

To the Graduate Council:

I am submitting herewith a thesis written by Ryan Connor entitled "Image-Based Statistical Volume Element Homogenization of Select Heterogeneous Materials." I have examined the final paper copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Mechanical Engineering.

Reza Abedi, Major Professor

We have read this thesis
and recommend its acceptance:

Reza Abedi

Stephanie TerMaath

Brett Compton

Accepted for the Council:

Dixie L. Thompson

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(Original signatures are on file with official student records.)

Image-Based Statistical Volume Element Homogenization of Select Heterogeneous Materials

A Thesis Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Ryan Connor

August 2025

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To the memory of my grandfathers, John Connor and Dr. James Johnston.

Both were remarkable men whose integrity, discipline, and curiosity continue to guide me. John's determination and deep passion for engineering set an enduring example of focus and perseverance. James's devotion to science, teaching, and his community reflected a rare combination of intellect and kindness.

Their influence has shaped how I approach work and life, and this work is dedicated to their memory with love and gratitude.

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To all of you—thank you.

“All models are wrong, but some are useful.”

—George E. P. Box

Abstract

Microstructural heterogeneity governs the strength, stiffness, and fracture behavior of materials. Predicting its influence requires linking local variability to macroscopic behavior while retaining the governing mechanisms that link behavior across scales.

A statistical volume element (SVE) framework is developed to connect microstructural variability and residual stresses to apparent material behavior. The approach is first established using a metallic microstructure from selective laser melting to quantify scale effects in elasticity and fracture, then extended to a multiphase ceramic composite where thermal mismatch generates internal residual fields. Building on prior experimental characterization of these stresses, the analysis incorporates them into a phase-field formulation that couples elasticity and fracture to compare thermally influenced and mechanical-only responses.

Residual stresses reduce peak strength but promote post-peak stability, reflecting how stored energy is redistributed between tensile inclusions and a compressive matrix. Anisotropy and variability diminish with increasing SVE size, revealing a common mechanism through which apparent homogeneity emerges from microstructural disorder. Variability follows a consistent scaling trend, with residual fields extending the length required for convergence in strength-related metrics. These findings demonstrate that effective properties are not fixed material constants but scale-dependent outcomes shaped by geometry, boundary conditions, and microstructural history.

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Chapter 1

Introduction

Recent advancements in manufacturing have redefined how structural materials are designed and modeled. This evolution reflects a shift from traditional process control to deliberate microstructural design. In both metals and ceramics, the ability to engineer features at the mesoscale opens new possibilities for tailoring properties but makes their mechanical response more difficult to predict [DebRoy et al. \(2018\)](#); [King et al. \(2017\)](#); [Carter et al. \(2014\)](#); [Pelz et al. \(2021a\)](#). For instance, what works for cast alloys may not work for advanced materials.

The key distinction lies in how thermal and mechanical fields develop during processing, giving rise to heterogeneous microstructures. Trying to capture these complexities often increases modeling cost and effort, creating a practical trade-off between fidelity and computational expense.

Capturing these effects within a unified modeling framework that remains tractable across scales is a central objective of modern computational mechanics. Numerical homogenization provides one such compromise, balancing the trade-offs between accuracy and efficiency.

1.0.1 Background and Motivation

Classical homogenization theories provide rigorous bounds and average property estimates for materials with heterogeneous microstructures Hashin and Shtrikman (1962); Eshelby (1957); Mori and Tanaka (1973). Modern computational methods, such as numerical homogenization and multiscale schemes, extend these ideas by directly linking local microstructural behavior to the macroscopic response under complex loading conditions Geers et al. (2010).

Despite these advances, challenges remain when applying these approaches to advanced materials. In these materials, microstructural features vary significantly across different regions and length scales, which causes the apparent elastic and fracture properties to depend on the size of the analyzed domain. This scale dependence has led to the development of Statistical Volume Element (SVE) approaches that quantify variability across different sampling windows rather than assuming the existence of a single Representative Volume Element (RVE) Kanit et al. (2003); Ostoja-Starzewski et al. (2007). Another major challenge involves the presence of internal stresses created during processing. In additively manufactured metals, these stresses arise from steep thermal gradients used during printing DebRoy et al. (2018); King et al. (2017). In multiphase ceramics, differences in thermal expansion between constituent phases lead to tensile and compressive zones that affect the effective mechanical response Pelz et al. (2021b). In particular, Shoulders et al. (2024) measured the microstructure and residual stress distributions in B_4C/SiC composites using X-ray diffraction (XRD) and Raman spectroscopy. Their work showed how thermal expansion mismatch creates tensile stresses in the inclusions and compressive stresses in the matrix, consistent with classical inclusion theory. These results also provided the microstructural data used to set up the present modeling framework. Building on that foundation, this study extends the residual-stress model to include fracture effects. The same residual stresses are built into the model and influence when and how cracks form and grow.

Representing such fracture behavior, however, introduces additional complexity. While phase-field and related fracture models robustly simulate crack initiation and growth [Miehe et al. \(2010a\)](#); [Borden et al. \(2012\)](#), their outcomes remain highly local and sensitive to the specific microstructure, residual stress field, and boundary conditions. As a result, connecting these local fracture simulations to effective, statistically representative material behavior remains an open challenge.

1.0.2 Objectives and Methodology

This work aims to develop and apply a Statistical Volume Element (SVE) framework that connects microstructural variability, residual stress, and fracture behavior. Building on experimental measurements of residual stress in B_4C/SiC composites [Shoulders et al. \(2024\)](#), the framework first establishes a mechanical SVE methodology using a selective laser melting (SLM) microstructure, then extends it to a thermomechanically informed ceramic system that includes eigenstrain-induced residual stresses. The work provides a basis for evaluating how microstructure heterogeneity influences effective stiffness, anisotropy, and fracture response.

1.0.3 Scope and Limitations

The remainder of this document is organized as follows. The first study (Chapter 2) focuses on the statistical homogenization of a selective laser melting (SLM) metallic microstructure, employing a cohesive-zone approach across melt pool boundaries to examine length scale effects in elasticity and fracture. Several limitations of this framework should be noted. The model was strictly mechanical and did not include thermal effects or residual stress evolution during processing. It used a simplified two-dimensional model based on experimental images, ignoring the grains' detailed crystal structure and three-dimensional shape. Fracture was represented using simplified cohesive interfaces and empirically calibrated properties, without direct linkage to process parameters.

The second study (Chapter 3) extends these concepts to a multiphase ceramic composite and partially includes thermomechanical coupling through eigenstrain-induced residual stresses. It begins with linear thermoelastic analyses across boundary conditions and SVE sizes to establish boundary treatments and quantify anisotropy. These results inform the cooling-stage simulations, where residual stresses drive nonlinear fracture captured through a diffusive phase-field formulation. A direct comparison of mechanical and thermomechanical responses is then performed to assess the influence of these residual fields. The concluding chapter connects these findings and discusses their broader implications for modeling and interpreting the behavior of complex manufactured materials.

