin{aligned} \langle {}^{ME}\Lambda_{ij}^p \mathcal{C}_{ijkl} {}^{ME}\Lambda_{kl}^m + {}^{ME}\Lambda_{ij}^p \mathcal{Q}_{kij} {}^{EE}\Gamma_k^m \rangle &= 0 \quad , \\ \langle {}^{EE}\Lambda_i^p \mathcal{Q}_{ijk} {}^{ME}\Lambda_{jk}^m - {}^{EE}\Lambda_i^p \mathcal{E}_{ij} {}^{EE}\Gamma_j^m \rangle &= 0 \quad . \end{aligned} \quad (3.9d)$$

After adding the vanishing averages (3.9a), (3.9c) and (3.9d) into the first part of (2.15a), the first part of (2.15b) and the second part of (2.15b) respectively and manipulating the indices, the following alternative expressions of the effective

macroscopic constitutive tensors (i.e. the quadratic forms) can be obtained:

$$\bar{\mathcal{C}}_{ijkl} = \langle {}^{MM}\Gamma_{pq}^{ij} \mathcal{C}_{pqmn} {}^{MM}\Gamma_{mn}^{kl} + {}^{EM}\Lambda_p^{ij} \mathcal{Q}_{pqm} {}^{MM}\Gamma_{qm}^{kl} + {}^{MM}\Gamma_{qm}^{ij} \mathcal{Q}_{pqm} {}^{EM}\Lambda_p^{kl} - {}^{EM}\Lambda_p^{ij} \mathcal{E}_{pq} {}^{EM}\Lambda_q^{kl} \rangle, \quad (3.10a)$$

$$\bar{\mathcal{Q}}_{ijk} = \langle {}^{ME}\Lambda_{pq}^i \mathcal{C}_{pqmn} {}^{MM}\Gamma_{mn}^{jk} + {}^{EE}\Gamma_p^i \mathcal{Q}_{pqm} {}^{MM}\Gamma_{qm}^{jk} + {}^{ME}\Lambda_{qm}^i \mathcal{Q}_{pqm} {}^{EM}\Lambda_p^{jk} - {}^{EE}\Gamma_p^i \mathcal{E}_{pq} {}^{EM}\Lambda_q^{jk} \rangle, \quad (3.10b)$$

$$\bar{\mathcal{E}}_{ij} = \langle -{}^{ME}\Lambda_{pq}^i \mathcal{C}_{pqmn} {}^{ME}\Lambda_{mn}^j - {}^{EE}\Gamma_p^i \mathcal{Q}_{pqm} {}^{ME}\Lambda_{qm}^j - {}^{ME}\Lambda_{qm}^i \mathcal{Q}_{pqm} {}^{EE}\Gamma_p^j + {}^{EE}\Gamma_p^i \mathcal{E}_{pq} {}^{EE}\Gamma_q^j \rangle. \quad (3.10c)$$

Here, the alternative forms of $\bar{\mathcal{C}}$ and $\bar{\mathcal{E}}$ clearly display the major symmetry and the symmetry respectively. Additionally, if the piezoelectric coupling is eliminated and electro-mechanical interactions are ignored, one can derive the quadratic forms of pure elastic and dielectric constitutive tensors from the relations above without employing asymptotic expansion from the beginning (cf. [42]). Adding vanishing (3.9b) into the second part of (2.15a) delivers

$$\bar{\mathcal{Q}}_{kij}^* = \langle {}^{ME}\Lambda_{pq}^k \mathcal{C}_{pqmn} {}^{MM}\Gamma_{mn}^{ij} + {}^{EE}\Gamma_p^k \mathcal{Q}_{pqm} {}^{MM}\Gamma_{qm}^{ij} + {}^{ME}\Lambda_{qm}^k \mathcal{Q}_{pqm} {}^{EM}\Lambda_p^{ij} - {}^{EE}\Gamma_p^k \mathcal{E}_{pq} {}^{EM}\Lambda_q^{ij} \rangle, \quad (3.11)$$

which concludes that $\bar{\mathcal{Q}}^{*T} = \bar{\mathcal{Q}}$, since $\bar{\mathcal{Q}}_{ijk}^{*T} = \bar{\mathcal{Q}}_{kij}^*$ by definition. After the derivation of these quadratic forms, their sensitivities with respect to a generic material variable ζ are derived next. Now, upon choosing $\{\bullet\}_{\eta_i}$ and $\{\bullet\}_{\omega}$ as judiciously chosen $\frac{\partial \{\bullet\}_{\mathbf{x}}}{\partial \zeta}$ results in the vanishing averages

$$\left\langle \frac{\partial {}^{MM}\Lambda_{ij}^{pq}}{\partial \zeta} \mathcal{C}_{ijkl} {}^{MM}\Gamma_{kl}^{mn} + \frac{\partial {}^{MM}\Lambda_{ij}^{pq}}{\partial \zeta} \mathcal{Q}_{kij} {}^{EM}\Lambda_k^{mn} \right\rangle = 0, \quad (3.12a)$$

$$\left\langle \frac{\partial {}^{EM}\Lambda_i^{pq}}{\partial \zeta} \mathcal{Q}_{ijk} {}^{MM}\Gamma_{jk}^{mn} - \frac{\partial {}^{EM}\Lambda_i^{pq}}{\partial \zeta} \mathcal{E}_{ij} {}^{EM}\Lambda_j^{mn} \right\rangle = 0; \quad (3.12b)$$

$$\left\langle \frac{\partial {}^{ME}\Lambda_{ij}^p}{\partial \zeta} \mathcal{C}_{ijkl} {}^{MM}\Gamma_{kl}^{mn} + \frac{\partial {}^{ME}\Lambda_{ij}^p}{\partial \zeta} \mathcal{Q}_{kij} {}^{EM}\Lambda_k^{mn} \right\rangle = 0, \quad (3.12c)$$

$$\left\langle \frac{\partial {}^{EE}\Lambda_i^p}{\partial \zeta} \mathcal{Q}_{ijk} {}^{ME}\Lambda_{jk}^m - \frac{\partial {}^{EE}\Lambda_i^p}{\partial \zeta} \mathcal{E}_{ij} {}^{EE}\Gamma_j^m \right\rangle = 0.$$

Now, taking the derivative of macroscopic constituents, invoking the vanishing averages and re-arranging indices together with the symmetries of macroscopic constituents produce the following compact forms:

$$\frac{\partial \bar{\mathcal{C}}_{ijkl}}{\partial \zeta} = \langle {}^{MM}\Gamma_{pq}^{ij} \frac{\partial \mathcal{C}_{pqmn}}{\partial \zeta} {}^{MM}\Gamma_{mn}^{kl} + {}^{EM}\Lambda_p^{ij} \frac{\partial \mathcal{Q}_{pqm}}{\partial \zeta} {}^{MM}\Gamma_{qm}^{kl} + \quad (3.13a)$$

$${}^{MM}\Gamma_{qm}^{ij} \frac{\partial \mathcal{Q}_{pqm}}{\partial \zeta} {}^{EM}\Lambda_p^{kl} - {}^{EM}\Lambda_p^{ij} \frac{\partial \mathcal{E}_{pq}}{\partial \zeta} {}^{EM}\Lambda_q^{kl} \rangle,$$

$$\frac{\partial \bar{\mathcal{Q}}_{ijk}}{\partial \zeta} = \langle {}^{ME}\Lambda_{pq}^i \frac{\partial \mathcal{C}_{pqmn}}{\partial \zeta} {}^{MM}\Gamma_{mn}^{jk} + {}^{EE}\Gamma_p^i \frac{\partial \mathcal{Q}_{pqm}}{\partial \zeta} {}^{MM}\Gamma_{qm}^{jk} + \quad (3.13b)$$

$${}^{ME}\Lambda_{qm}^i \frac{\partial \mathcal{Q}_{pqm}}{\partial \zeta} {}^{EM}\Lambda_p^{jk} - {}^{EE}\Gamma_p^i \frac{\partial \mathcal{E}_{pq}}{\partial \zeta} {}^{EM}\Lambda_q^{jk} \rangle,$$

$$\frac{\partial \bar{\mathcal{E}}_{ij}}{\partial \zeta} = \langle -{}^{ME}\Lambda_{pq}^i \frac{\partial \mathcal{C}_{pqmn}}{\partial \zeta} {}^{ME}\Lambda_{mn}^j - {}^{EE}\Gamma_p^i \frac{\partial \mathcal{Q}_{pqm}}{\partial \zeta} {}^{ME}\Lambda_{qm}^j - \quad (3.13c)$$

$${}^{ME}\Lambda_{qm}^i \frac{\partial \mathcal{Q}_{pqm}}{\partial \zeta} {}^{EE}\Gamma_p^j + {}^{EE}\Gamma_p^i \frac{\partial \mathcal{E}_{pq}}{\partial \zeta} {}^{EE}\Gamma_q^j \rangle.$$

In addition to the computational advantage, due to the variational structure of FEM, this form generates exact sensitivity values regardless of FE mesh resolution. Note that these sensitivity expressions have exactly the same forms as (3.10a), (3.10b) and (3.10c).

3.2.1.1 Material Distribution Design Variable

Within the topology optimization framework, obtaining an optimal material density distribution is one of the main goals. In the essence of design parametrization, the material density is determined as if an image is constructed through determining the colors of pixels for rendering [33]. To this end, $s(\mathbf{y})$ denotes the so-called design function, responsible for the material distribution within the microstructure. In order to cooperate with FEM framework, the design function is similarly discretized as an element function:

$$s^e = \sum_I^{n_e} (s^e)^I N^I(\mathbf{y}), \quad (s^e)^I \in [0, 1]. \quad (3.14)$$

In this work, the discretized s^e is selected to be a constant at each point within an element. Since Lagrangian basis functions admit the partition of unity, for convenience, s^e notation is selected to represent the element design function implying

$s^e \in [0, 1]$.

In order to avoid checkerboard patterns and mesh dependence, filtering operation $\mathcal{F}$ is employed on s^e , which delivers the *morphology* variable ρ^e (see [33, 53]):

$$\rho^e = \mathcal{F}(\mathcal{D}^e, s) \quad . \quad (3.15)$$

$\mathcal{D}^e$ represents the filter domain encapsulating neighboring elements within a sphere with radius R . Various types of filters have been defined and explored (e.g. see [54–56] for morphology-based filters and [57] for PDE-based filters). In this work, linear morphology based filter with conic weights is utilized:

$$\rho^K = \sum_I w^{KI} s^I \quad \text{and} \quad w^{KI} = \begin{cases} \frac{R-d(K,I)}{\sum_{J \in \mathcal{D}^K} R-d(K,J)} & I \in \mathcal{D}^K \\ 0 & \text{otherwise} \end{cases} \quad . \quad (3.16)$$

Here, $\sum_I w^{KI} = 1$ and $d(K, I)$ represents the distance function operating on the centroids of the corresponding elements [55]. Furthermore, the sensitivity of the morphology variable yields

$$\frac{\partial \rho^K}{\partial s^I} = w^{KI} \quad . \quad (3.17)$$

Capturing a discrete 0\1 material density distribution for a smooth design [55] while controlling the minimum length scale can be challenging with a standard filtering method; thus, various techniques have been proposed, such as sensitivity filtering and projection methods [55, 58–60]. In this study, the threshold projection method is adopted for 0\1 projection:

$$\tilde{\rho}^I = \frac{\tanh(\beta\eta) + \tanh(\beta(\rho^I - \eta))}{\tanh(\beta\eta) + \tanh(\beta(1 - \eta))} \quad . \quad (3.18)$$

Here, the morphology variable $\eta \in [0, 1]$ operates as a dilation (i.e. for $\eta = 0$) or an erosion operator (i.e. for $\eta = 1$), while highlighting that $\eta = 0.5$ is the optimal choice for smooth design without enforcing any minimum length scale [60]. The projection parameter β manages the discreteness of the design. β is gradually incremented like a continuation method to avoid getting stuck at local minima [53, 58]². Ultimately, the sensitivity of the threshold projection can be derived

²Continuation method is a design evolution procedure in which the penalization in (3.21) is incremented in some way (see [58])

as

$$\frac{\partial \tilde{\rho}^I}{\partial \rho^J} = \begin{cases} \frac{\beta(1-\tanh^2(\beta(\rho^I-\eta)))}{\tanh(\beta\eta)+\tanh(\beta(1-\eta))} & I = J \\ 0 & \text{otherwise} \end{cases} . \quad (3.19)$$

In order to determine the discreteness of the design, i.e. whether the material density distribution is fully converged to 0\1 design or not, *measure of non-discreteness* (M_{nd}) is adopted:

$$M_{nd} = \frac{\sum_I^{N_e} 4\tilde{\rho}^I(1-\tilde{\rho}^I)}{N_e} \times 100\% . \quad (3.20)$$

It suggests that $M_{nd} = 0\%$ highlights the intermediate density values are eliminated (i.e. fully discrete design) whereas $M_{nd} = 100\%$ implies all density values are equal to 0.5 [55]. In this work, the measure M_{nd} is calculated and shared in each example to assess the discreteness.

The material constitutive fields are explicitly constructed through the projected and filtered variables for FEM and optimization based on two-material SIMP model that is utilized as the so-called design function (see [61,62] for alternative approaches). SIMP creates a fictitious material model with predetermined material properties to represent the actual (or physical) material via the interpolation scheme [33,53]:

$$\mathcal{A} = (\tilde{\rho}^e)^p \mathcal{A}^{(1)} + (1 - (\tilde{\rho}^e)^p) \mathcal{A}^{(0)} . \quad (3.21)$$

Here, $\mathcal{A} \in \{\mathcal{C}, \mathcal{Q}, \mathcal{E}\}$ and $\tilde{\rho}^e$ represents the design function at the centroid of an element with exponent of penalization factor $p \geq 1$. Since the distribution of material within an element remains constant, the interpolation is computed once for all quadrature points within the element. Hence, the sensitivity of two-material SIMP model reads

$$\frac{\partial \mathcal{A}}{\partial \tilde{\rho}^e} = p(\tilde{\rho}^e)^{(p-1)} (\mathcal{A}^{(1)} - \mathcal{A}^{(0)}) + \mathcal{A}^{(0)} . \quad (3.22)$$

3.2.1.2 Material Orientation Design Variable

Working with anisotropic constituents requires additional design variables to completely characterize the macroscopic behavior of the material, such as the angle of

rotation of the material axes (the axes of the cell) [33,61]. However, cooperating the axes of the cell with the anisotropy axes creates deficiencies and practical challenges for optimization purposes, which are elaborated later in this and next section comparatively. Therefore, the axis responsible for the material orientation is treated as an independent design variable compared to the orientation of the unit cell.