Chapter 2

Statistical Homogenization of Elastic and Fracture Properties of a Sample Selective Laser Melting Material

2.1 Introduction

Selective Laser Melting (SLM) is an additive manufacturing method where components are formed directly from metal powder [Carter et al. \(2014\)](#). Components formed using SLM are built layer-by-layer by a high-powered laser, localized to a select area, fusing metallic powder together. This methodology is of particular interest to industries that require complex geometry or intricate hollow designs [Qiu et al. \(2013\)](#). Such complex geometries find value in applications such as aerospace, biomedical, and other industries [Carter et al. \(2014\)](#). Considering the diverse applications of components manufactured through SLM, a notable focus has been on the modeling and simulation aspects.

The area affected by the radiation of the laser can be sectioned into three regions: the fusion zone (FZ), heat-affected zone (HAZ), and substrate [Zou et al. \(2022\)](#). In the fusion zone, metallic powder is briefly liquidized to form pools of melted powder known as melt pools [Zou et al. \(2022\)](#). The melt pools, once resolidified, form the layer-by-layer construction of the SLM component. A 3D conceptual drawing of a melt pool is shown in Figure 2.1 from [Zou et al. \(2022\)](#).

Melt pool boundaries change size and shape depending on the parameters used in the SLM process, such as laser power and laser scanning speed. These parameters greatly influence induced residual stresses, hierarchical layout, and severity of defects such as voids and cracks [Choo et al. \(2019\)](#). The inclusion of melt pools, however, dramatically increases the complexities of the microstructure of SLM materials, making it difficult to establish a correlation between microstructures and mechanical response [Andani et al. \(2018, 2019\)](#); [Wang et al. \(2014\)](#); [Riedlbauer et al. \(2017\)](#).

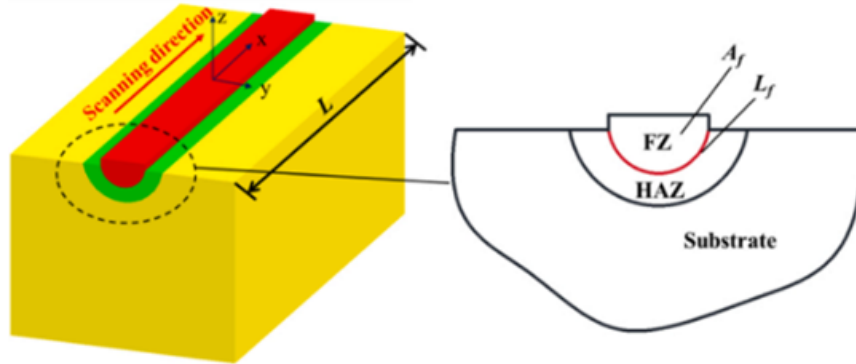


Figure 2.1: 3D conceptual drawing of a melt pool [Zou et al. \(2022\)](#).

Current works have simulated this microstructure using Voronoi tessellation approximating the polycrystalline geometry of the printed microstructure [Andani et al. \(2018\)](#); [Belotti et al. \(2022\)](#); [Pilgar et al. \(2022\)](#). Notably, these studies focus on accurately representing the complex microstructural features inherent to AM processes. From [Belotti et al. \(2022\)](#), a modular methodology is used to obtain representative microstructural cells, encompassing feature-based representations and

morphological shape analyses for different AM processes and materials. Analogously, additional works introduce a novel technique that models columnar and equiaxial grains, alongside melt pools, using crystal plasticity and finite element (FE) modeling for SLM components [Andani et al. \(2018\)](#). Additionally, a crystal plasticity-based Fast Fourier Transform (CP-FFT) framework captures microstructural influences on mechanical responses in SLM-fabricated materials, highlighting the role of grain features [Pilgar et al. \(2022\)](#). From this perspective, crystal plasticity furnishes the essential microstructural insight required for mechanical analysis, while FFT augments the ability to scrutinize and visualize the spatial distribution of microstructural features.

Other crystal plasticity models are presented in [Cao et al. \(2022\)](#) extending the focus to comprehend the impact of crack nucleation behavior on mechanical attributes, specifically, the assessment of fatigue life in materials produced through SLM printing. This would suggest that process parameters leading to the formation of different pore types can significantly influence the initiation of fatigue cracks, which directly impacts the mechanical behavior of the material. Moreover, researchers in [Ji et al. \(2022\)](#); [Hao et al. \(2023\)](#) conduct a morphological analysis that directly assesses inherent physical traits, thereby reinforcing the substantial connection between processing parameters and the resulting material behavior.

Even with the extensive literature outlining the effect of various process parameters and demonstrating the impacts within approximated domains, there exists a gap in our understanding of the mechanical behavior at different length scales for metal SLM material. This work introduces a framework to employ a high-fidelity meshing approach to comprehensively represent the intricate complexities of SLM microstructures. Additionally, the variation of mechanical properties is examined across various length scales, elucidating the intricate connection between these fluctuations and specific regions within the melt pool.

Numerical homogenization has proven to be an effective means to quantify material properties, given a microstructure with such complexities [Li et al. \(2015\)](#).

Numerical homogenization aims to upscale the effect of all microstructural details into the effective or apparent material properties that can be used in continuum-level models [Zou et al. \(2020\)](#). In homogenization theory, representative volume element (RVE) refers to a large enough domain for which a target material property can be considered converged versus the volume element size [Hill \(1963, 1972\)](#); [Mandel \(1966\)](#); [Ogden \(1974\)](#). There are various perspectives in defining convergence [Sab \(1992\)](#); [Gitman et al. \(2007\)](#); [Pelissou et al. \(2009\)](#). For example, one can examine if the given property is almost independent of the choice of boundary conditions used [Ostoja-Starzewski \(1998\)](#); [Ostoja-Starzewski et al. \(2007\)](#), whether the mean value has stabilized versus the volume size, or whether the variation of the homogenized properties over a population of volume elements (VEs) of the same size is small enough [Kanit et al. \(2003\)](#). Depending on the mechanical properties in question, however, constructing an appropriately sized RVE can prove sufficiently challenging, if not impractical [Abedi et al. \(2022a\)](#). For example, fracture-related properties have very large RVE sizes.