First the explicit forms of the microscopic materials must be derived; therefore, constituents of any piezoelectric material showing transversely isotropic symmetry can be represented as (see [51])

$$\begin{aligned}\mathcal{E}_{ij} &= (\lambda_2^\mathcal{E} - \lambda_1^\mathcal{E})n_i n_j + \lambda_1^\mathcal{E}\delta_{ij}, & \mathcal{Q}_{ijk} &= \lambda_1^\mathcal{Q}(\delta_{ij}n_k + \delta_{ik}n_j) + \lambda_2^\mathcal{Q}n_i\delta_{jk} + \lambda_3^\mathcal{Q}n_i n_j n_k, \\ \mathcal{C}_{ijkl} &= \lambda_1^\mathcal{C}\delta_{ij}\delta_{kl} + \lambda_5^\mathcal{C}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + (\lambda_2^\mathcal{C} - 4\lambda_4^\mathcal{C})n_i n_j n_k n_l + \lambda_3^\mathcal{C}(\delta_{ij}n_k n_l + n_i n_j \delta_{kl}) \\ &\quad + \lambda_4^\mathcal{C}(n_i \delta_{jk} n_l + n_i \delta_{jl} n_k + \delta_{ik} n_j n_l + \delta_{il} n_j n_k) \quad .\end{aligned}\tag{3.23}$$

Here, the anisotropy axis $\mathbf{n}$ is a unit vector perpendicular to the isotropy plane satisfying $\|\mathbf{n}\| = 1$ by definition and $\lambda_{\{\bullet\}}^{\{\bullet\}}$ represents the material constants. For instance, since transversally isotropic class encapsulates the isotropic class, the material constants imply Lamé constants via setting $\lambda_2^\mathcal{C} = \lambda_3^\mathcal{C} = \lambda_4^\mathcal{C} = 0$ [51]. Parametrizing $\mathbf{n}$ suffices for optimization purposes without introducing additional design parameters to interpret the orientation of the anisotropy direction. Hence, this parametrization may be done through introducing the spherical coordinates; thus, let (ρ, θ, ϕ) be radial, polar and azimuthal positions, respectively (cf. [63]). From the definition of the anisotropy axis, enforcing $\rho = 1$ delivers

$$n_i(\theta, \phi) = \begin{bmatrix} \cos(\theta) \sin(\phi) \\ \sin(\theta) \sin(\phi) \\ \cos(\phi) \end{bmatrix} .\tag{3.24}$$

Furthermore, $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$ may be selected to fully cover the unit sphere, because $\mathcal{Q}$ is not quadratically dependent on $\mathbf{n}$ which highlights that any reflection operation applied on tensor $\mathcal{Q}$ with respect to the isotropy plane will alter the sign of the tensor, which does not hold for $\mathcal{C}$ and $\mathcal{E}$. In order to maintain the bounds of the design variables, a similar interpolation in (3.21) can be utilized as well without enforcing the penalization via choosing $\theta^{min} = 0$, $\theta^{max} = \pi$ and

$$\phi^{min} = 0, \phi^{max} = 2\pi:$$

$$\theta = (\theta^{max} - \theta^{min})\mathcal{O}_\theta + \theta^{min} \quad \text{and} \quad \phi = (\phi^{max} - \phi^{min})\mathcal{O}_\phi + \phi^{min}. \quad (3.25)$$

Here, the design variables $\mathcal{O}_\theta \in [0, 1]$ and $\mathcal{O}_\phi \in [0, 1]$ satisfy the same bounds. Ultimately, a standard chain rule operation can be carried out for sensitivity analysis purposes:

$$\frac{\partial n_i}{\partial \mathcal{O}_\theta} = (\theta^{max} - \theta^{min}) \begin{bmatrix} -\sin(\theta) \sin(\phi) \\ \cos(\theta) \sin(\phi) \\ 0 \end{bmatrix}, \quad \frac{\partial n_i}{\partial \mathcal{O}_\phi} = (\phi^{max} - \phi^{min}) \begin{bmatrix} \cos(\theta) \cos(\phi) \\ \sin(\theta) \cos(\phi) \\ -\sin(\phi) \end{bmatrix}. \quad (3.26)$$

Plugging (3.23) into (3.21) delivers the final form of the fictitious material model at the microscale. Note that in general each transversally isotropic material requires introducing an independent set of orientation design variables. Optimization of the material axes for macroscopic topology optimization problems have been attempted via adjusting fiber or cell orientation through applying a certain rotation on the cell configuration or utilizing the Euler angle representation (e.g. [33, 39, 64]). However, the aforementioned methodologies have various disadvantages (see [33, 41]). On the other hand, the spherical representation via covering the full range may eliminate polarity issues and undesirable mathematical discontinuities due to odd powers of $\mathbf{n}$ appearing in the construction of the piezoelectric tensor, while admitting non-uniqueness and ambiguity issues of the bounds of angles (see [41] for the Cartesian formulation).

3.2.2 Geometry Design Variable

Design space may be restrictive without adjusting the geometry of the unit cell, which may negatively impact the evolution of the microstructure; thus, overall design iteration may converge to a suboptimal design (see [42, 65]). Therefore, the adaptation of the cell geometry is conducted through an uniform linear transformation $\mathbf{A}$, which maps the referential unit cell $\mathcal{Y}_0$ to the current unit cell $\mathcal{Y}$. Since the components of $\mathbf{A}$ admits different parametrization, in addition to the generic design variable ζ , a new design variable γ which parameterizes $\mathbf{A}$ must be introduced. The macroscopic constitutive tensors are now indicated as $\bar{\mathcal{C}}[\zeta; \gamma]$, $\bar{\mathcal{Q}}[\zeta; \gamma]$

and $\bar{\mathcal{E}}[\zeta; \gamma]$ to emphasize the functional dependence of macroscopic materials with respect to γ .

For this purpose, $\langle \bullet \rangle_0 = |\mathcal{Y}_0|^{-1} \int_{\mathcal{Y}_0} \bullet dv_0$ notation is introduced to represent the cell averages on the referential unit cell. Before deriving the sensitivity expressions, it should be noted that in order to minimize non-uniqueness, $\mathbf{A}$ is enforced to be isochoric, meaning that $\det(\mathbf{A}) = 1$ will be constrained for the optimization purposes because the development of the homogenization methodology is not affected by the absolute size of the unit cell. Thus, it is convenient and accurate to use $\langle \bullet \rangle_0 = \langle \bullet \rangle$ for the upcoming theoretical developments, while highlighting that the equality may not hold between optimization iterations for implementation purposes.

First step is to derive a compact sensitivity expression for $\bar{\mathcal{C}}$ from (3.10a); thus, each term in the sensitivity expression is analyzed:

$$\begin{aligned} \frac{\partial \bar{\mathcal{C}}_{pqmn}}{\partial \gamma} = & \left\langle \frac{\partial^{MM} \Lambda_{ij}^{pq}}{\partial \gamma} \mathcal{C}_{ijkl} {}^{MM} \Gamma_{kl}^{mn} + {}^{MM} \Gamma_{ij}^{pq} \mathcal{C}_{ijkl} \frac{\partial^{MM} \Lambda_{kl}^{mn}}{\partial \gamma} \right. \\ & + \frac{\partial^{MM} \Lambda_{ij}^{pq}}{\partial \gamma} \mathcal{Q}_{kij} {}^{EM} \Lambda_k^{mn} + {}^{MM} \Gamma_{ij}^{pq} \mathcal{Q}_{kij} \frac{\partial {}^{EM} \Lambda_k^{mn}}{\partial \gamma} \\ & + \frac{\partial {}^{EM} \Lambda_i^{pq}}{\partial \gamma} \mathcal{Q}_{ijk} {}^{MM} \Gamma_{jk}^{mn} + {}^{EM} \Lambda_i^{pq} \mathcal{Q}_{ijk} \frac{\partial {}^{MM} \Lambda_{jk}^{mn}}{\partial \gamma} \\ & \left. - \frac{\partial {}^{EM} \Lambda_i^{pq}}{\partial \gamma} \mathcal{E}_{ij} {}^{EM} \Lambda_j^{mn} - {}^{EM} \Lambda_i^{pq} \mathcal{E}_{ij} \frac{\partial {}^{EM} \Lambda_j^{mn}}{\partial \gamma} \right\rangle_0 . \end{aligned} \quad (3.27)$$

Before simplifying further, it should be noted that $\mathbf{B} := \mathbf{A}^{-1} = \frac{\partial \mathbf{y}_0}{\partial \mathbf{y}}$ and

$${}^{MM} \Upsilon_{mn}^{kl} = \frac{\partial {}^{MM} \chi_m^{kl}}{\partial y_{0_n}} , \quad {}^{MM} \Lambda_{mn}^{kl} = {}^{MM} \Upsilon_{mr}^{kl} B_{rn} , \quad (3.28a)$$

$${}^{EM} \Upsilon_k^{mn} = \frac{\partial {}^{EM} \chi^{mn}}{\partial y_{0_k}} , \quad {}^{EM} \Lambda_k^{mn} = {}^{EM} \Upsilon_r^{mn} B_{rk} . \quad (3.28b)$$

After defining these new quantities, next step is to substitute them into (3.27)

and then, mapping the integration domain, also rearranging indices deliver

$$\begin{aligned}
\frac{\partial \bar{\mathcal{C}}_{pqmn}}{\partial \gamma} = & \left\langle \frac{\partial}{\partial y_j} \left(\frac{\partial^{MM} \chi_i^{pq}}{\partial \gamma} \right) [\mathcal{C}_{ijkl}^{MM} \Gamma_{kl}^{mn} + \mathcal{Q}_{kij}^{EM} \Lambda_k^{mn}] \right. \\
& + \frac{\partial}{\partial y_i} \left(\frac{\partial^{EM} \chi^{pq}}{\partial \gamma} \right) [\mathcal{Q}_{ijk}^{MM} \Lambda_{jk}^{mn} - \mathcal{E}_{ij}^{EM} \Lambda_j^{mn}] \\
& + [\mathcal{C}_{ijkl}^{MM} \Gamma_{kl}^{pq} + \mathcal{Q}_{kij}^{EM} \Lambda_k^{pq}] \frac{\partial}{\partial y_j} \left(\frac{\partial^{MM} \chi_i^{mn}}{\partial \gamma} \right) \\
& + [\mathcal{Q}_{ijk}^{MM} \Gamma_{jk}^{pq} - \mathcal{E}_{ij}^{EM} \Lambda_j^{pq}] \frac{\partial}{\partial y_i} \left(\frac{\partial^{EM} \chi^{mn}}{\partial \gamma} \right) \\
& + \frac{\partial B_{rj}}{\partial \gamma} [{}^{MM}\Upsilon_{ir}^{pq} \mathcal{C}_{ijkl}^{MM} \Gamma_{kl}^{mn} + {}^{MM}\Gamma_{kl}^{pq} \mathcal{C}_{ijkl}^{MM} \Upsilon_{ir}^{mn}] \\
& + \frac{\partial B_{rj}}{\partial \gamma} [{}^{MM}\Upsilon_{ir}^{pq} \mathcal{Q}_{kij}^{EM} \Lambda_k^{mn} + {}^{EM}\Lambda_k^{pq} \mathcal{Q}_{kij}^{MM} \Upsilon_{ir}^{mn}] \\
& + \frac{\partial B_{ri}}{\partial \gamma} [{}^{EM}\Upsilon_r^{pq} \mathcal{Q}_{ijk}^{MM} \Gamma_{jk}^{mn} + {}^{MM}\Gamma_{jk}^{pq} \mathcal{Q}_{ijk}^{EM} \Upsilon_r^{mn}] \\
& \left. - \frac{\partial B_{ri}}{\partial \gamma} [{}^{EM}\Upsilon_r^{pq} \mathcal{E}_{ij}^{EM} \Lambda_j^{mn} + {}^{EM}\Lambda_j^{pq} \mathcal{E}_{ij}^{EM} \Upsilon_r^{mn}] \right\rangle .
\end{aligned} \tag{3.29}$$

Here, first four terms vanish upon choosing ${}^M\eta_i$ and ${}^M\omega$ as $\frac{\partial^{MM} \chi_i^{pq}}{\partial \gamma}$ and $\frac{\partial^{EM} \chi^{pq}}{\partial \gamma}$, respectively in (3.1a). Now, introducing $\{\bullet\} \mathbb{A}_{ij}^{\{\bullet\}} := -\{\bullet\} \Lambda_{ik}^{\{\bullet\}} \frac{\partial A_{kl}}{\partial \gamma} B_{lj}$, utilizing the identity $\frac{\partial \mathbf{B}}{\partial \gamma} = -\mathbf{B} \frac{\partial \mathbf{A}}{\partial \gamma} \mathbf{B}$ and manipulating indices result in the final compact form of (3.29):

$$\begin{aligned}
\frac{\partial \bar{\mathcal{C}}_{ijkl}}{\partial \gamma} = & \left\langle {}^{MM}\mathbb{A}_{pq}^{ij} \mathcal{C}_{pqrs}^{MM} \Gamma_{rs}^{kl} + {}^{MM}\Gamma_{pq}^{ij} \mathcal{C}_{pqrs}^{MM} \mathbb{A}_{rs}^{kl} \right. \\
& + {}^{MM}\mathbb{A}_{qr}^{ij} \mathcal{Q}_{pqr}^{EM} \Lambda_p^{kl} + {}^{EM}\Lambda_p^{ij} \mathcal{Q}_{pqr}^{MM} \mathbb{A}_{qr}^{kl} \\
& + {}^{EM}\mathbb{A}_p^{ij} \mathcal{Q}_{pqr}^{MM} \Gamma_{qr}^{kl} + {}^{MM}\Gamma_{qr}^{ij} \mathcal{Q}_{pqr}^{EM} \mathbb{A}_p^{kl} \\
& \left. - {}^{EM}\mathbb{A}_p^{ij} \mathcal{E}_{pq}^{EM} \Lambda_q^{kl} - {}^{EM}\Lambda_p^{ij} \mathcal{E}_{pq}^{EM} \mathbb{A}_q^{kl} \right\rangle .
\end{aligned} \tag{3.30}$$

Similar methodology is employed for the rest of the constitutive tensors. Next, the sensitivity of the piezoelectric tensor is derived:

$$\begin{aligned}
\frac{\partial \bar{\mathcal{Q}}_{pmn}}{\partial \gamma} = & \left\langle \frac{\partial {}^{ME}\Lambda_{ij}^p}{\partial \gamma} \mathcal{C}_{ijkl}^{MM} \Gamma_{kl}^{mn} + {}^{ME}\Lambda_{ij}^p \mathcal{C}_{ijkl} \frac{\partial {}^{MM}\Lambda_{kl}^{mn}}{\partial \gamma} \right. \\
& + \frac{\partial {}^{EE}\Lambda_i^p}{\partial \gamma} \mathcal{Q}_{ijk}^{MM} \Lambda_{jk}^{mn} + {}^{EE}\Gamma_i^p \mathcal{Q}_{ijk} \frac{\partial {}^{EE}\Lambda_{jk}^{mn}}{\partial \gamma} \\
& + \frac{\partial {}^{ME}\Lambda_{ij}^p}{\partial \gamma} \mathcal{Q}_{kij}^{EM} \Lambda_k^{mn} + {}^{ME}\Lambda_{ij}^p \mathcal{Q}_{kij} \frac{\partial {}^{EM}\Lambda_k^{mn}}{\partial \gamma} \\
& \left. - \frac{\partial {}^{EE}\Lambda_i^p}{\partial \gamma} \mathcal{E}_{ij}^{EM} \Lambda_j^{mn} - {}^{EE}\Gamma_i^p \mathcal{E}_{ij} \frac{\partial {}^{EM}\Lambda_j^{mn}}{\partial \gamma} \right\rangle_0 .
\end{aligned} \tag{3.31}$$

Now, the counter parts of (3.28a) and (3.28b) are defined similarly as

$${}^{EE}\Upsilon_k^m = \frac{\partial {}^{EE}\chi_k^m}{\partial y_{0_k}} \quad , \quad {}^{EE}\Lambda_k^m = {}^{EE}\Upsilon_r^m B_{rk} \quad , \quad (3.32a)$$

$${}^{ME}\Upsilon_{kl}^m = \frac{\partial {}^{ME}\chi_k^m}{\partial y_{0_l}} \quad , \quad {}^{ME}\Lambda_{kl}^m = {}^{ME}\Upsilon_{kr}^m B_{rl} \quad . \quad (3.32b)$$

Substituting the counter parts, grouping the similar terms and altering the integration domain in (3.31) as done before deliver

$$\begin{aligned} \frac{\partial \bar{\mathcal{Q}}_{pmn}}{\partial \gamma} = & \left\langle \frac{\partial}{\partial y_j} \left(\frac{\partial {}^{ME}\chi_i^p}{\partial \gamma} \right) [\mathcal{C}_{ijkl} {}^{MM}\Gamma_{kl}^{mn} + \mathcal{Q}_{kij} {}^{EM}\Lambda_k^{mn}] \right. \\ & + \frac{\partial}{\partial y_i} \left(\frac{\partial {}^{EE}\chi^p}{\partial \gamma} \right) [\mathcal{Q}_{ijk} {}^{MM}\Lambda_{jk}^{mn} - \mathcal{E}_{ij} {}^{EM}\Lambda_j^{mn}] \\ & + [\mathcal{C}_{ijkl} {}^{ME}\Lambda_{kl}^p + \mathcal{Q}_{kij} {}^{EE}\Gamma_k^p] \frac{\partial}{\partial y_j} \left(\frac{\partial {}^{MM}\chi_i^{mn}}{\partial \gamma} \right) \\ & + [\mathcal{Q}_{ijk} {}^{ME}\Lambda_{jk}^p - \mathcal{E}_{ij} {}^{EE}\Gamma_j^p] \frac{\partial}{\partial y_i} \left(\frac{\partial {}^{EM}\chi^{mn}}{\partial \gamma} \right) \\ & + \frac{\partial B_{rj}}{\partial \gamma} [{}^{ME}\Upsilon_{ir}^p \mathcal{C}_{ijkl} {}^{MM}\Gamma_{kl}^{mn} + {}^{ME}\Lambda_{kl}^p \mathcal{C}_{ijkl} {}^{MM}\Upsilon_{ir}^{mn}] \\ & + \frac{\partial B_{rj}}{\partial \gamma} [{}^{ME}\Upsilon_{ir}^p \mathcal{Q}_{kij} {}^{EM}\Lambda_k^{mn} + {}^{EE}\Gamma_k^p \mathcal{Q}_{kij} {}^{MM}\Upsilon_{ir}^{mn}] \\ & + \frac{\partial B_{ri}}{\partial \gamma} [{}^{EE}\Upsilon_r^p \mathcal{Q}_{ijk} {}^{MM}\Gamma_{jk}^{mn} + {}^{ME}\Lambda_{jk}^p \mathcal{Q}_{ijk} {}^{EM}\Upsilon_r^{mn}] \\ & \left. - \frac{\partial B_{ri}}{\partial \gamma} [{}^{EE}\Upsilon_r^p \mathcal{E}_{ij} {}^{EM}\Lambda_j^{mn} + {}^{EE}\Gamma_j^p \mathcal{E}_{ij} {}^{EM}\Upsilon_r^{mn}] \right\rangle \quad . \end{aligned} \quad (3.33)$$

Lastly, all possible combinations of $\{\bullet\}\boldsymbol{\eta}$ and $\{\bullet\}\boldsymbol{\omega}$ must be chosen as corresponding admissible $\frac{\partial \{\bullet\}\boldsymbol{\chi}}{\partial \gamma}$ to deduce the final form via employing the same identities used before. Then, the resultant equations imply that first four terms of (3.33) must vanish:

$$\begin{aligned} \frac{\partial \bar{\mathcal{Q}}_{ijk}}{\partial \gamma} = & \left\langle {}^{ME}\mathbb{A}_{lp}^i \mathcal{C}_{lpqr} {}^{MM}\Gamma_{qr}^{jk} + {}^{ME}\Lambda_{lp}^i \mathcal{C}_{lpqr} {}^{MM}\mathbb{A}_{qr}^{jk} \right. \\ & + {}^{ME}\mathbb{A}_{pq}^i \mathcal{Q}_{lpq} {}^{EM}\Lambda_l^{jk} + {}^{EE}\Gamma_l^i \mathcal{Q}_{lpq} {}^{MM}\mathbb{A}_{pq}^{jk} \\ & + {}^{EE}\mathbb{A}_l^i \mathcal{Q}_{lpq} {}^{MM}\Gamma_{pq}^{jk} + {}^{ME}\Lambda_{pq}^i \mathcal{Q}_{lpq} {}^{EM}\mathbb{A}_l^{jk} \\ & \left. - {}^{EE}\mathbb{A}_l^i \mathcal{E}_{lp} {}^{EM}\Lambda_p^{jk} - {}^{EE}\Gamma_l^i \mathcal{E}_{lp} {}^{EM}\mathbb{A}_p^{jk} \right\rangle \quad . \end{aligned} \quad (3.34)$$

Finally, the sensitivity of the dielectric tensor is formulated. First step is to take the derivative of the dielectric tensor with respect to γ in the reference unit cell,

since the linear transformation affects the current position of the cell:

$$\begin{aligned}
\frac{\partial \bar{\mathcal{E}}_{pm}}{\partial \gamma} = & \langle -\frac{\partial^{ME} \Lambda_{ij}^p}{\partial \gamma} \mathcal{C}_{ijkl} {}^{ME} \Lambda_{kl}^m - {}^{ME} \Lambda_{ij}^p \mathcal{C}_{ijkl} \frac{\partial^{ME} \Lambda_{kl}^m}{\partial \gamma} \\
& - \frac{\partial^{EE} \Lambda_i^p}{\partial \gamma} \mathcal{Q}_{ijk} {}^{ME} \Lambda_{jk}^m - {}^{EE} \Gamma_i^p \mathcal{Q}_{ijk} \frac{\partial^{ME} \Lambda_{jk}^m}{\partial \gamma} \\
& - \frac{\partial^{ME} \Lambda_{ij}^p}{\partial \gamma} \mathcal{Q}_{kij} {}^{EE} \Gamma_k^m - {}^{ME} \Lambda_{ij}^p \mathcal{Q}_{kij} \frac{\partial^{EE} \Lambda_k^m}{\partial \gamma} \\
& + \frac{\partial^{EE} \Lambda_i^p}{\partial \gamma} \mathcal{E}_{ij} {}^{EE} \Gamma_j^m + {}^{EE} \Gamma_i^p \mathcal{E}_{ij} \frac{\partial^{EE} \Lambda_j^m}{\partial \gamma} \rangle_0 .
\end{aligned} \tag{3.35}$$

Invoking the counter parts of (3.28a) and (3.28b) introduced previously results in

$$\begin{aligned}
\frac{\partial \bar{\mathcal{E}}_{pm}}{\partial \gamma} = & \langle -\frac{\partial}{\partial y_j} \left(\frac{\partial^{ME} \chi_i^p}{\partial \gamma} \right) [\mathcal{C}_{ijkl} {}^{ME} \Lambda_{kl}^m + \mathcal{Q}_{kij} {}^{EE} \Gamma_k^m] \\
& - \frac{\partial}{\partial y_i} \left(\frac{\partial^{EE} \chi^p}{\partial \gamma} \right) [\mathcal{Q}_{ijk} {}^{ME} \Lambda_{jk}^m - \mathcal{E}_{ij} {}^{EE} \Gamma_j^m] \\
& - [\mathcal{C}_{ijkl} {}^{ME} \Lambda_{kl}^p + \mathcal{Q}_{kij} {}^{EE} \Gamma_k^p] \frac{\partial}{\partial y_j} \left(\frac{\partial^{ME} \chi_i^m}{\partial \gamma} \right) \\
& - [\mathcal{Q}_{ijk} {}^{ME} \Lambda_{jk}^p - \mathcal{E}_{ij} {}^{EE} \Gamma_j^p] \frac{\partial}{\partial y_i} \left(\frac{\partial^{EE} \chi^m}{\partial \gamma} \right) \\
& - \frac{\partial B_{rj}}{\partial \gamma} [{}^{ME} \Gamma_{ir}^p \mathcal{C}_{ijkl} {}^{ME} \Lambda_{kl}^m + {}^{ME} \Lambda_{kl}^p \mathcal{C}_{ijkl} {}^{ME} \Gamma_{ir}^m] \\
& - \frac{\partial B_{rj}}{\partial \gamma} [{}^{ME} \Gamma_{ir}^p \mathcal{Q}_{kij} {}^{EE} \Gamma_k^m + {}^{EE} \Gamma_k^p \mathcal{Q}_{kij} {}^{ME} \Gamma_{ir}^m] \\
& - \frac{\partial B_{ri}}{\partial \gamma} [{}^{EE} \Gamma_r^p \mathcal{Q}_{ijk} {}^{ME} \Lambda_{jk}^m + {}^{ME} \Lambda_{jk}^p \mathcal{Q}_{ijk} {}^{EE} \Gamma_r^m] \\
& + \frac{\partial B_{ri}}{\partial \gamma} [{}^{EE} \Gamma_r^p \mathcal{E}_{ij} {}^{EE} \Lambda_j^m + {}^{EE} \Gamma_j^p \mathcal{E}_{ij} {}^{EE} \Gamma_r^m] \rangle .
\end{aligned} \tag{3.36}$$

Here, instead of all possible combinations of the selection in the weak form, it suffices to select ${}^M \eta_i$ and ${}^E \omega$ as $\frac{\partial^{ME} \chi_i^p}{\partial \gamma}$ and $\frac{\partial^{EE} \chi^p}{\partial \gamma}$ respectively, which leads to disappearance of the first four terms. Ultimately, employing the symmetry properties and $\frac{\partial \mathbf{B}}{\partial \gamma}$ -identity, the final form of the sensitivity of the dielectric tensor

is obtained:

$$\begin{aligned}
\frac{\partial \bar{\mathcal{E}}_{ij}}{\partial \gamma} = & \langle -{}^{ME}\mathbb{A}_{kl}^i \mathcal{C}_{klpq} {}^{ME}\Lambda_{pq}^j - {}^{ME}\Lambda_{kl}^i \mathcal{C}_{klpq} {}^{ME}\mathbb{A}_{pq}^j \\
& - {}^{ME}\mathbb{A}_{lp}^i \mathcal{Q}_{klp} {}^{EE}\Gamma_k^j - {}^{EE}\Gamma_k^i \mathcal{Q}_{klp} {}^{ME}\mathbb{A}_{lp}^j \\
& - {}^{EE}\mathbb{A}_k^i \mathcal{Q}_{klp} {}^{ME}\Lambda_{lp}^j - {}^{ME}\Lambda_{lp}^i \mathcal{Q}_{klp} {}^{EE}\mathbb{A}_k^j \\
& + {}^{EE}\mathbb{A}_k^i \mathcal{E}_{kl} {}^{EE}\Gamma_l^j + {}^{EE}\Gamma_k^i \mathcal{E}_{kl} {}^{EE}\mathbb{A}_l^j \rangle .
\end{aligned} \tag{3.37}$$

After deriving the final forms of the sensitivities with respect to an arbitrary component of $\mathbf{A}$, next step is to explicitly state the parametrization of the linear transformation:

$$\mathbf{A} = \begin{bmatrix} g_{max}\gamma_1 + g_{min}(1 - \gamma_1) & 2g_d(\gamma_2 - 0.5) & 2g_d(\gamma_3 - 0.5) \\ 2g_d(\gamma_4 - 0.5) & g_{max}\gamma_5 + g_{min}(1 - \gamma_5) & 2g_d(\gamma_6 - 0.5) \\ 2g_d(\gamma_7 - 0.5) & 2g_d(\gamma_8 - 0.5) & g_{max}\gamma_9 + g_{min}(1 - \gamma_9) \end{bmatrix} . \tag{3.38}$$

Here, the set of constants (g_{max}, g_{min}, g_d) are responsible for the scaling of $\mathbf{A}$ that is parameterized through the optimization variable $\gamma_i \in [0, 1]$ (see [42] for the determination of the scaling constants). Since the explicit form of $\mathbf{A}$ is presented, one may apply Jacobi's formula to compute the sensitivity of the given constraint or may prefer to use a direct approach.

The significance of the cell geometry has recently been discussed and elaborated for various physical settings (see [42, 43]). However, it becomes vital while dealing with anisotropic materials. The reason of this is basically that the rotation of the material axes intrinsically implies the rotation of the whole configuration (i.e. the unit cell axes and the material axes), which may be problematic and restrictive. Since a rotation tensor must be orthogonal by definition, it cannot impose a deformation on the unit cell, which may lead to convergence to a sub-optimal design (see [42, 65]). Moreover, if one tries to interchange the rotation tensor with an arbitrary linear transformation to overcome the issue, it may result in the generation of nonphysical materials due to potential violations of the material symmetries or invariants (see [41]). Therefore, separating the relaxation of the unit cell geometry and the material axes to design microstructures with anisotropic constituents is advantageous, because this treatment can stretch the

unit cell geometry, while adjusting the orientation of the material without any violation of the aforementioned principles.

3.3 Performance Variables

Even if the optimization problems have not been rigorously defined so far, the ultimate goal of this work is simply to capture macroscopic target structural behavior of the piezoelectric solids. Solely designing a microstructure may not be sufficient to model complex structural behavior due to the insufficient number of optimization DOFs. Therefore, additional optimization variables have to be included within the optimization framework, which is elaborated next.

3.3.1 Macroscopic Field Variable

Before attempting to capture macroscopic structural behavior, a target macroscopic stress signal at a point is optimized under prescribed cyclic loading of the macroscopic strain. Capturing an arbitrarily prescribed macroscopic stress-strain path has been attempted via tunable microstructures via cooperating temporal design variable with the material coefficients (e.g. see [42,47]). In this work, the workload of this tunability transferred directly into the actual temporal fields. Therefore, from (2.5), any macroscopic stress behavior can be described via

$$\bar{\sigma}(\zeta, \tau, t) = \bar{\mathcal{C}}[\zeta]\bar{\epsilon}(t) - \bar{\mathcal{Q}}^T[\zeta]\bar{\mathbf{E}}(\tau) . \quad (3.39)$$

Here, the performance variable is selected to be the electric field parameterized by the discrete temporal variable $\tau_i \in [0, 1]$ and $\zeta \in \{\tilde{\rho}, \mathbf{O}, \gamma\}$. The notation is adapted to highlight that the macroscopic electric field is not functionally, but rather directly parameterized through the temporal variable for each direction:

$$\bar{E}_i(\tau) = (E_{max} - E_{min})\tau_i + E_{min} . \quad (3.40)$$

Here, the classical linear interpolation scheme is utilized without introducing the penalization while noting that all directions share the same scaling bounds

(see [42] for an alternative scheme). The number of optimization variables for each τ_i corresponds to the number of time steps used in the discretization of continuous time interval. Since the main goal is to achieve target stress behavior, stress-based formulation is emphasized. However, one can employ the same formulation for the electric displacement and attempt to achieve an optimal strain distribution over the time interval via recalling (2.5):

$$\overline{D}(\zeta, \tau, t) = \overline{Q}[\zeta]\overline{\epsilon}(\tau) + \overline{\mathcal{E}}[\zeta]\overline{E}(t) . \quad (3.41)$$

3.3.2 Macroscopic Boundary-Value Variable

Capturing certain macroscopic structural behavior may not be maintained by only optimizing the microstructure. Hence, as discussed above, additional optimization variables should be introduced. To this end, optimizing macroscopic boundary conditions accompanied by the microstructure design may overcome this shortcoming. Since the structural behavior of the piezoelectric medium is targeted, instead of attempting to optimize both the mechanical and the electrical parts of the boundary, specifically Dirichlet portion of the electrical boundary is studied and Neumann portion is assigned to be traction-free. Before developing further mathematical expressions, it must be highlighted that the electric potential based BC formulation should not involve the spatial variation of the electric potential on neighboring FE nodes, which would degrade the physical interpretation (see [12]). The reason is that essential BCs on electrical boundary physically imply electroded sections and the rest may be denoted as unelectroded. The electric potential over each electroded section should be a constant. Therefore, instead of attempting to parameterize $\partial\mathcal{B}_e^E$, it may be separated into regions such that a boundary-value $B^{(I)}$ can parameterize the electric potential within the non-neighboring subregions $\partial\mathcal{B}_e^{E(I)} \subset \partial\mathcal{B}_e^E$ and $\partial\mathcal{B}_e^E \equiv \bigcup_I \partial\mathcal{B}_e^{E(I)}$, where $I \in \{1, \dots, N_b\}$ and N_b represents the number of boundary regions, satisfying $\partial\mathcal{B}_e^{E(I)} \cap \partial\mathcal{B}_e^{E(J)} \equiv \emptyset$, in which $I \neq J$.