An alternative approach, one that attempts to consider the variability of the microstructure, is the concept of a statistical volume element (SVE), first introduced in [Huyse and Maes \(2001\)](#); [Segurado and Llorca \(2006\)](#); [Tregger et al. \(2006\)](#) for homogenizing elastic properties. SVE-homogenization partitions a large domain into VEs much smaller than the RVE size limit for a given property. Understanding the variation of mechanical properties versus VE (SVE) size and homogenizing properties by SVEs, as opposed to RVEs, have multiple benefits. First, many mechanical properties have a specific form of size effect, that is the trends at which the mean and variation of the given property change versus the observation (SVE) size [Bažant and Planas \(1998\)](#); [Genet et al. \(2014\)](#). Second, RVE-based homogenization has rendered ineffective in many fracture analyses as all material heterogeneities that play a key role in crack nucleation, propagation, and coalescence are lost in the homogenization process. For example, lack of convergence or convergence to an incorrect value is reported for fracture pattern [Al-Ostaz and Jasiuk \(1997\)](#) and fracture energy [Kozicki](#)

and Tejchman (2007). In the method of moving window Baxter and Graham (2000); Graham and Baxter (2001), a window (SVE) traverses a macroscopic domain and each time at the centroid of the SVE assigns the homogenized properties. Unlike RVEs, the homogenized values at different locations are not uniform (or almost uniform), hence the corresponding mesoscopic property fields generated are inhomogeneous and address the aforementioned problem. Third, many interesting mechanical responses of a material are stochastic. For example, for the same sample geometry and loading, different fracture patterns and strain-stress curves are reported in Ming et al. (2021); Liu et al. (2009), respectively. The smaller size of SVEs (compared to RVEs) ensures that the homogenized properties are stochastic and maintain the mentioned sample-to-sample variation. In short, the SVE-based properties maintain a certain level of material heterogeneity and randomness and are a promising tool in multiscale material modeling. For this purpose, the size of SVE can be viewed as the resolution of the homogenization scheme and acts as a gauge between RVE-based homogenization and direct numerical simulation (DNS) in terms of accuracy and efficiency.

The intent of this work is to explore the effects of SVE size against published experimental results of elastic and fracture properties of SLM material and explore the size effect of these properties. The SVE-based homogenization will also examine the effect of the geometry of the melt pools and their intrinsic length scale on homogenized properties at different sizes. Investigating the correlation between microstructure and mechanical properties can prove instrumental in establishing fundamental relationships that govern a material’s behavior.

2.2 Materials and Methods

The layer-by-layer construction, shown in Figure 2.2, depicts rows of melt pools atop one another to form the microstructure typical of an SLM material. Consider the cross-section shown in Figure 2.2 from Hanzl et al. (2015) of an SLM material, referred to as the RVE from hereon.

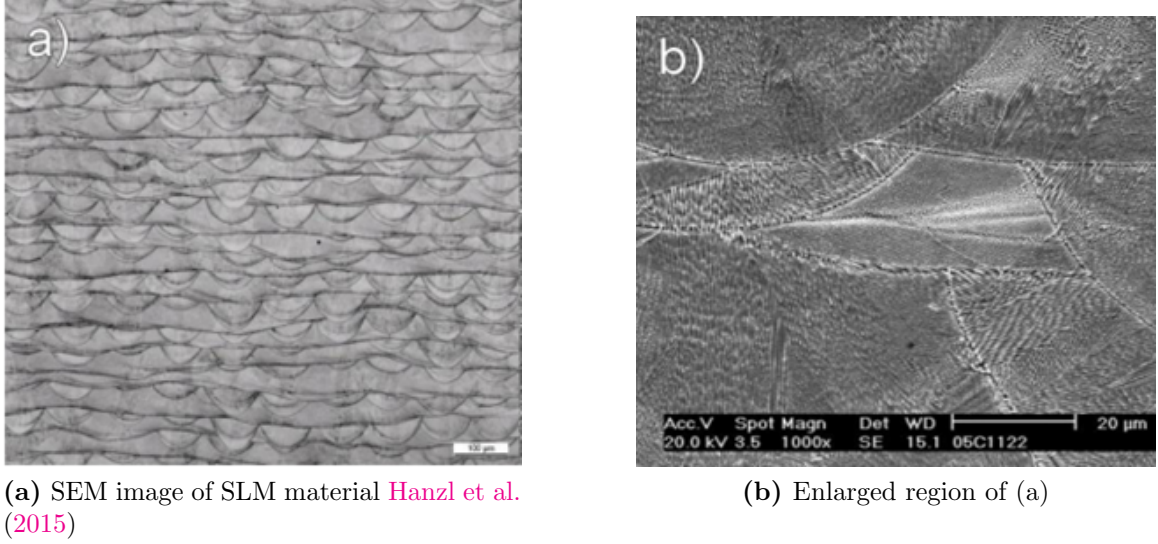


Figure 2.2: SLM microstructure: (a) SEM image; (b) Enlarged sub-region.

Figure 2.3b shows the FE mesh constructed by the Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) method [Soghrati et al. \(2017a,b\)](#). CISAMR is a non-iterative mesh generation algorithm that transforms an initial structured mesh of rectangular elements into a high-quality hybrid conforming mesh consisting of rectangular and triangular elements. The meshing process involves three phases: (1) h-adaptive refinement of background elements intersecting material interfaces to minimize geometric discretization error; (2) r-adaptivity of refined element nodes intersecting interfaces, which on average transforms 50% of these elements into conforming elements; and (3) sub-triangulation of the remaining non-conforming elements with hanging nodes. The effect of each phase is illustrated in Figure 2.3.

A unique feature of CISAMR is the ability to generate high-quality meshes for problems with complex morphologies [Bahmani et al. \(2019\)](#). However, sharp geometrical features in the microstructure required algorithmic modifications. As shown in Figure 2.4, after the h-adaptivity phase, background elements containing sharp corners of melt pools were identified and the closest mesh node snapped to the

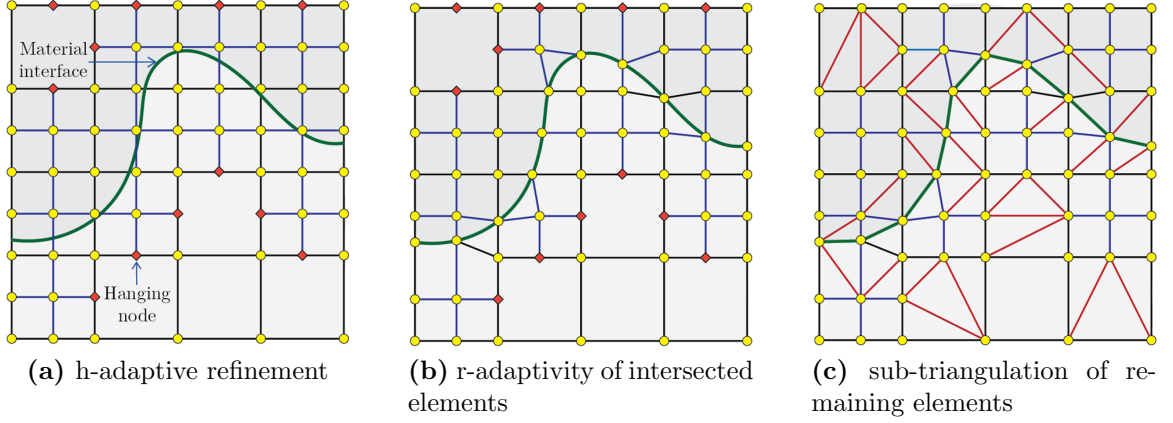


Figure 2.3: Transformation of a structured quadrilateral mesh into a conforming mesh using CISAMR. Adapted from [Soghrati et al. \(2017a\)](#).

sharp corner. Subsequent r-adaptivity and sub-triangulation were then carried out normally. This modification preserves sharp features of melt pools.