An interpolation scheme that is similar to those which have been employed in

earlier chapters can be utilized for this optimization variable:

$$B^{(I)} = (B_{max} - B_{min})b^{(I)} + B_{min} . \quad (3.42)$$

Here, $b^{(I)} \in [0, 1]$ and the other relevant terms represent scaling coefficients. In order to derive the sensitivity expression, the well-known adjoint method is carried out [33]. Before rigorously defining the optimization problems, the adjoint method can be explained via introducing a representative objective function. For this purpose, let $J := J(\bar{\mathbf{x}}^*)$ be a representative objective function of the solution of a macroscopic problem constructed through FEM formulation:

$$\bar{K}_{IJ}\bar{x}_J = \bar{b}_I . \quad (3.43)$$

Hence, imposing Dirichlet conditions alters the linear system as

$$\bar{K}_{\alpha\beta}^*\bar{x}_\beta^* = \bar{b}_\alpha^* - \left(\sum_I^{N_b} \bar{K}_{I\alpha}\bar{x}_I^\circ \right) . \quad (3.44)$$

Here, $\{\bullet\}^*$ expressions represent the reduced forms whereas $\mathbf{x}^\circ$ is the prescribed Dirichlet BC on the element nodes. Furthermore, implicitly differentiating both hand-sides with respect to boundary variable B delivers

$$\frac{\partial \bar{x}_\theta^*}{\partial B} = \bar{K}_{\theta\alpha}^{*-1} \left[\frac{\partial \bar{b}_\alpha^*}{\partial B} - \sum_I^{N_b} \left(\frac{\partial \bar{K}_{I\alpha}}{\partial B} \bar{x}_I^\circ + \bar{K}_{I\alpha} \frac{\partial \bar{x}_I^\circ}{\partial B} \right) - \frac{\partial \bar{K}_{\alpha\beta}^*}{\partial B} \bar{x}_\beta^* \right] . \quad (3.45)$$

Since the solution of the linear system is dependent on the applied BCs, employing the chain rule on the sensitivity of the representative objective function and substituting the above expression implies

$$\frac{\partial J}{\partial B} = \lambda_\alpha \left[\frac{\partial \bar{b}_\alpha^*}{\partial B} - \sum_I^{N_b} \left(\frac{\partial \bar{K}_{I\alpha}}{\partial B} \bar{x}_I^\circ + \bar{K}_{I\alpha} \frac{\partial \bar{x}_I^\circ}{\partial B} \right) - \frac{\partial \bar{K}_{\alpha\beta}^*}{\partial B} \bar{x}_\beta^* \right] , \quad (3.46)$$

where λ_α is the so-called adjoint variable (or vector), which solves the linear system of equations formulated through the symmetry of the stiffness matrix:

$$\bar{K}_{\theta\alpha}^* \lambda_\alpha = \frac{\partial J}{\partial \bar{x}_\theta^*} . \quad (3.47)$$

It should be noted that the generic form (3.46) can be simplified further which eventually delivers

$$\frac{\partial J}{\partial B} = \lambda_\alpha \left[\sum_I^{N_b} \bar{K}_{I\alpha} \frac{\partial \bar{x}_I^\circ}{\partial B} \right] , \quad (3.48)$$

since the optimization variable $b^{(I)}$ does not contribute to the right hand-side and the stiffness matrix. Nevertheless, the form is presented as generically as possible, in order to highlight that the derivative of the macroscopic stiffness matrix with respect to the microscopic design variables can be computed through (3.46) by omitting the partial derivatives of $\bar{b}_\alpha^*$ and $\bar{x}_I^\circ$. If objective function J is selected to be at most quadratic in $\bar{\mathbf{x}}^*$ without introducing any microscopic variable, it is straightforward to show that the overall optimization problem degrades to a system of linear equations. Consequently, the ultimate purpose of the methodology described is based on optimizing the boundary values inherited on the fixed boundary regions rather than designing the distribution of the regions, in order to characterize the structural behavior of the macroscopic solid. In other words, the distribution of the regions are not designed but the boundary-values that inhibit on the regions are included in the optimization.

Chapter 4

Numerical Investigations

In this chapter, various types of optimization problems are introduced regarding both scales. First, determination of corresponding FEM and optimization constants are explained for the completeness of the subject and reproducible results. Next, examples of smooth piezoelectric microstructure designs are illustrated based on the previous mathematical derivations. Lastly, numerically optimized stress response and structural behavior of a macroscopic solid are presented. Throughout this chapter, formulation of different objective functions are presented according to the corresponding section. In the following examples, $3 \times 3 \times 3$ unit cells are depicted and relevant cyclic functions (e.g. stress signal) are plotted on consecutive three periods with a specified number of time steps stated later in this chapter. For the design of microstructure, transparent blue represents the distribution of isotropic matrix (e.g. Epoxy), whereas opaque red denotes the distribution of transversally isotropic inclusion (e.g. PZT-5A), where in-between represents the fictitious material.

4.1 Optimization Parameters

Before appointing certain values to the constants mentioned earlier, the optimization algorithm that has been used in the essence of this study should be introduced. Within the optimization scheme, the well-known first gradient based non-linear optimizer, Method of Moving Asymptotes (MMA) by Svanberg, is adopted due its consistent performance on topology optimization problems (see [33, 66]). While preserving default values of MMA, `movlim` parameter is selected as 0.2. Due to the intrinsic structure of MMA, limits of all design variables are assigned to 0-1, and also the computed objective function at each design iteration is scaled to 1-100 by a constant.

Isoparametric linear Lagrange elements with 2 quadrature points per direction are selected and N_e is determined as 40^3 for microscopic FE mesh structure. The result of homogenization is compared with a micromechanics approach to ensure its accuracy and the sensitivity values are verified with 2nd and 4th-order central finite difference.

Penalization factor p is selected as 1 for two-material SIMP model. Filter radius R is calculated based on the mesh size while maintaining 5% ratio for the domain size. For the threshold projection, η is selected as 0.5 and β is multiplied by 2 at every 100th design cycle until $\beta = 256$ or $M_{nd} = 3\%$, unless otherwise stated (see [55]). As mentioned before, $\theta^{min} = 0$, $\theta^{max} = \pi$ and $\phi^{min} = 0$, $\phi^{max} = 2\pi$ are assigned for the material orientation and the remaining material constants are selected as

$$\begin{aligned}
 \lambda_i^{\mathcal{E}^{(0)}} &= \{7.97 \times 10^{-2}, 7.97 \times 10^{-2}\} \frac{\text{nF}}{\text{m}}, \\
 \lambda_i^{\mathcal{Q}^{(0)}} &= \{0, 0, 0\} \frac{\text{N}}{\text{V m}}, \\
 \lambda_i^{\mathcal{C}^{(0)}} &= \{2.57, 0, 0, 0, 0.64\} \text{GPa}; \\
 \lambda_i^{\mathcal{E}^{(1)}} &= \{8.11, 7.35\} \frac{\text{nF}}{\text{m}}, \\
 \lambda_i^{\mathcal{Q}^{(1)}} &= \{12.30, -5.40, -3.40\} \frac{\text{N}}{\text{V m}}, \\
 \lambda_i^{\mathcal{C}^{(1)}} &= \{75.40, -9.60, -0.20, -1.70, 22.80\} \text{GPa},
 \end{aligned} \tag{4.1}$$

which conveniently delivers the well-known Epoxy and PZT-5A respectively by substituting $\mathbf{n} = \mathbf{e}_3$ in (3.23) (see [28]). The set of (g_{max}, g_{min}, g_d) is determined as $(1.5, 1/1.5, 0.8)$ to parameterize the linear transformation $\mathbf{A}$ and $\det \mathbf{A} = 1$ is constrained for the cell geometry optimization. In order to visualize the current cell configuration and the material orientation, each microstructure is demonstrated with a coordinate axis indicated with colored unit vectors (i.e. red, yellow and blue) and a gray unit vector for the direction of the material orientation.

4.2 Computational Microstructure Design

In this section, generic objective function is constructed to perform a parametric analysis over various design variables to isolate their effects on the optimization scheme. Since the ultimate purpose is to characterize the structural behavior of piezoelectric solids, the macroscopic strain and electric fields are described through harmonic functions that such solids typically operate under [67]:

$$\bar{\epsilon}_{ij}^*(t) = \bar{\epsilon}_{ij}^m \sin\left(\frac{2\pi}{T^\epsilon}t\right) \quad \text{and} \quad \bar{E}_i^*(t) = \bar{E}_i^m \cos\left(\frac{2\pi}{T^E}t\right) \quad . \quad (4.2)$$

Here, $\{\bullet\}^m$ represents the mean of prescribed signals, whereas T^ϵ and T^E are the periods of the strain and electric field respectively. The examples presented in this section is selected to capture the effects of the relaxation of various design variables. Therefore, the periods of the fields are not varied and are both assigned to 1.0s with 20 time steps N_t which delivers 0.05s step size, in order to fully isolate the alteration of the microstructure design. Ultimately, substituting the expressions in (4.2) into the stress (2.6) delivers

$$\bar{\sigma}_{ij}(\tilde{\boldsymbol{\rho}}, \mathbf{O}, \boldsymbol{\gamma}, t) = \bar{\mathcal{C}}_{ijkl}[\tilde{\boldsymbol{\rho}}; \mathbf{O}; \boldsymbol{\gamma}] \bar{\epsilon}_{kl}^*(t) - \bar{\mathcal{Q}}_{kij}[\tilde{\boldsymbol{\rho}}; \mathbf{O}; \boldsymbol{\gamma}] \bar{E}_k^*(t) \quad , \quad (4.3)$$

where $\bar{\epsilon}_{ij}^m = 10^{-4}$ and $\bar{E}_i^m = 1.0 \text{ kV/mm}$ are prescribed, while noting that *small* temporal variation of the macroscopic strain and electric fields does not violate the quasistatic assumptions as explained earlier. Consequently, the objective function is defined through the time-average of tracking error on temporally varying target

macroscopic stress signal with the prescribed strain and electric field:

$$\begin{aligned}
\min. \quad & \Xi[\tilde{\boldsymbol{\rho}}; \boldsymbol{\mathcal{O}}; \boldsymbol{\gamma}] = \sum_{i,j} \left[\frac{1}{T} \int_{t-T}^t (\bar{\sigma}_{ij}(\tilde{\boldsymbol{\rho}}, \boldsymbol{\mathcal{O}}, \boldsymbol{\gamma}, t) - \bar{\sigma}_{ij}^*(t))^2 dt \right], \\
\text{s.t.} \quad & s_I \in [0, 1], \mathcal{O}_\alpha \in [0, 1], \gamma_i \in [0, 1]; \\
& \det \mathbf{A} = 1 \quad .
\end{aligned} \tag{4.4}$$

Since MMA requires the computation of the first derivative of the objective function and constraints with respect to the design variables, the sensitivity of Ξ with respect to $\boldsymbol{\zeta} \in \{\mathbf{s}, \boldsymbol{\mathcal{O}}, \boldsymbol{\gamma}\}$ can be derived via recalling (3.22), (3.26), (3.30) and (3.34) as follows:

$$\frac{\partial \Xi}{\partial \boldsymbol{\zeta}} = 2 \sum_{i,j} \left[\frac{1}{T} \int_{t-T}^t (\bar{\sigma}_{ij}(\tilde{\boldsymbol{\rho}}, \boldsymbol{\mathcal{O}}, \boldsymbol{\gamma}, t) - \bar{\sigma}_{ij}^*(t)) \left(\frac{\partial \bar{\mathcal{C}}_{ijkl}}{\partial \boldsymbol{\zeta}} \bar{\epsilon}_{kl}^*(t) - \frac{\partial \bar{\mathcal{Q}}_{kij}}{\partial \boldsymbol{\zeta}} \bar{E}_k^*(t) \right) dt \right] \quad . \tag{4.5}$$

Here, the sensitivity of $\tilde{\boldsymbol{\rho}}$ with respect to $\mathbf{s}$ can be calculated through the chain rule based on the combination of (3.17) and (3.19). It should be highlighted that the sensitivity of the filter domain with respect to the linear transformation is not attempted to be calculated due to potential discontinuities in the sensitivity which may occur during the transformation. In other words, the filter domain occupied by the elements in referential configuration may not be the same elements after the transformation, which implies that the corresponding derivatives may become undefined due to the discrete nature of filtering process. Therefore, the filter domain selected in referential configuration remains constant. As a result of this, rather than perfect spherical particles, deformed ellipsoid particles may appear according to applied stretch by the linear transformation. In order to overcome this shortcoming, one may adopt a PDE-based filter which intrinsically satisfies the continuity criterion (see [57]). Eventually, the time integral is discretized with the parameters discussed above and Riemann summation is applied for a computational framework.

4.2.1 Unit Cell Topology Optimization

According to (4.4), target stress signal $\bar{\boldsymbol{\sigma}}^*$ is generated based on a unit cell with fixed geometry and material orientation via prescribed strain and electric fields

(Figure 4.1). Then, optimization is conducted based on 6 independent components of the stress for $\mathbf{s}$ with 500 design iterations, which approximately results in 10% tracking error on the maximum deviation (Figure 4.2). Since the volume fraction is not constrained for the optimization, the optimizer prefers to construct additional topological features without attempting to directly construct fibers along $\mathbf{e}_2$, which correlates with the shear components of the stress (Figure 4.2b, 4.2d, 4.2f). This tracking error may verify the convergence of the optimization as an acceptable design (see [42]). Nevertheless, even if the objective is decreased by a certain amount, the resultant topology should not be considered as a smooth design in Figure 4.1b due to checkerboard patterns appearing within the design of unit cell, which should be expected (see [33, 53]).

Next, the same objective function with the same parameters is minimized via filtering the design in each design iteration to eliminate the checkerboard issue. Ratio of the filter domain with respect to the domain of the unit cell remains fixed and it is selected as 5%. The total number of the design iteration is determined as 500 same as with non-modified design. The design iteration is terminated with approximately 3% tracking error for all six components (Figure 4.2). The application of filtering results in eliminating the checkerboard patterns and aiding the optimizer to eliminate the local topological features, which ultimately delivers fiber-like design with approximately 7% decrement in the objective function (Figure 4.1c and 4.2). However, even if the value of the objective function is within the convergence tolerance, the application of filtering generates intermediate topological densities which are not desired, that ultimately increases M_{nd} (Figure 4.1c). In order to highlight the elimination of mesh dependence of the optimized microstructure through filtering, the same objective function is minimized with a different discretization scheme (Figure 4.1c and 4.3). Since it is hard to obtain the same objective value within the design iterations for different mesh structures, the optimization is carried out for 500 design iterations. Since a microstructure with less elements in discretization has less design variables for optimization, the optimized microstructure with less design variables has a lower objective value for the same number of design iterations. This explains the subtle nuances between the microstructures with different mesh sizes (Figure 4.1c and

4.3). Due to higher value of M_{nd} of the filtered unit cell, compared with non-modified design, the application of the threshold projection becomes inevitable (see [55, 58]).

Eventually threshold projection is invoked based on the description shared previously. As a result of the projection, M_{nd} of the optimized topology is decreased significantly, while maintaining the accuracy of the tracking error as 10^{-4} . Since the threshold projection modifies the sensitivity values at the iterations where β is incremented, the decreasing trend of the objective function is altered as if the new design cycle begins freshly at each corresponding iteration. Therefore, one has to avoid aggressive increments in β , which may negatively affect the objective. Next step is to highlight the significance of the material orientation within the optimization framework.

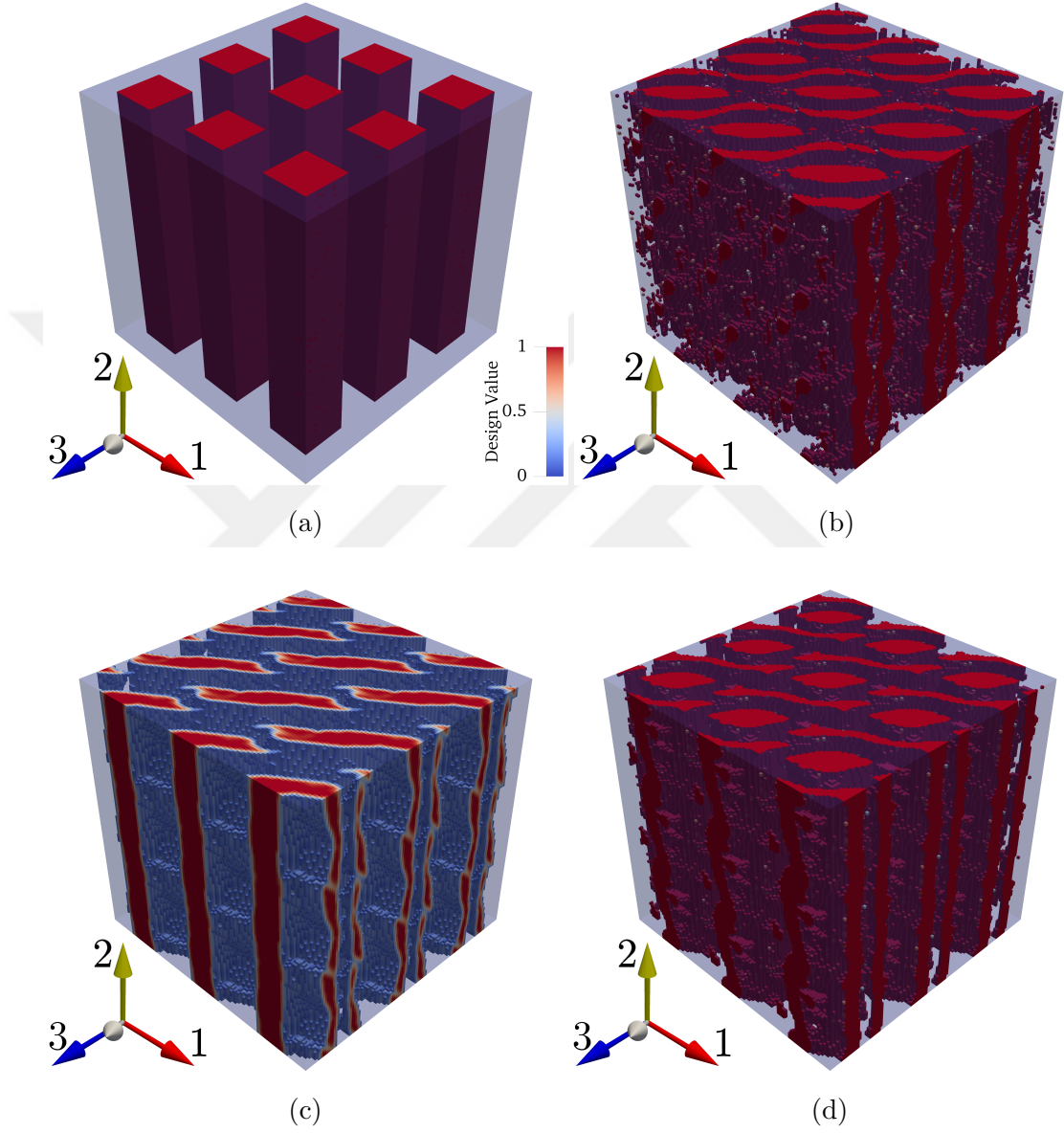


Figure 4.1: Stress signal optimization results for different density distribution strategies are summarized based on a target microstructure (a). Non-modified (b), filtered (c) , filtered and projected (d) designs are captured with M_{nd} values approximately 0.3%, 13% and 0.03% respectively.

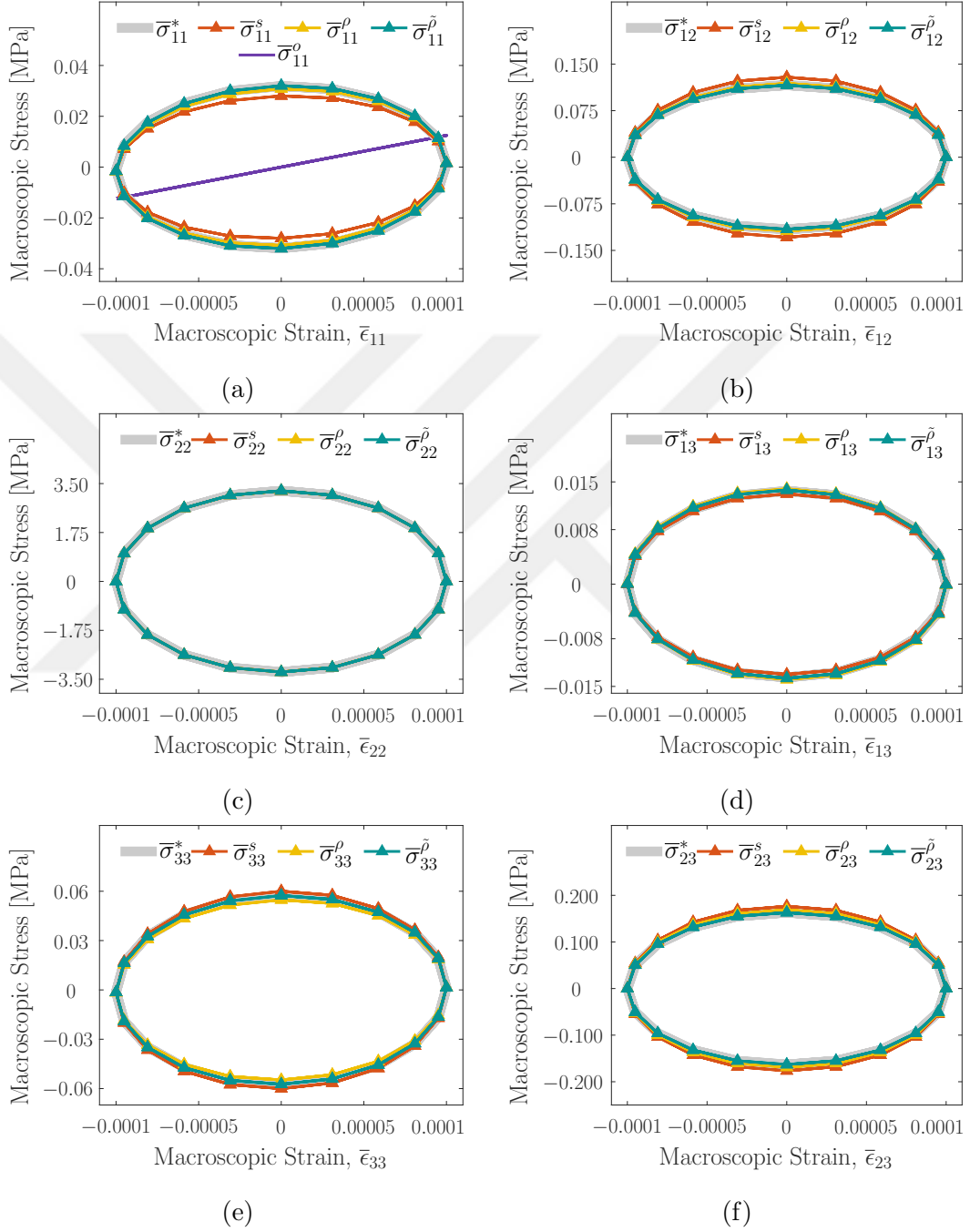


Figure 4.2: Acquired macroscopic stress-strain paths of Figure 4.1 are presented, while separating the paths based on the different design treatments with a superscript: $\{\bullet\}^s$, $\{\bullet\}^\rho$ and $\{\bullet\}^{\tilde{\rho}}$ represent non-modified, filtered and both filtered and projected designs respectively. A reference stress signal $\bar{\sigma}_{11}^o$ computed for the target microstructure in Figure 4.1a by eliminating electrical contributions is illustrated in macroscopic path-normal 1, (a).

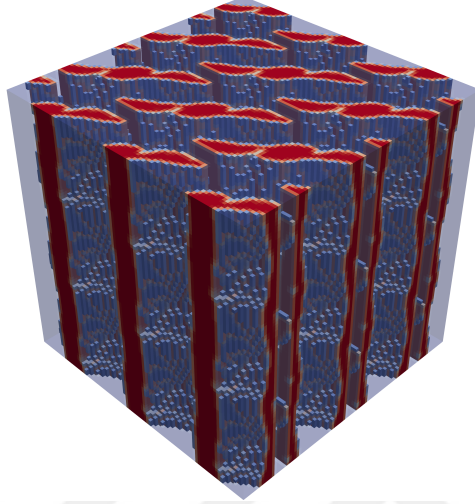


Figure 4.3: Stress signal optimization is carried out based on the target microstructure in Figure 4.1a. The optimized microstructure design with the same filter radius-domain ratio based on a different mesh size, $N_e = 30^3$, is summarized.

4.2.2 Material Orientation Optimization

The ultimate purpose of this example is to highlight the influence of the relaxation of material orientation direction. Therefore, in this example, target stress signal is generated via laminated unit cell where the direction of the material orientation is selected to coincide with the orientation of laminates, in order to acquire challenging target stress response along $\mathbf{e}_2$ -direction (Figure 4.4a). For the first optimization strategy, the material orientation is selected to be constant along $\mathbf{e}_1$ -direction and the volume fraction of the target design is constrained over $\tilde{\rho}$ (i.e. $\langle \tilde{\rho} \rangle = s^*$) to enforce the optimizer to generate a particular design. As a result of this, the optimizer is enforced to generate a microstructure with non-acceptable objective value (Figure 4.5). However, since the optimizer attempts to minimize the objective function, it generates laminated structure with a certain angle, in order to distribute accumulated stiffness along $\mathbf{e}_1$ -direction (Figure 4.4c). Nevertheless, $\bar{\sigma}_{1\bullet}$ components cannot track the relevant components of the

target stress signal (Figure 4.5a, 4.5b, 4.5d).

In order to overcome this issue and obtain lower objective values, material orientation is introduced as a new design variable to the optimizer. Within this approach, since the orientation is relaxed, the optimizer attempts to construct a microstructure similar to the target (Figure 4.4b). However, it should be noted that since the volume fraction of the target is not constrained for this approach, the exact topological microstructure of the target may not be obtained as the result of the optimization due to the non-uniqueness of the problem. Since the material orientation is relaxed, the macroscopic target stress signal is finally captured with 10^{-5} accuracy for all stress components (Figure 4.5). MMA tends to construct a similar laminated structure with a similar material orientation (Figure 4.4b).

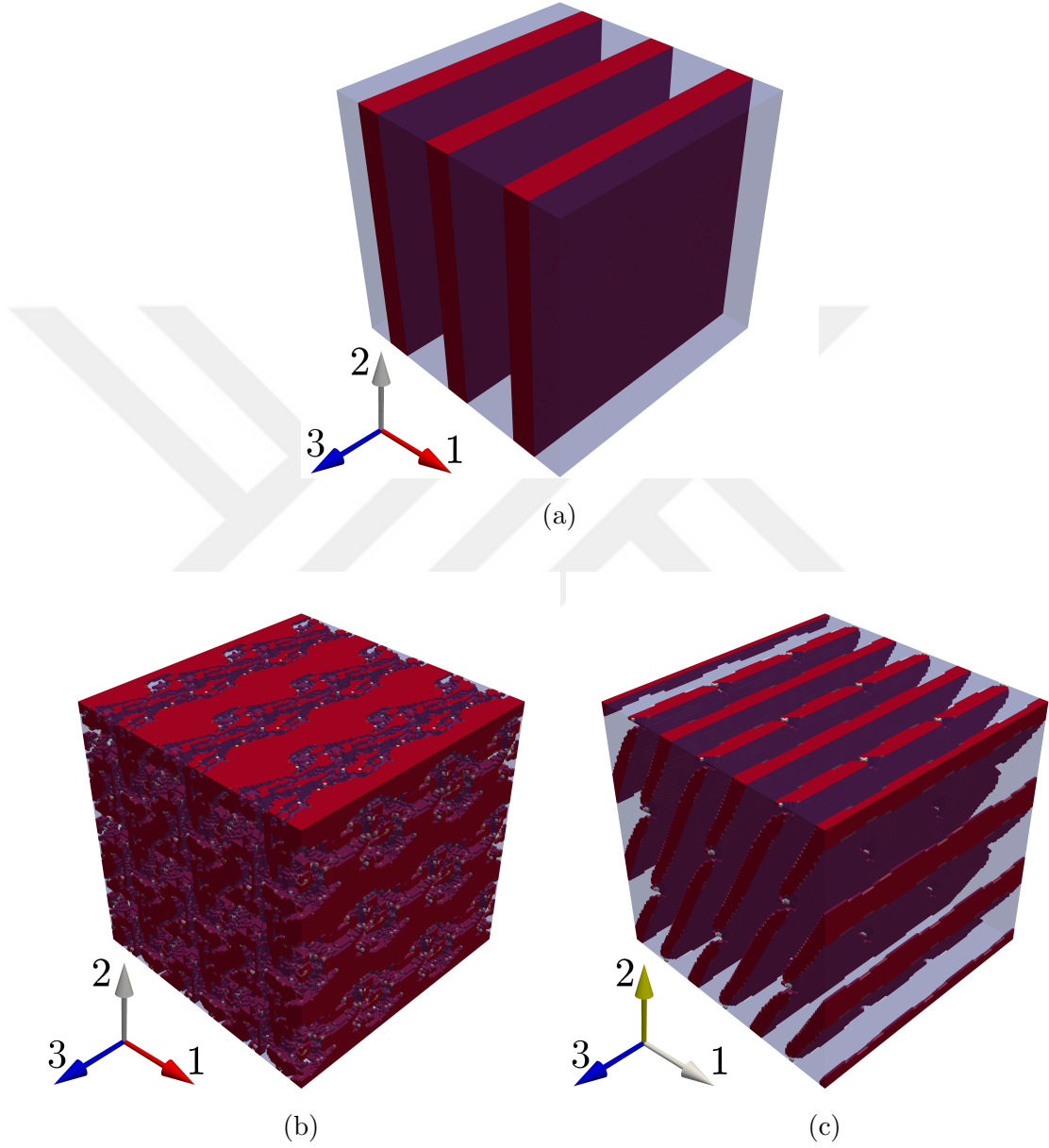


Figure 4.4: Stress signal optimization is carried out based on fixed unit cell geometry (a) for relaxed topology and material orientation. The unit cell with optimized material orientation (b) and fixed material orientation (c) are captured with M_{nd} values approximately 1.0% and 1.5% respectively, while the resultant material orientation directions are indicated with a gray arrow

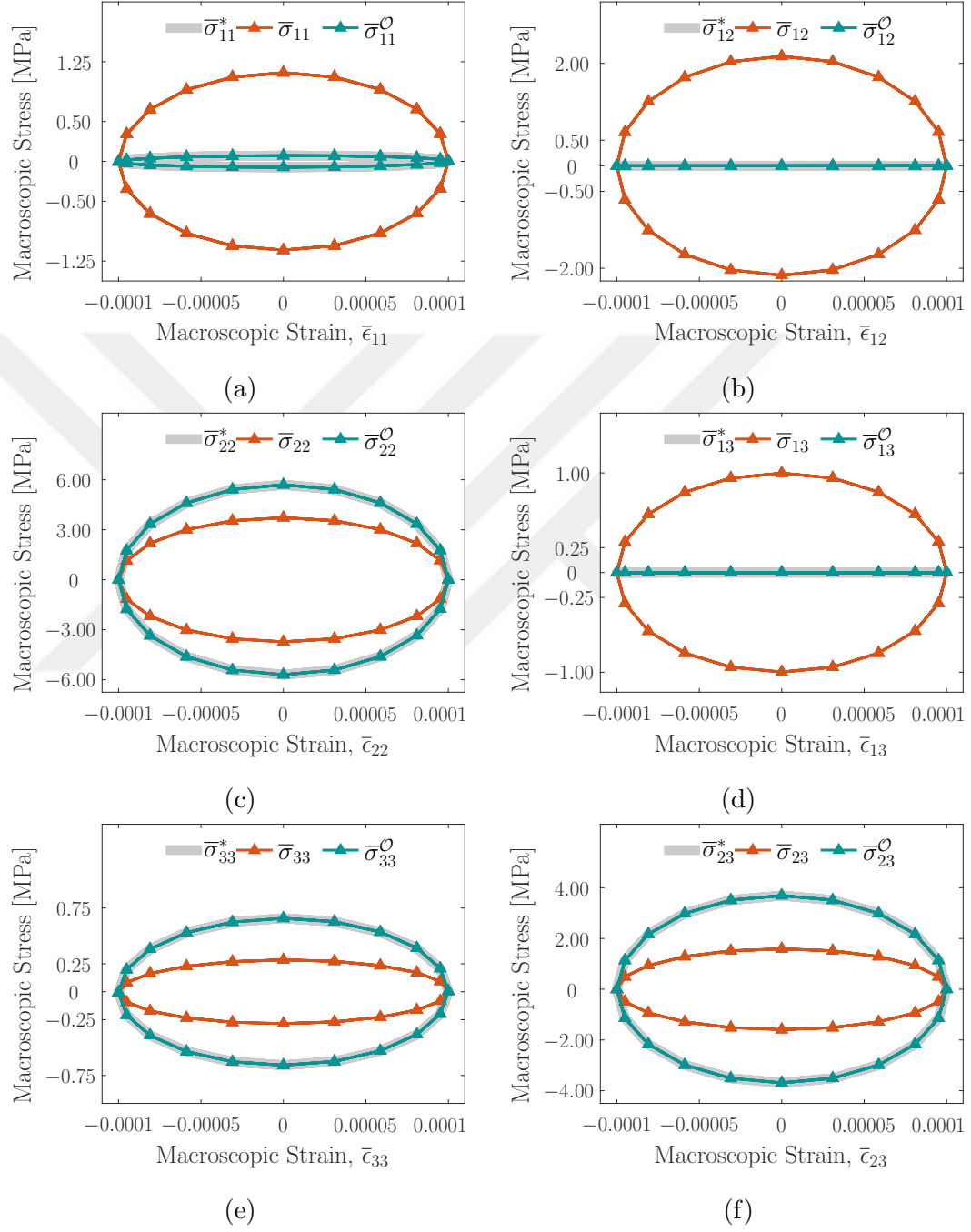


Figure 4.5: Acquired macroscopic stress-strain paths of Figure 4.4 are presented, while separating the paths based on the different optimization strategies with a superscript. $\mathcal{O}$ indicates the stress signal obtained under the relaxation of the material orientation.