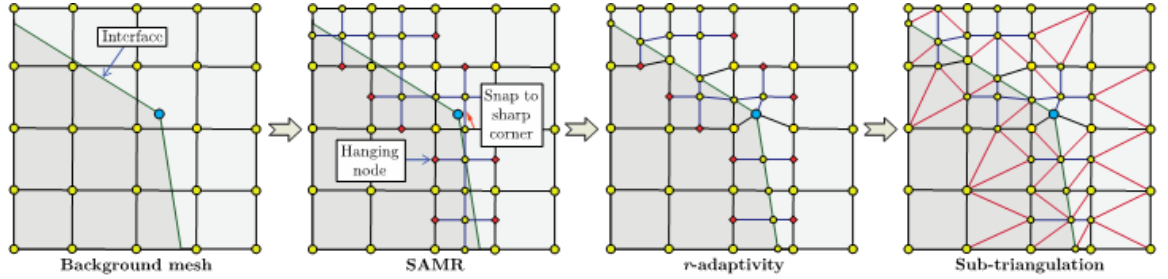


Figure 2.4: Modification of the CISAMR algorithm to preserve sharp corners along melt pool interfaces. Adapted from [Soghrati et al. \(2017b\)](#).

Figure 2.5a shows the geometrical model constructed for the $924 \mu\text{m} \times 840 \mu\text{m}$ RVE image shown in Figure 2.2a, in which melt pool boundaries are characterized using non-uniform rational B-splines (NURBS) curves. This domain comprises 239 melt pools and is discretized using the CISAMR algorithms, resulting in a conforming mesh consisting of 1.31 million elements and a maximum aspect ratio of 4.4. The RVE mesh is then partitioned into several smaller SVEs. Four different SVE sizes are analyzed in this work, i.e., $L_{\text{SVE}} = 56, 84, 112$, and $140 \mu\text{m}$. These sizes correspond to 240, 110, 56, and 36 SVE counts, respectively.

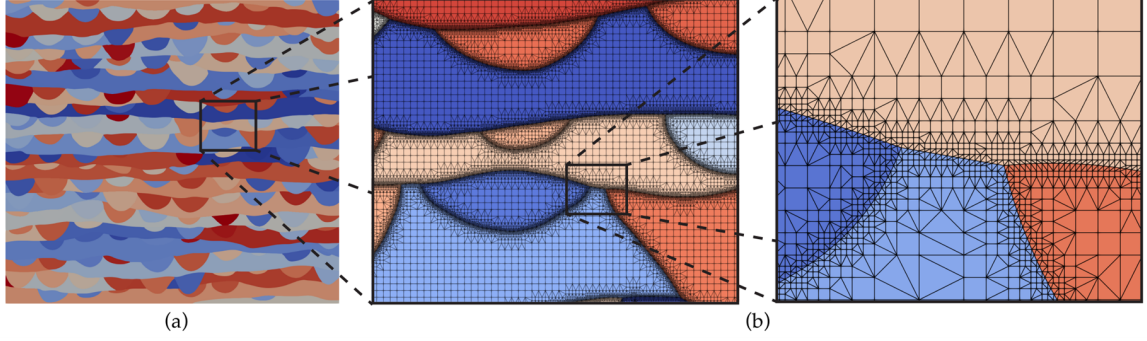


Figure 2.5: (a) Geometrical model of SLM microstructure (239 melt pools). (b) Sample SVE extracted from CISAMR mesh with inset showing mesh refinement.

Since the RVE mesh contains 239 melt pools, the smallest to largest SVEs contain an average of about 1, 2.2, 4.2, and 6.6 melt pools in each SVE. Accordingly, $L_{SVE} = 56$ is the minimum size below which there will be less than one melt pool in average within an SVE. As sub-melt pool length scale, the model ideally should incorporate grain level mechanisms and crystal plasticity or other more accurate physics-based model are more appropriate to investigate the failure response of the SVE. In the following, we use a cohesive model to model failure between the melt pools. Accordingly, due to the lack of more accurate grain-scale models in this work, we limited the smallest SVE size to $L_{SVE} = 56$. As for the largest size, SVEs larger than $L_{SVE} = 140 \mu\text{m}$ would result even in fewer than 36 SVEs which may be a too small number to accurately calculate the mean and standard deviation of homogenized properties. We refer the reader to (Abedi et al., 2022a) on why this is especially a concern for fracture properties due to their slower convergence relative to L_{SVE} compared with elastic properties. In short, while ideally we could model larger SVEs (if starting with a larger experimental image shown in Figure 2a, the chosen sizes still manifest distinct mechanical behaviors. Larger sizes are valuable for revealing interactions between multiple melt pools, while mid-range sizes shed light on interactions between select boundaries.

The microstructure and the corresponding conforming mesh for one of the SVEs with $L_{SVE} = 140 \mu\text{m}$ are illustrated in Figure 5b. For reference, the CISAMR mesh

is generated on a background structured mesh with an element size of $2.8 \mu\text{m}$, with two levels of h-adaptive refinement along melt pool boundaries. Accordingly, the SVEs of sizes $L_{\text{SVE}} = 56, 84, 112, \text{ and } 140 \mu\text{m}$ correspond to 20, 30, 40, and 50 background elements along the edge, respectively. The calibration of material and interface properties and finite element analysis of the SVEs are discussed next.

Finite element analysis by Abaqus (Abaqus, 2006) was used to analyze the derived SVEs under three different load cases to characterize the response for tensile loading in vertical and horizontal directions (denoted by v and h subscripts), and the shear loading. The most common boundary conditions (BCs) for the homogenization of elastic properties are Kinematic Uniform Boundary Condition (KUBC) and Stress Uniform Boundary Condition (SUBC). In KUBC, two displacements of the boundary nodes are specified consistent with a macroscopic strain tensor. In SUBC, traction values corresponding to a constant macroscopic stress tensor are applied on the boundary of VE. KUBC and SUBC provide the upper and lower limits for the homogenized elastic properties, with the properties converging to unique values as the SVE size increases (Huet, 1990; Hazanov and Huet, 1994; Hazanov and Amieur, 1995)). KUBC is not appropriate for the nonlinear failure problem as it does not permit a crack to completely tear vertically or horizontally through the domain. SUBC is also not appropriate for failure simulations as it cannot model the unloading portion of the homogenized strain-stress response. We have used a Mixed Boundary Condition (MBC) (Abedi et al., 2022a) for homogenization. The MBC condition is preferred over KUBC and SUBC for multiple reasons. First, the homogenized elastic properties are in between KUBC and SUBC values and thus are not overly over- or under-estimated for small SVE sizes. Second, it allows cracks to completely go through the VE and can model the unloading portion of strain-stress response, and the problems of KUBC and SUBC, respectively.

To apply the MBC for the tensile loading in the horizontal direction, the top and bottom sides of the SVE are modeled as rollers (zero tangential traction and normal direction), whereas the left and right sides are gradually taken apart by applying

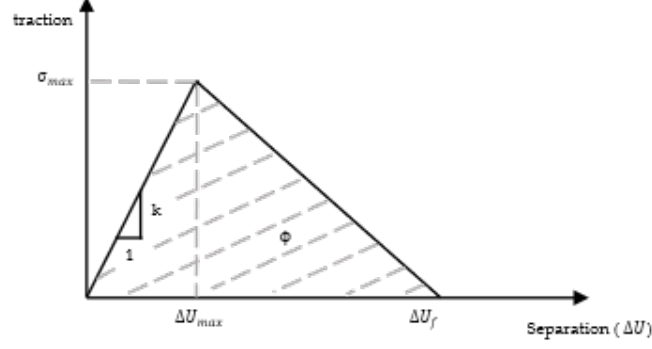


Figure 2.6: Bilinear traction–separation relation (TSR) used to model cohesive failure along melt pool boundaries [Abaqus \(2006\)](#).

opposing spatially uniform and temporally increasing displacement values across all nodes. The terminal value of the applied displacement of SVEs in the horizontal direction is chosen large enough so that most SVEs undergo failure through the loading process. For the tangential direction, zero traction is specified for these sides too. We refer the reviewer to ([Abedi et al., 2022a](#)) for a more thorough description of MBC and its comparison with KUBC and SUBC.

The average strains and stresses of the SVEs were computed using a Python script. By having the average stresses and strains of the three load cases, the elasticity stiffness is computed using the process described in ([Abedi et al., 2022a](#)). The compliance matrix is computed as the inverse of the stiffness matrix. Finally, the vertical and horizontal elastic moduli, denoted by E_v and E_h , are computed from the compliance matrix.

To establish an effective failure model for each SVE, one must consider the interaction between each melt pool, i.e., the boundary between melt pools in Figure 5a (corresponding to melt pools in Figure 2a). Since the fusion zone is melted and deposited on top of the heat-affected zone, there must exist an interface between the two ([Zou et al., 2022](#)). Several works including ([Andani et al., 2018](#); [Belotti et al., 2022](#); [Pilgar et al., 2022](#)) treat such melt pool boundaries as weak interfaces, whose failure response is represented by a cohesive Traction-Separation Relation (TSR).

Figure 2.6 shows the bilinear TSR used for this study. This TSR is characterized by the initial tangent modulus k , strength value $\sigma_{\max}$, and the work of separation (fracture energy) ϕ , which is the area under the traction–separation relation.

Table 2.1 shows experimentally measured vertical and horizontal elastic moduli and strengths for the sample shown in Figure 2.2a from Hanzl et al. (2015). Our objective is to calibrate the elastic and fracture properties of SLM at the melt pool scale, e.g., bulk properties and melt pool boundary TSR parameters, so that the computationally homogenized elastic and fracture properties for the RVE match the results shown in this table. The last two columns of the table show our computational results for a domain that is half the size of the domain shown in Figure 2.5a in each direction. As evident, there is a good match between experimental and computational elastic and fracture properties. The details of the calibration process are provided below. Since the experimentally reported stiffnesses and strengths are in GPa and the RVE size in Figure 2.2a is expressed in μm , we use GPa and μm as units of stiffness/strength and length for the remainder of the paper.

Table 2.1: Experimental vs. computational elastic moduli and strengths for the SLM RVE Hanzl et al. (2015).

	Experimental		Calibrated	
	Horizontal	Vertical	Horizontal	Vertical
Young’s Modulus (GPa)	172	160	171.75	160.80
Yield Strength (GPa)	1.09	1.08	1.27	1.07

For multiphase composites, the volume fractions and topologies of individual phases contribute to the overall elastic and fracture properties of the material at a given SVE (observation) size. Herein, similar to (Andani et al., 2018; Belotti et al., 2022; Pilgar et al., 2022) the additively manufactured material is treated as single-phase with the melt pool boundaries being the dominant feature responsible for material nonlinear response. From this perspective, there are two aspects that contribute to the compliance of SLM material: bulk compliance and

traction–separation model compliance. This is due to the fact that the cohesive model is intrinsic, that is it has the initial slope of k in Figure 2.6. To make explicit how the cohesive interface contributes to the effective stiffness, consider the one-dimensional schematic shown in Figure 2.7, where equal-length elastic regions of thickness ℓ and modulus E_m are separated by cohesive models with stiffness k . Under a uniform stress σ , the total elongation of a representative period of thickness ℓ can be written as the sum of the elastic and cohesive contributions:

$$\frac{\sigma}{E_{\text{eff}}} \ell = \frac{\sigma}{E_m} \ell + \frac{\sigma}{k}, \quad (2.1)$$

which directly leads to the series-compliance relation

$$\frac{1}{E_{\text{eff}}} = \frac{1}{E_m} + \frac{1}{k \ell}. \quad (2.2)$$

This expression is exact for an ideal laminate with horizontal melt-pool boundaries separated by ℓ ; for the measured SLM topology with curved or oblique pools, it serves as a first-order proxy that guides the selection of (E_m, k) pairs used in the calibration below.

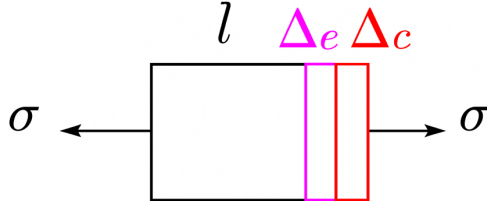


Figure 2.7: Schematic illustrating elastic (Δ_e) and cohesive (Δ_c) contributions over a period ℓ under stress σ .