4.2.3 Unit Cell Geometry Optimization

For this example, the significance of the relaxation of the cell geometry is highlighted via constructing two separate optimization schemes as done previously. In order to generate target stress signal, target unit cell is constructed and rotated with 45° angle about $+\mathbf{e}_1$ -direction which perfectly coincides with the material orientation (Figure 4.6a). The reason of this selection is to highlight the relevance of the cell geometry compared to the material orientation via building rotated constituents through applying the same rotation enforced on the cell to the material orientation. In other words, as noted before, applying the same rotation onto both the cell and the material axis intrinsically implies the rotation of the whole configuration, which emphasizes the need of relaxation of the cell geometry. Therefore, in order to visualize this unification strategy, the rotation is denoted via the rotation of the coordinate axes in Figure 4.6a. The volume fraction constraint is solely invoked for the cell with fixed geometry in 4.6c.

Since the relaxation of the cell geometry is not introduced to the optimization yet, MMA attempts to modify the projected density values to minimize the objective function and simultaneously satisfy the volume fraction constraint even if the material orientation is accurately captured (Figure 4.6c). Even though the resultant tracking error on the stress is approximately 2%, unfavorable M_{nd} and the appearance of the local topological features conclude that the converged design is undesirable (Figure 4.7, 4.6c). Next, as a second approach, the relaxation of the cell geometry is introduced to MMA with the same optimization parameters as discussed above. Hence, MMA successfully minimizes the tracking error with 10^{-3} accuracy for all stress components, while maintaining an acceptable M_{nd} (Figure 4.6b, 4.7). One can observe that if the representative coordinate axes in Figure 4.6b is mapped to match the axes of Figure 4.6a, the material orientation of the target design and the optimized design are nearly colinear. This observation justifies the previous discussion on the relation between the design variables and the rotation of the configuration.

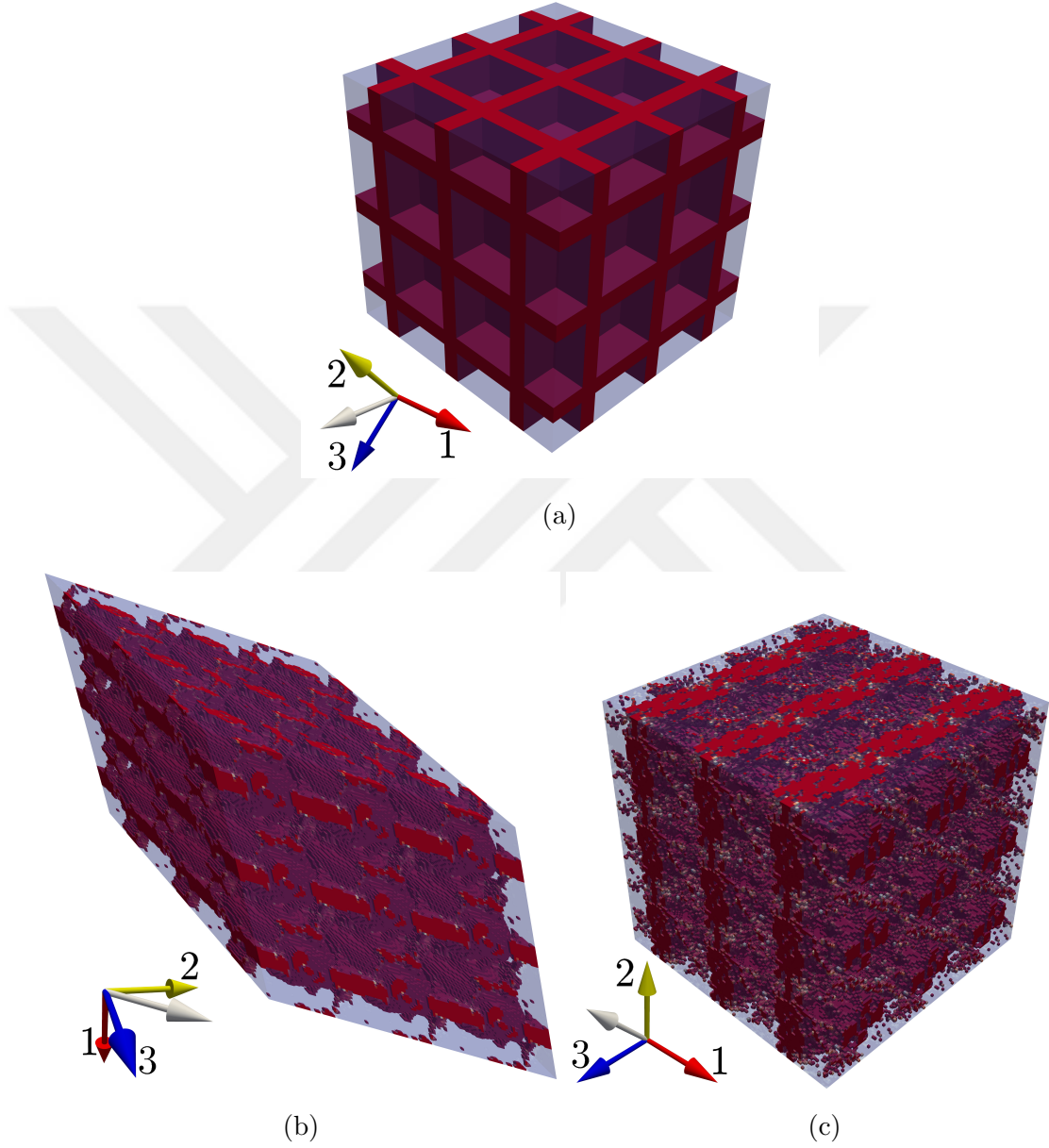


Figure 4.6: Stress signal optimization is carried out based on a rotated cell geometry (a). The unit cell with relaxed cell geometry (b) and fixed cell geometry (c) are captured with M_{nd} values approximately 1.5% and 8% respectively. The optimized material orientation is indicated with a gray arrow, whereas the orientation of the cell is described by the colored axes.

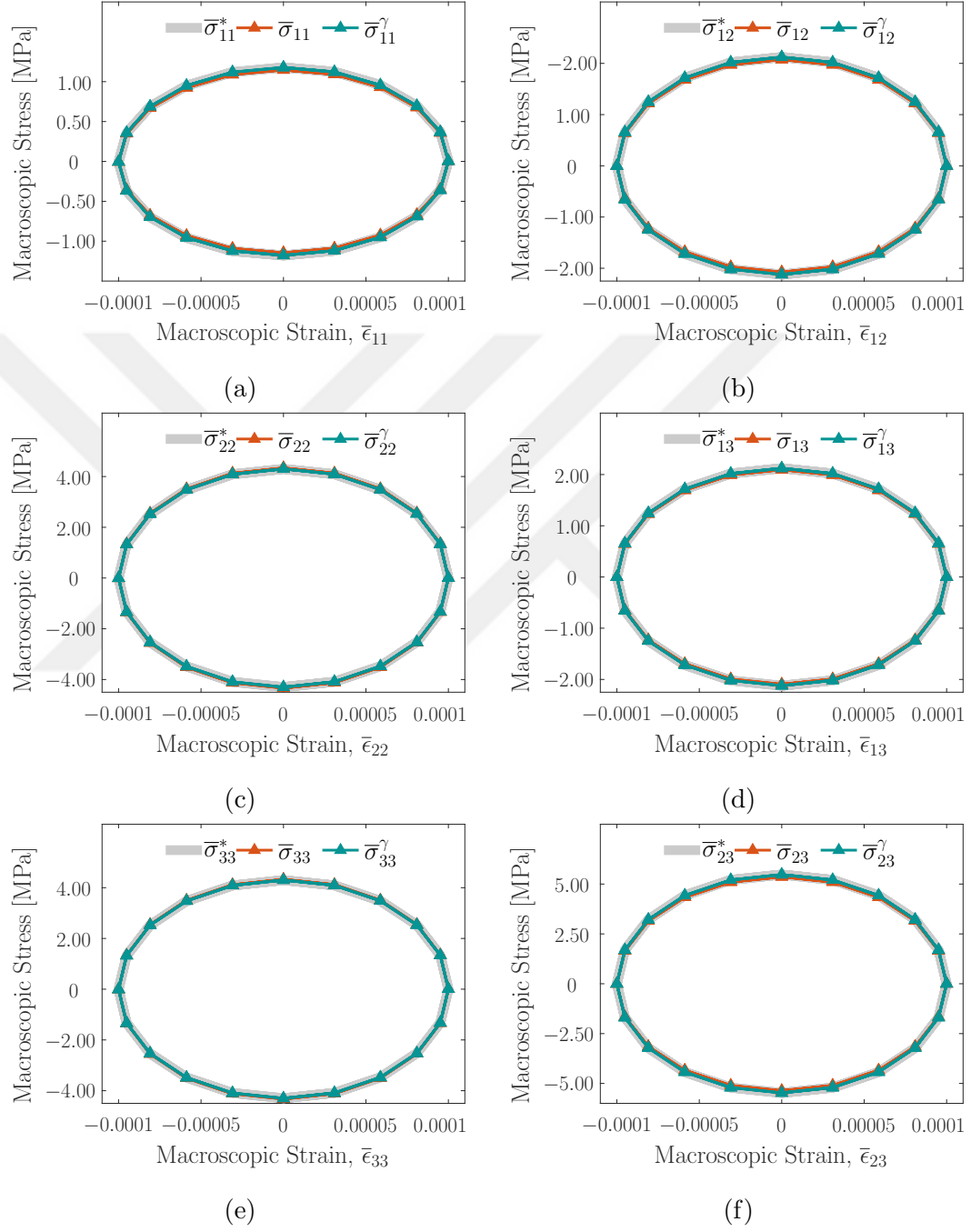


Figure 4.7: Acquired macroscopic stress-strain paths of Figure 4.6 are presented, while separating the paths based on the different design treatments with a superscript. γ indicates the stress signal obtained under the relaxation of the cell geometry.

4.3 Micro Performance Optimization

Generating intriguing stress-strain paths from a target unit cell and fixed macroscopic fields has limited applications, because one has to find the exact microstructure and corresponding fields to produce the desired stress signal which may not be straightforward. Hence, since the microstructure and the material parameters are not allowed to vary in time within the limits of linear theory, any time-dependent stress path may not be captured with the predetermined time-independent material parameters. Therefore, in order to overcome this limitation, adaption of temporal electric field should be introduced to the framework, which temporally modifies the system such that the target stress signal may be apprehended with a particular microstructure. Before numerically investigating the problem, the optimization problem mentioned in (4.4) must be modified via recalling (3.39) and (3.40):

$$\begin{aligned}
\min. \quad & \Xi[\zeta] = \sum_{i,j} \left[\frac{1}{T} \int_{t-T}^t (\bar{\sigma}_{ij}(\zeta, \boldsymbol{\tau}, t) - \bar{\sigma}_{ij}^*(t))^2 dt \right], \\
\text{s.t.} \quad & \zeta \in \{\tilde{\rho}, \boldsymbol{\mathcal{O}}, \boldsymbol{\gamma}\}; \\
& \tau_i \in [0, 1], s_I \in [0, 1], \mathcal{O}_\alpha \in [0, 1], \gamma_i \in [0, 1]; \\
& \langle \tilde{\rho} \rangle = \rho^*; \\
& \det \mathbf{A} = 1 \quad .
\end{aligned} \tag{4.6}$$

Here, the volume fraction is explicitly constrained with a target volume fraction $\rho^* = 0.5$ for the examples below. Next, the number of time steps N_t is selected as 108 to present the resultant signals smoothly, while preserving the prescribed strain signal in 4.2. For the numerical investigation of the micro performance, $\bar{E}_{max}$ and $\bar{E}_{min}$ constants are determined as 1 kV/mm and -1 kV/mm respectively. In order to calculate the sensitivity of the objective, one has to include additionally the partial derivative of the stress with respect to performance variable $\boldsymbol{\tau}$ in (4.5). In this section, two examples are demonstrated based on the number of components of the stress that are introduced to the objective. It should be noted that the maximum number of stress components is selected to be three, in order to avoid from an overconstrained optimization problem.

In the first example, $\bar{\sigma}_{11}$ and $\bar{\sigma}_{12}$ signals are targeted. Unlike the stress signals that are presented in the previous section, the frequencies and phases of the signals are altered. $3T_{11}^\epsilon$ with a phase difference of $\pi/2$ and $2T_{12}^\epsilon$ with a phase difference of $-\pi/3$ are selected for the corresponding stress signals with a mean of 1 MPa (Figure 4.8).

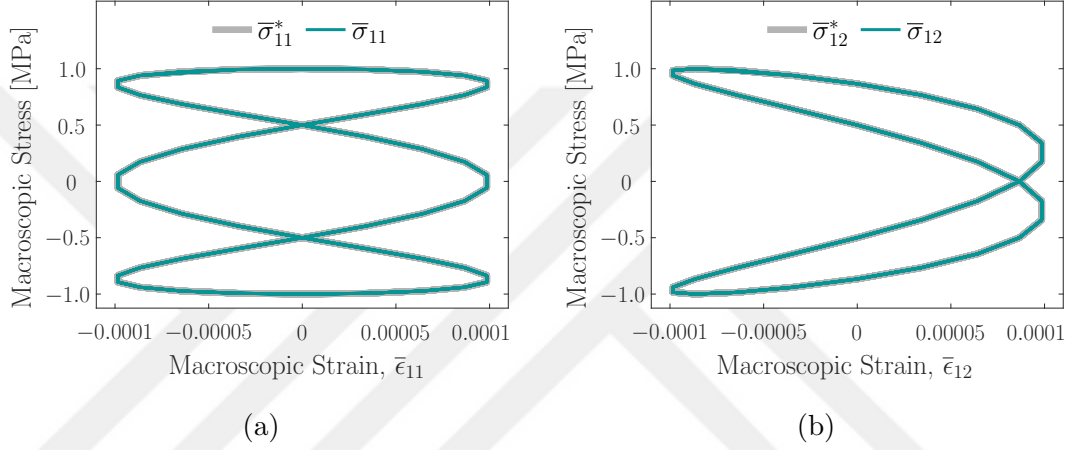


Figure 4.8: Stress signal optimization is carried out based on active target stress components: (a) macroscopic path-normal and (b) macroscopic path-shear.

Since the number of the stress components are less than the performance variables that are linear in the stress, the target is captured with 10^{-3} accuracy with a nearly discrete design (Figure 4.9a). Due to the linearity, the objective becomes highly sensitive to the performance variables in the macroscopic electric field. Therefore, without heavily modifying the design variables, MMA severely alters the performance variables that are initially prescribed constant for the optimization (Figure 4.11b, 4.11c and 4.11d). Even if the different phases and frequencies are invoked to pose a challenging optimization problem, MMA eventually minimizes the objective within the convergence tolerance. Therefore, in order to test the limits of MMA and the framework, another stress component is targeted as well for the next example.

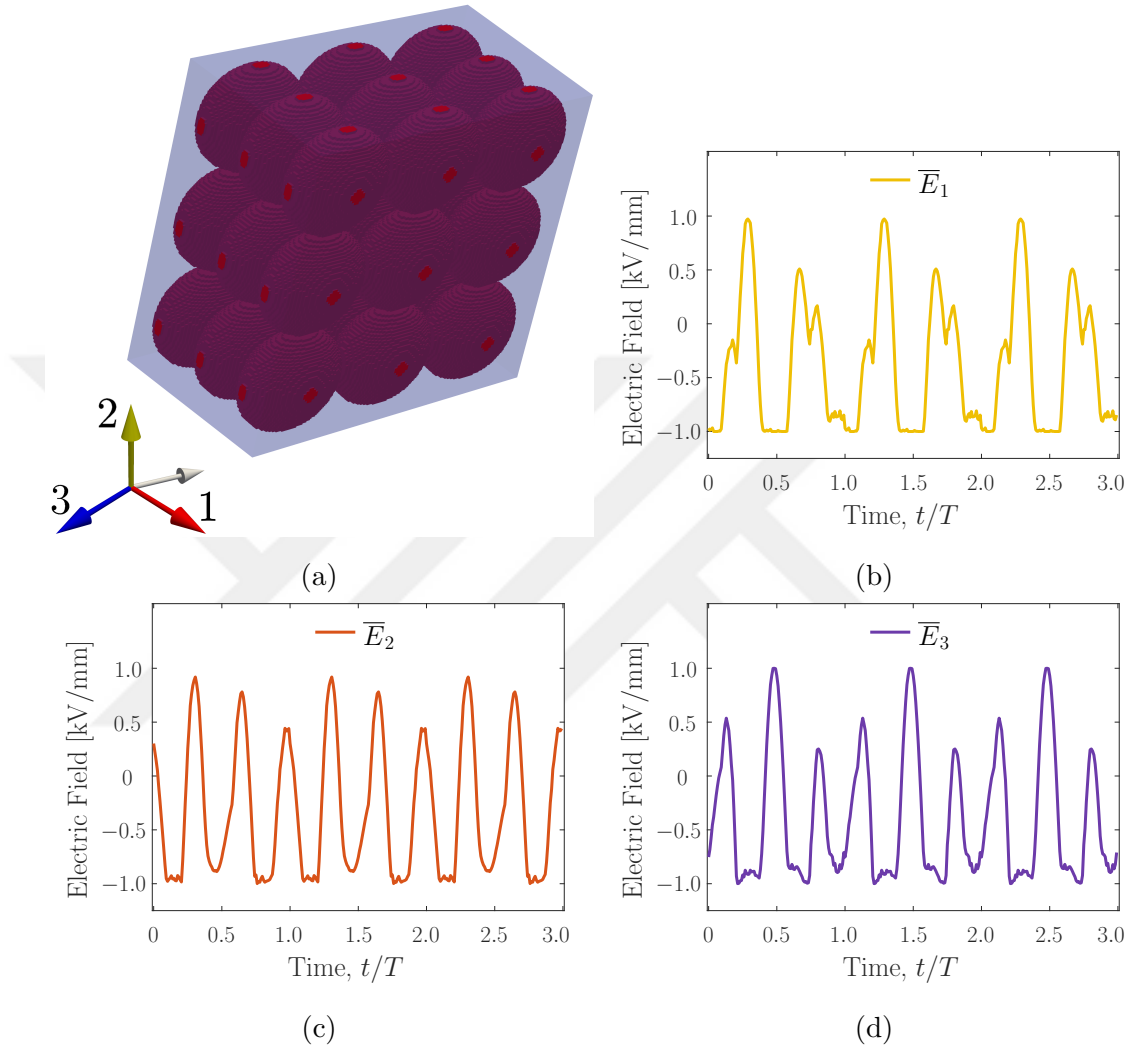


Figure 4.9: Resultant optimization variables generate stress-strain paths in Figure 4.8: (a) optimized unit cell with approximately 0.001% M_{nd} and (b),(c),(d) components of the temporally adapted macroscopic electric field.

In the second example, in addition to the already prescribed stress signals $\bar{\sigma}_{11}$ and $\bar{\sigma}_{12}$, a new component of the stress $\bar{\sigma}_{13}$ is cast into the objective. The additionally prescribed stress signal has the same mean value with the others but $1.5T_{22}^c$ period without a phase shift (Figure 4.10c). Due to the intrinsic complexity of the problem that arises from the increment in the number of the stress components, MMA now begins to deteriorate and deliver approximately 1% tracking error (Figure 4.10 and 4.12).

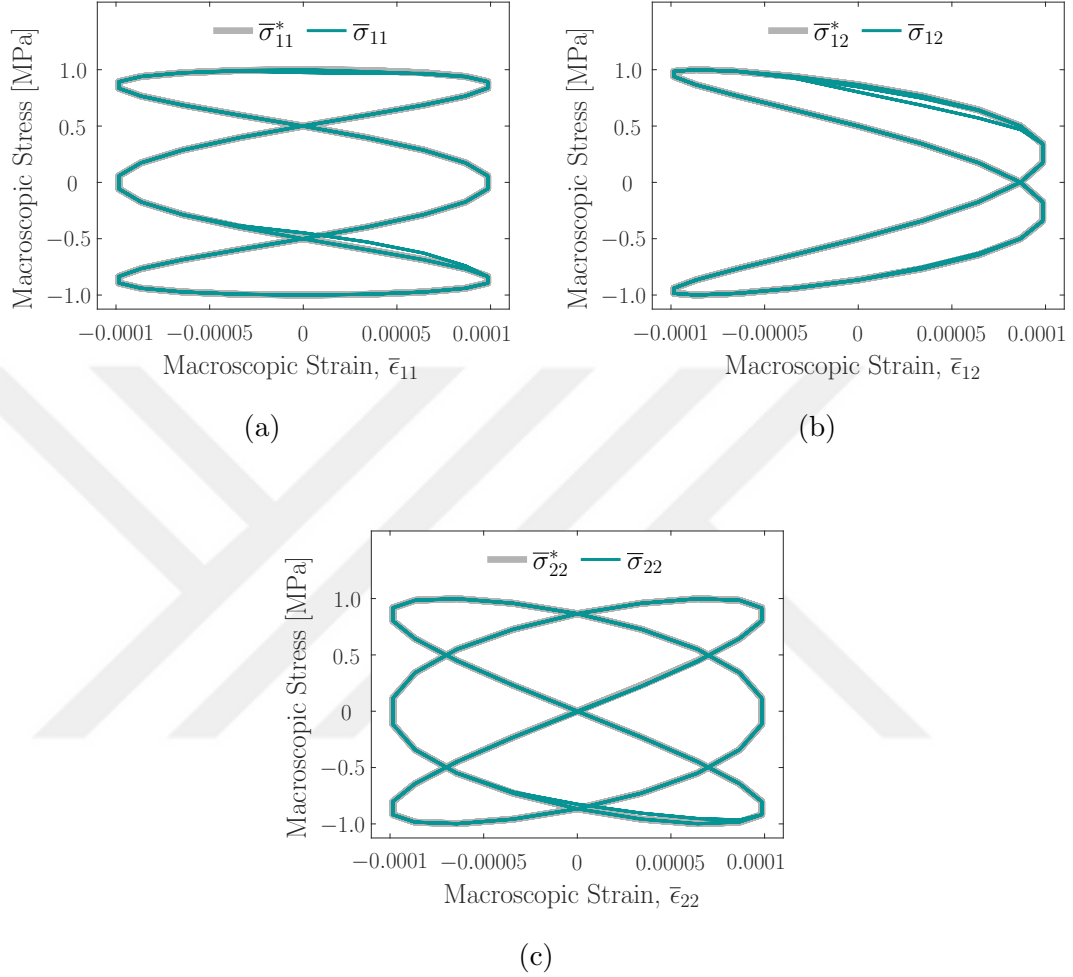


Figure 4.10: Stress signal optimization is carried out based on active target stress components: (a) macroscopic path-normal 1, (b) macroscopic path-shear and (c) macroscopic path-normal 2.

In this example, since all three components affect the objective with alternating frequencies, the design variables become more influential compared to previous example. Subsequently, instead of generating a design with particles, MMA attempts to build more of a laminated design with a non-standard interface (Figure 4.11a). Here, it is not straightforward to describe the interaction between the design and the resultant macroscopic electric field (Figure 4.11b, 4.11c and 4.11d). However, the reason of the formation of the less frequent electric fields compared to the first example might be grounded by the inclusion of the less frequent stress

signal cast into the objective.

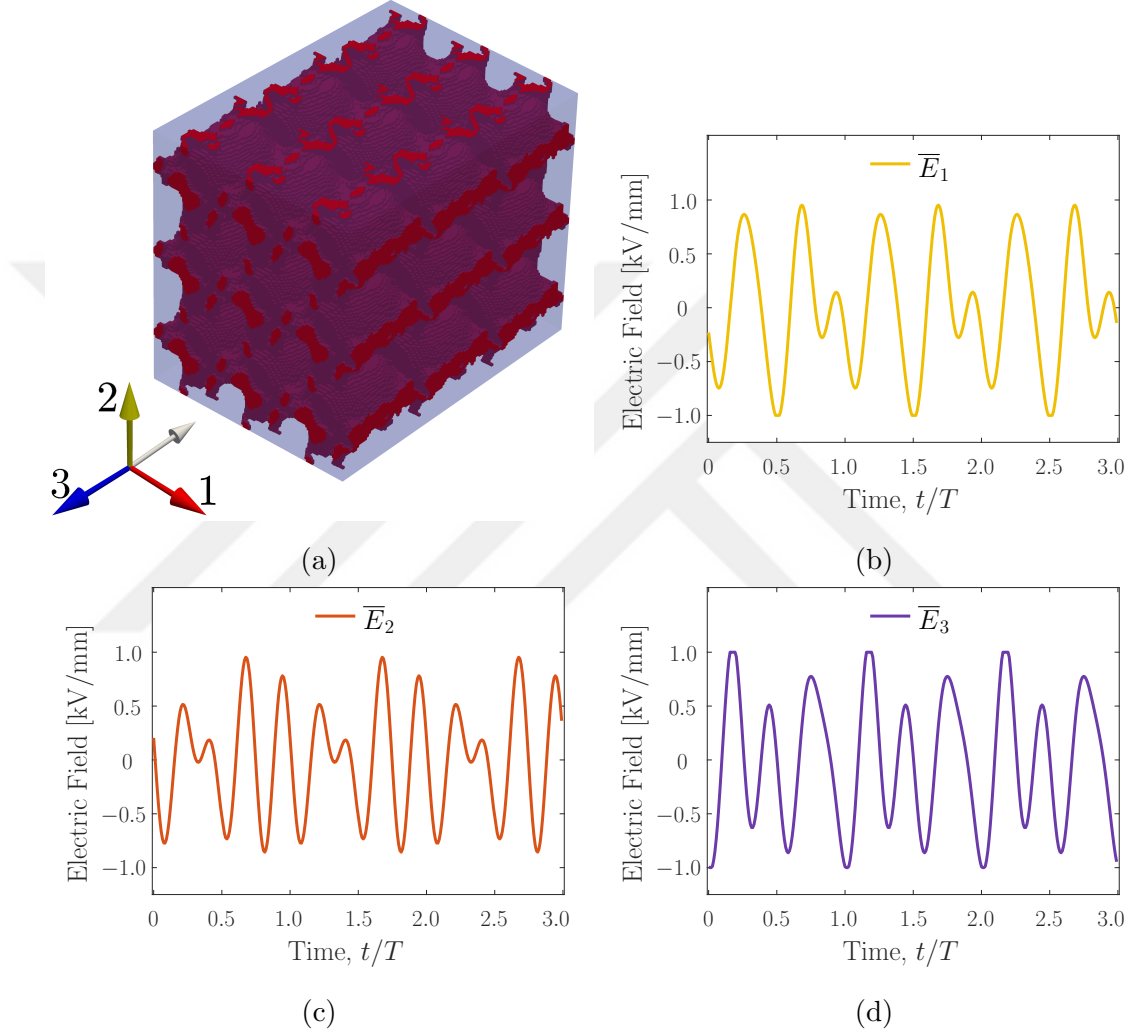


Figure 4.11: Resultant optimization variables generate stress-strain paths in Figure 4.10: (a) optimized unit cell with 0.8% M_{nd} and (b),(c),(d) components of the temporally adapted macroscopic electric field.

At this point, after concluding the effects of the performance variables in this framework, as a last step, the heuristic update scheme of β is discussed. In order to highlight the influence of the non-discrete design on the objective, a cut-off

filter operator $\tilde{\mathcal{F}}^I := \tilde{\mathcal{F}}(\mathcal{R}, \tilde{\rho}^I)$ is defined where $\mathcal{R}$ is the cut-off radius:

$$\tilde{\mathcal{F}}^I = \begin{cases} 1 & \tilde{\rho}^I \geq \mathcal{R} \\ 0 & \text{otherwise} \end{cases}. \quad (4.7)$$

The standard cut-off operation is employed on the filtered and projected material densities at the iterations in which β is updated without interfering the optimization. Since the sensitivities of the objective with respect to the material densities are interrupted at the specified iterations, the objectives that are computed under the cut-off filter are gathered to summarize the behavior of the corresponding objective values (Figure 4.12). One can observe that when the objective approaches to the convergence tolerance, the material distributions become similar which ultimately explains the trend of the decay in the computed objectives (Figure 4.13 and 4.12). Additionally, the spikes of the objective values in between the updates may be resulted from the change in the other optimization variables, since the projected variables are gradually modified (Figure 4.12).

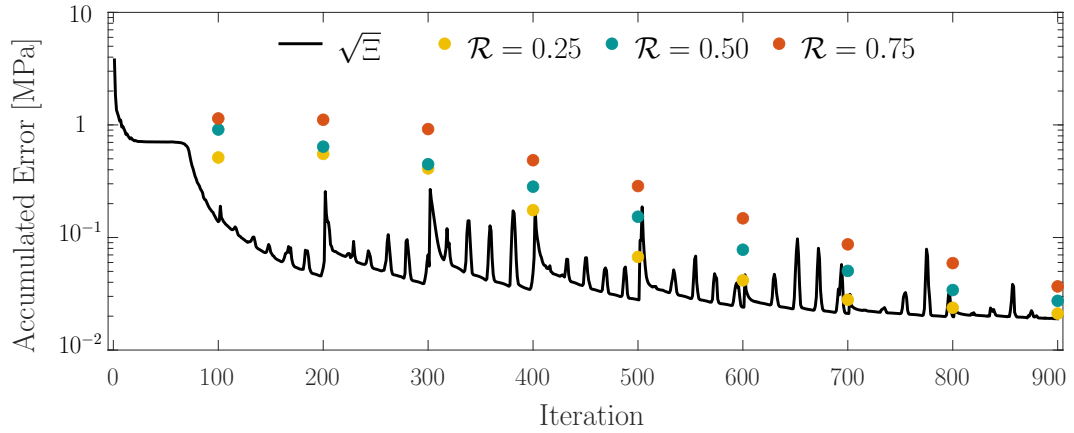


Figure 4.12: Convergence history of the optimization variables in Figure 4.11 is presented based on the tracking error. The resultant errors are indicated for microstructures on which cut-off filters with different radii are employed.