Equation (2.2) provides the relationship between the bulk modulus E_m , cohesive stiffness k , and the effective modulus E_{eff} . To relate this 1D model to the SLM microstructure in Figure 2.2a, ℓ is set to the average vertical spacing between melt pools, E_m represents the bulk modulus within the pools, and E_{eff} corresponds to the measured vertical stiffness of 160.8 GPa from Table 2.1. This relation was used in

the calibration process to estimate suitable (E_m, k) pairs capable of reproducing the experimental response. Specifically, $\hat{\sigma}_{\max}$ was fixed to the vertical strength of 1.08 GPa and $\beta = 2$ to ensure numerical stability, while k was varied and the corresponding E_m was obtained from Equation (2.2). Each (E_m, k) pair was then tested in VE simulations to evaluate the resulting vertical modulus $E_v(k)$ and strength $\sigma_{v,\max}(k)$, and the optimal value of k was identified where both matched the experimental targets, as summarized in Table 2.2.

Interestingly, the 1D equation relating k, E_m has worked well in the calibration process by varying k , calculating E_m from (1), and assigning reasonable values for $\hat{\sigma}_{\max}$ and ϕ , the other two parameters of the TSR in Figure 2.6. Specifically, we choose $\hat{\sigma}_{\max}$ equal to the macroscopic vertical strength of the bulk material equal to 1.08 GPa in Table 2.1. Unfortunately, no energy measure was provided in the experimental results of (Hanzl et al., 2015), thus there is direct means to assign the value of ϕ . However, computational results provided some guidance on choosing a reasonable value for ϕ ; in Figure 2.6, the area under the unloading line represents the energy reserve past the maximum strength of the interface; the smaller β defined as the ratios of the unloading to loading energies, the more brittle the behavior of the TSR. From the simulation of SVEs of different sizes, we encountered nonconvergence problems when $\beta \lesssim 2$.

In short, in the calibration process we only varied the value of k , with the corresponding value of E_m obtained from equation (2.2), $\hat{\sigma}_{\max} = 1.08$ GPa and ϕ obtained from $\beta = 2$. Figure 2.8a and Figure 2.8b show how the computed vertical stiffness E_v and strength $\sigma_{v,\max}$ as a function of k . Interestingly, for the same value of $k \approx 72$ GPa/ μm , vertical E_v and $\sigma_{v,\max}$ from Table 2.1 are matched simultaneously. Having chosen $k = 72$ GPa/ μm , other parameters are obtained from the process explained earlier and are reported in Table 2.2, noting that $\phi = 0.025$ GPa $\cdot\mu\text{m}$ is the rounded-up fracture energy corresponding to $\beta = 2$ and the Poisson ratio of $\nu = 0.3$ is a typical value chosen for steel.

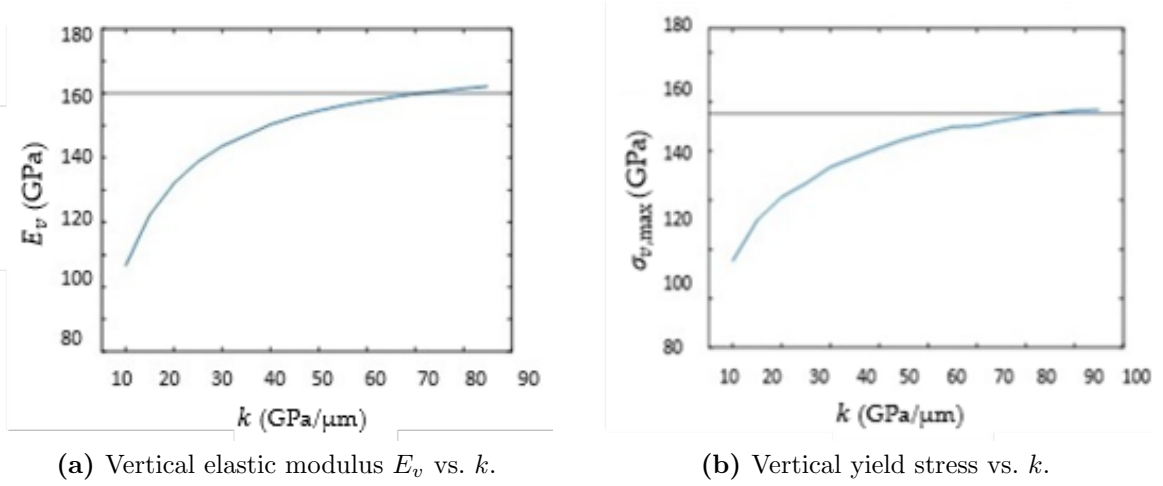
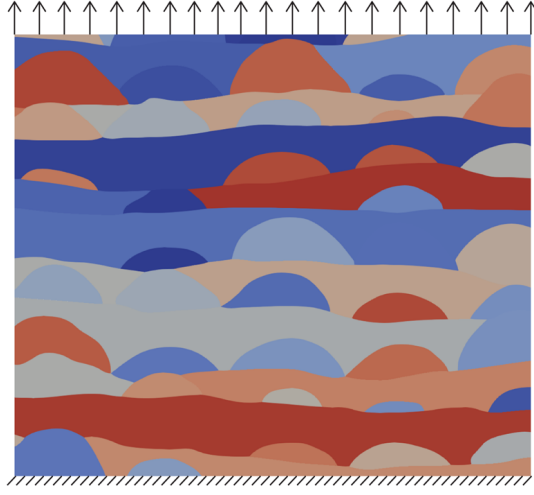


Figure 2.8: Calibration of cohesive model stiffness: (a) Vertical elastic modulus E_v vs. k ; (b) Vertical yield stress vs. k .

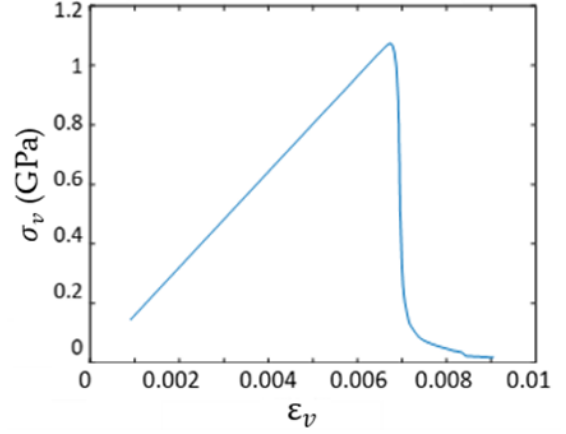
Table 2.2: Material properties set from the calibration process.

Property	Value
Bulk modulus E_m (GPa)	175
Poisson's ratio ν	0.3
Cohesive stiffness k (GPa/ μm)	72
Cohesive strength $\hat{\sigma}_{\max}$ (GPa)	1.08
Fracture energy ϕ (GPa- μm)	0.025

Figure 2.9a shows the VE geometry and boundary conditions used to calibrate the material properties discussed above. Displacement boundary conditions were applied to the top of the domain with a fixed BC at the bottom. Traction-free BCs are used on the left and right sides to match the experimental setup. The corresponding vertical stress-strain response is depicted in Figure 2.9b for the final calibrated parameters. The slope of the linear part matches $E_v = 160.80$ GPa and the maximum strength matches $\sigma_{v,\max} = 1.08$ GPa in Table 2.1 from Hanzl et al. (2015) (see the last two columns).



(a) Domain and BCs for vertical calibration.



(b) Stress-strain curve with calibrated parameters.

Figure 2.9: (a) Domain and boundary condition for vertical loading for parameter calibration; (b) Vertical stress versus strain for the domain in (a) with calibrated parameters.

For large enough domains such as the one shown in Figure 2.9a, the material fails across the boundaries between the melt pools. However, for smaller domains, like the partitioned SVEs, the likelihood of a melt pool boundary permeating across the domain, thus resulting in cohesive fracture along the corresponding TSR interfaces, significantly reduces. As a result, realistically other modes of material degradation must be included to handle the failure of small SVEs. Accordingly, a bulk failure mechanism is needed to handle the failure of all SVE sizes, especially in the horizontal direction. For this reason, we have employed a bulk plasticity model in addition to TSR-based decohesion across melt pool boundaries. Due to the inherent microstructure of SLM materials, the effect of bulk degradation, i.e., plastic yielding, is more evident for the horizontal load case than the vertical load case.

2.3 Results

To interpret the effect of SVE size on mechanical properties, we first select a few mechanical quantities of interest (QoIs) and examine the results as SVE size increases. The variation of QoIs is discussed in the context of graphical overlays of stress versus strain, and the size effect of the homogenized QoI, that is the variation of its mean, minimum, and maximum versus the SVE size. The remainder of this section is divided into two sections. The first examines the vertical load case and the second handles the horizontal load case. We consider elastic and fracture QoIs.

2.3.1 Vertical Direction

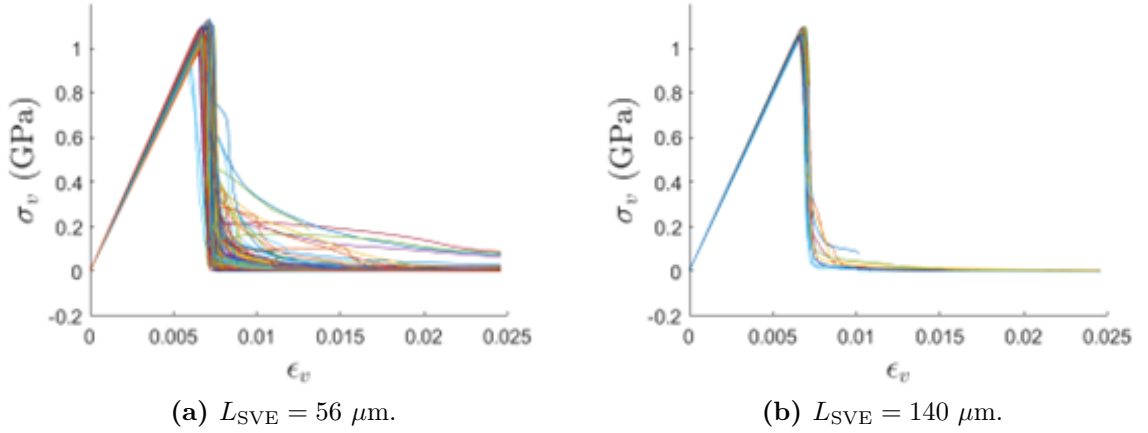


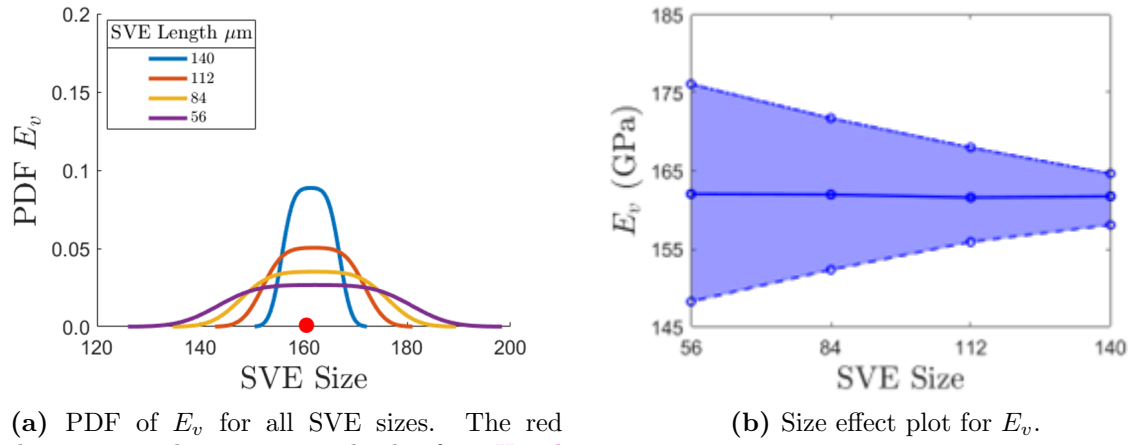
Figure 2.10: Vertical stress–strain overlays for (a) $L_{\text{SVE}} = 56 \mu\text{m}$; (b) $L_{\text{SVE}} = 140 \mu\text{m}$.

Figure 2.10 shows strain versus stress results in the vertical direction for all SVEs of sizes $L_{\text{SVE}} = 56 \mu\text{m}$ and $L_{\text{SVE}} = 140 \mu\text{m}$, respectively. The elastic property corresponds to the slope of the linear part of the response and is the elastic modulus of SLM material in the vertical direction (E_v). Two key fracture properties correspond to the maximum stress ($\sigma_{v,\text{max}}$) and fracture energy (the area under the strain–stress curve).

A few trends can be observed. First, for both sizes, there are more variations in fracture (maximum and post-maximum stress) than elastic response. Second, the variations of both elastic and fracture properties are more noticeable for the smaller SVEs in Figure 2.10a. Third, the captured response is relatively brittle pre-maximum stress level. In Ming et al. (2021) several brittleness indicators are defined based on the ratios of initiation (i.e., where stress-strain response before maximum stress significantly deviates from linear response), maximum (where stress is maximum), and final (the first instance when stress reaches zero) strains or energies. For example, in Figure 2.10, the ratio of strain at the initiation stage to the maximum stage is very close to one, reflecting the little softening response before the elastic branches reach the maximum stress level, and indicating a brittle failure response.