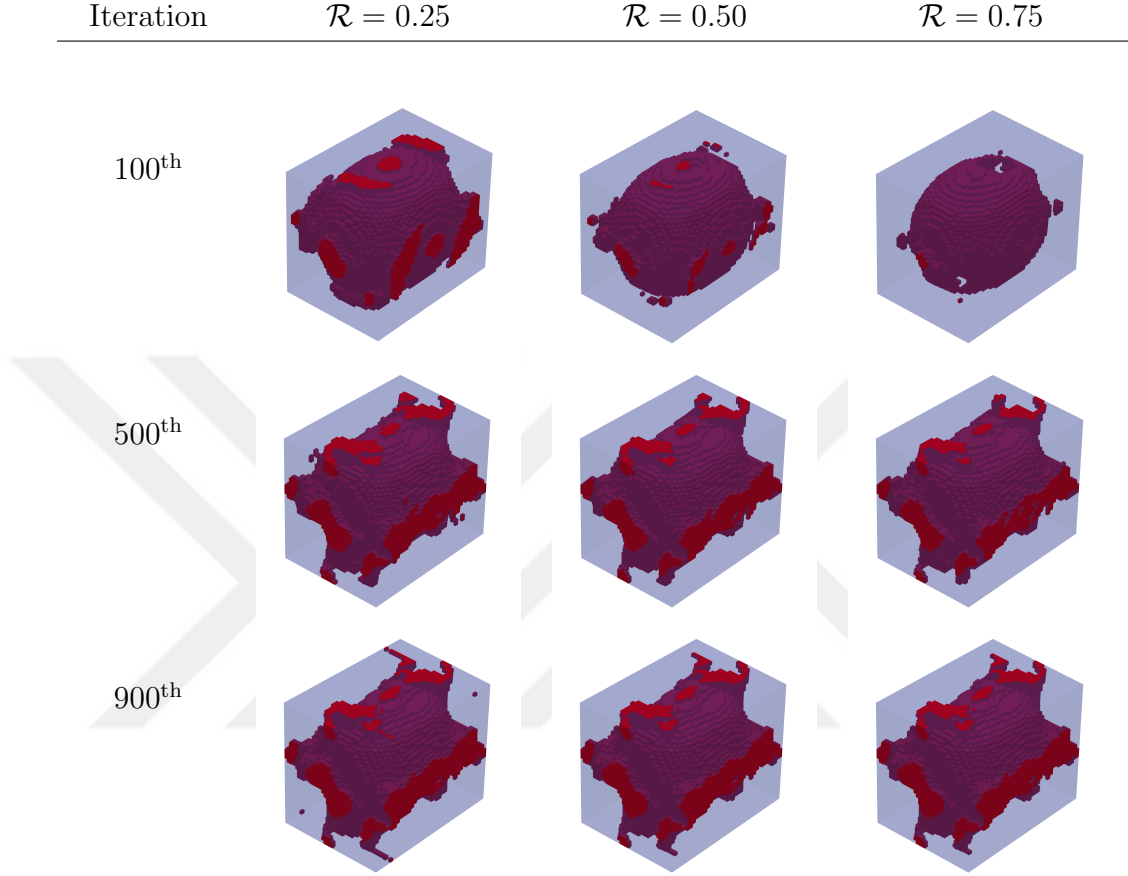


Figure 4.13: Unit cells of the corresponding material distributions summarized in Figure 4.12 are illustrated based on different iterations and cut-off filter radii.

4.4 Macro Performance Optimization

In this section, a more generic case is investigated with an additional macroscopic analysis. Before elaborating on the investigation, it should be noted that when practical concerns are taken into consideration, one may not precisely control the electric field at each point on the macroscopic solid. However, the modification of the boundary conditions may become more convenient practically. To this end, in order to enhance the behavior of the piezoelectric actuators, the optimization of the electrodes may be a reasonable approach without modifying the microscale (see [45]). However, the significance of the two-scale treatment in piezoelectric

actuators is highlighted in a 2D setting [44]. Therefore, in order to exploit the advantages of the two-scale treatment, a two-scale problem is constructed by slightly modifying the objective in (4.4), where $(\bar{\mathbf{u}}(t))^*$ is the targeted macroscopic nodal displacement on the macroscopic FE mesh and $\bar{\mathbf{u}}(t)$ is the representative displacement field defined on the corresponding node (Figure 4.14a):

$$\begin{aligned}
\min. \quad & \Xi[\boldsymbol{\zeta}, \mathbf{b}] = \sum_i \left[\frac{1}{T} \int_{t-T}^t [\bar{u}_i(\boldsymbol{\zeta}, \mathbf{b}, t) - (\bar{u}_i(t))^*]^2 dt \right], \\
\text{s.t.} \quad & \boldsymbol{\zeta} \in \{\tilde{\boldsymbol{\rho}}, \boldsymbol{\mathcal{O}}, \boldsymbol{\gamma}\}; \\
& s_I \in [0, 1], \mathcal{O}_\alpha \in [0, 1], \gamma_i \in [0, 1]; \\
& b^{(I)} \in [0, 1] \text{ over } \partial B^{(I)}; \\
& \det \mathbf{A} = 1.
\end{aligned} \tag{4.8}$$

Here, the sensitivities of the objective with respect to the optimization variables are calculated by applying the adjoint method that is discussed in (3.46). Within the application of the adjoint method, one has to consider the derivative of the stiffness matrix with respect to the microscopic design variables. It should be emphasized that this computation immensely increases the computational cost, while noting that the discretization parameters for FE meshes and time escalates the wall time of the execution linearly. The discretization parameters are determined such that the wall time of both the microscopic and macroscopic optimization problems is similar up to a certain order. Therefore, $\bar{N}_e$, N_e and N_t are selected as $5 \times 3 \times 5$, 20^3 and 10 respectively. The update scheme of the threshold projection is preserved, whereas the filter-domain ratio is degraded to 10%. Both the cell geometry and material orientation parameters are kept constant. Even though no dimension is invoked for the unit cell taht is assumed to be *small*, the corresponding dimensions of the macroscopic solid are selected as 100.0 mm $\times$ 3.0 mm $\times$ 25.0 mm (Figure 4.14a). The period T is determined as 1.0 s, which results in approximately 0.11 s step size. In order to consistently correlate the results of the macroscopic problem with the microscopic one, B_{max} and B_{min} are selected as 1.0 kV and -1.0 kV respectively. For additional details, the depiction of the macroscopic problem is summarized in Figure 4.14a.

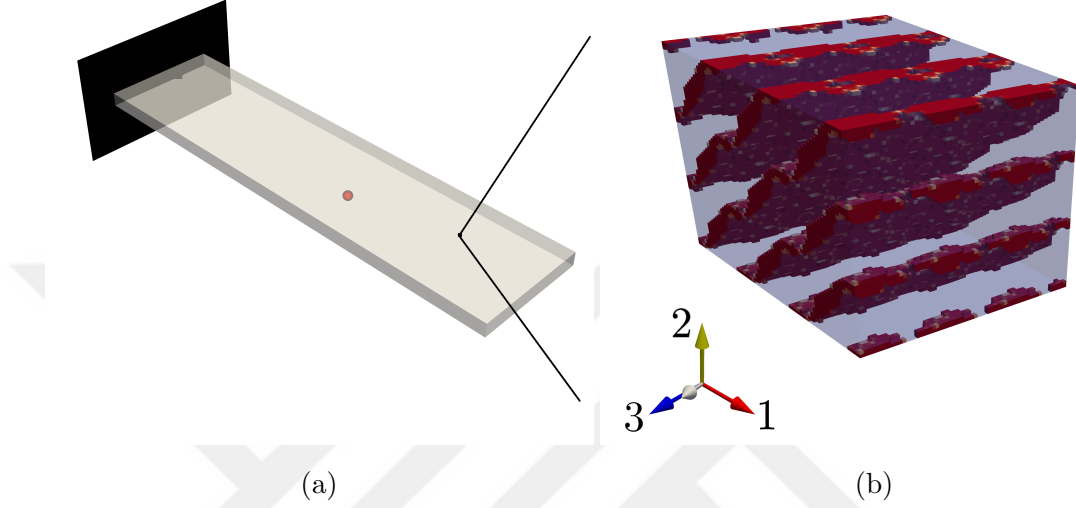


Figure 4.14: Depiction of the two-scale design problem (a) and the resultant microstructure design (b) with approximately 1.2% M_{nd} are illustrated. The top surface ($\partial B^{(2)}$) and the bottom surface ($\partial B^{(1)}$) are electroded and the rest represents the unelectroded surfaces. Mechanically, the left surface is enforced to be fixed and the remaining portions are traction-free. The red dot indicates the target node on the macroscopic mesh.

The ultimate purpose of this example is to present the significance of the multiphase nature of the composites. To this end, the example is built to identify the multi-directional behavior of the macroscopic solid under a single excitation (Figure 4.14a). Since the relevant quantities of the microstructure is kept time-independent, the behavior of time-varying target is only controlled with the macroscopic boundary-value variable. However, the need of the piezocomposite is manifested through the multi-directional behavior in Figure 4.15, which may not be realized with a homogeneous material with the predetermined topology, cell geometry and material orientation.

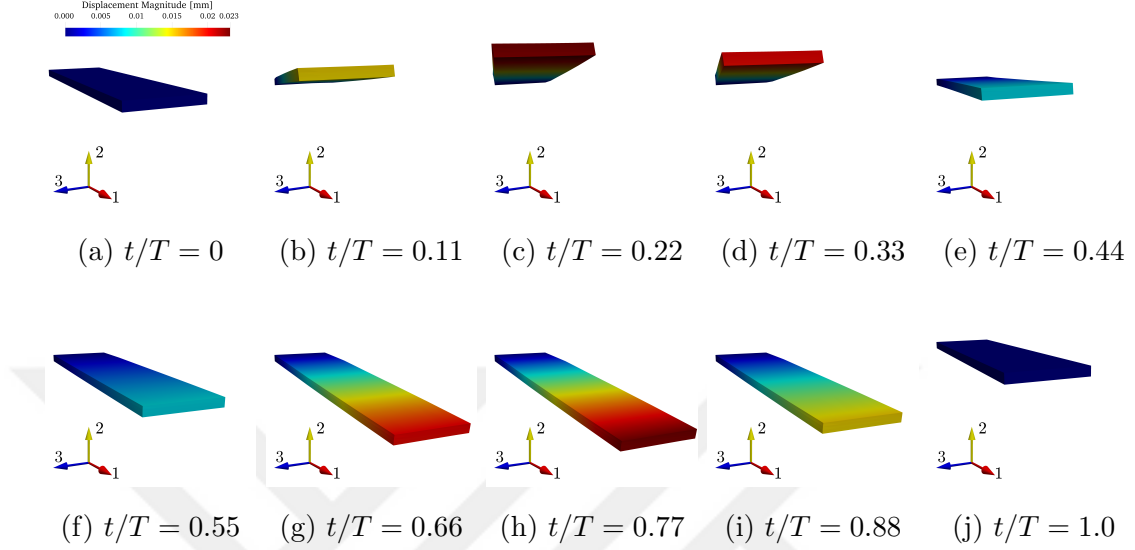


Figure 4.15: The resultant displacement magnitude variation is presented based on non-dimensionalized time scale. The corresponding behavior of the macroscopic structure is magnified with a scale factor of 1000.

In view of the target displacement components in Figure 4.16c and 4.16d and the time variation of the boundary-value variables in Figure 4.16a and 4.16b, it should be highlighted that since the components of the target displacement are harmonically synchronized without any phase or period shift, the resultant macroscopic boundary-value variables must share the same signal properties. Due to time-independent design variables, they cannot affect the time variation of the macroscopic fields. Therefore, one has to be careful about the time distribution of the components of the target displacement. If one introduces any phase or period shift within the components of the displacement, the target may become inadmissible under a single excitation. Consequently, MMA successfully minimizes the objective with approximately 10^{-13} accuracy and generates an acceptably discrete design (see Figure 4.16 and 4.14b).

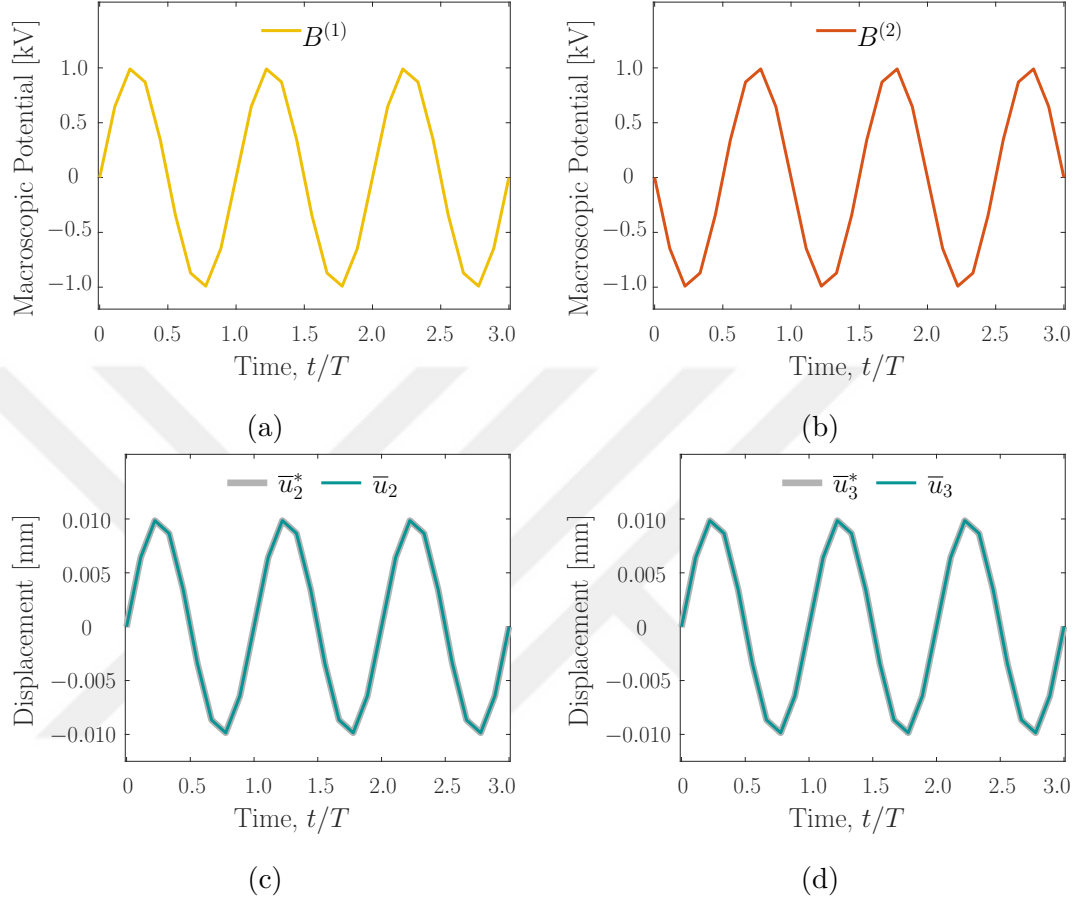


Figure 4.16: The resultant macroscopic optimization variables (a), (b) and displacement paths (c), (d) are demonstrated based on a non-dimensional time scale. The targeted variables are indicated with a superscript.

Chapter 5

Conclusion

Piezocomposites in the context of smart materials have truly showed their promising capabilities to enhance the overall behavior of the macroscopic solid. Many studies have reported different optimization schemes and design frameworks to improve the characteristics of piezoelectric materials. In this study, the classical topology optimization framework is extended to anisotropic material orientation and the unit cell geometry optimization. The significance of this development is realized by conducting comparative numerical studies in which the cyclic macroscopic stress response and structural behavior are targeted. Initially, an additional optimization variable is invoked to control the time-varying macroscopic electric field to characterize intriguing stress-strain paths. In order to test the framework and present its applicability, multi-directional behavior of a macroscopic solid under single excitation is captured by invoking a distinct performance variable that controls the time-varying macroscopic voltage imposed on the boundary. As a future work in the short term, PDE-based filters may be developed to obtain non-deformed inclusions when the unit cell geometry optimization is invoked. Even though this approach may not enrich the design space, it may enable the framework to deliver more symmetrical inclusions. In the long term, instead of optimizing spatially fixed boundary-values, the design of the distribution of boundary conditions may be attempted which may enrich the design space of the macroscopic behavior of the solid by allowing multiple excitation simultaneously.

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