Figure 2.11a shows the Probability Distribution Function (PDF) plots of E_v for all relative SVE sizes. As can be seen, the variation of E_v decreases as the SVE size increases. This agrees with the second observation above for the two relative SVE sizes of $L_{\text{SVE}} = 56$ and $L_{\text{SVE}} = 140 \mu\text{m}$. Interestingly, the mean and mode of E_v are relatively unaffected as a function of SVE size. Another important vertical elastic material property is C_{22} , the vertical normal component of the elasticity stiffness matrix. Due to Poisson effects, C_{22} is not equal to E_v . For brevity, we do not present the results for C_{22} , but note that similar trends to E_v are observed for C_{22} . The red dot corresponds to the experimental value reported in Table 2.1 from Hanzl et al. (2015) and is provided as a reference point for other sample size results. The experimental sample, called RVE in this paper, is about 6 times larger than the largest SVE size of $140 \mu\text{m}$. Thus, if we had more experimental images for this material, we would have expected the PDF for this size to be a narrower bell-shape curve than that of $L_{\text{SVE}} = 140 \mu\text{m}$, around the red dot.

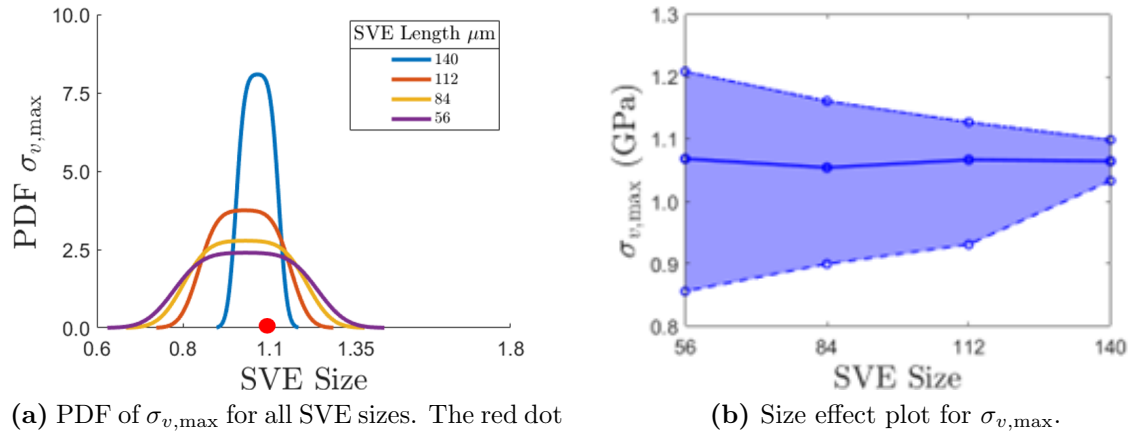
Size effect relation of vertical stiffness is shown in Figure 2.11b. The minimum and maximum values of homogenized stiffness for the population of SVEs at any given size are shown by the dashed and dot-dashed lines. The mean value of the homogenized property is shown by the solid line inside this region. As implied by the



(a) PDF of E_v for all SVE sizes. The red dot serves as the experimental value from Hanzl et al. (2015).

(b) Size effect plot for E_v .

Figure 2.11: Vertical results for E_v : (a) PDF of E_v for all SVE sizes; the red dot marks the experimental value from Hanzl et al. (2015); (b) size-effect plot for E_v .



(a) PDF of $\sigma_{v,\max}$ for all SVE sizes. The red dot serves the experimental value from Hanzl et al. (2015).

(b) Size effect plot for $\sigma_{v,\max}$.

Figure 2.12: Vertical results for $\sigma_{v,\max}$: (a) PDF of $\sigma_{v,\max}$ for all SVE sizes; the red dot marks the experimental value from Hanzl et al. (2015); (b) size-effect plot for $\sigma_{v,\max}$.

PDFs in Figure 2.11a, we observe that the mean value of E_v is quite stable among all SVE sizes. Moreover, there exists a relative difference of only .0027 across means values for each SVE size, highlighting that E_v is not size sensitive. In Abedi et al. (2022a), a mean-based RVE size limit criterion is proposed, wherein the RVE size for a property is defined as the size at which the mean value of the given property is close enough to its terminal value (in the limit of infinite VE size). We observe that from this perspective, even the smallest relative SBE, $L_{\text{SVE}} = 56 \mu\text{m}$, can be considered an RVE size for E_v whose mean value closely aligns with that of published value in Table 2.1. The variations of E_v gradually decrease from about 10% to 2.5% of the mean value as the SVE size increases. The decrease of the variations is expected as in the limit of SVE size equal to infinity all VEs have the same response and the variation tends to zero.

PDF and size effect plots of vertical strength $\sigma_{(v,\text{max})}$ are shown in Figure 2.12. The size effect plot in $\sigma_{(v,\text{max})}$ in Figure 2.12b shows a similar trend to vertical stiffness in Figure 2.11b, although the mean value is not as stable as E_v across all SVE sizes and the variations are higher for the smallest SVE sizes (15% for $\sigma_{(v,\text{max})}$ compared to 10% for E_v for the SVE size, $L_{\text{SVE}} = 56 \mu\text{m}$). This instability in the mean for $\sigma_{(v,\text{max})}$ is more evident in the PDFs of strengths (Figure 2.12a). This is expected as fracture properties are more sensitive to minute differences in the layout of material at the microscale and in general higher variations are experienced for fracture properties than elastic ones Abedi et al. (2022a). Like Figure 2.11a, the experimental value for the RVE (Figure 2.2a) is shown by the red dot in Figure 2.12a, for comparison with the PDFs of the results of different SVE sizes.

2.3.2 Horizontal Direction

Figure 2.13 shows strain versus stress results in the horizontal direction for SVEs of sizes $L_{\text{SVE}} = 56$ and $L_{\text{SVE}} = 140 \mu\text{m}$, respectively. Compared to the corresponding results for vertical loading in Figure 2.11, there is less variation in elastic modulus and

a delayed softening past the maximum stress for the horizontal loading results. We contribute these features to the topology of the melt pools in Figure 2.2a. The melt pool boundaries are more favorably opened when the loading is along the vertical direction compared to the horizontal direction. This is due to the fact that for horizontal loading there are long stretches of material from left to right that carry the load and contain no melt pool lines. Accordingly, separation along the cohesive surfaces is not activated as much. The results show less variation and unloading past maximum stress given that the response is mostly driven by elastoplasticity of the bulk material.

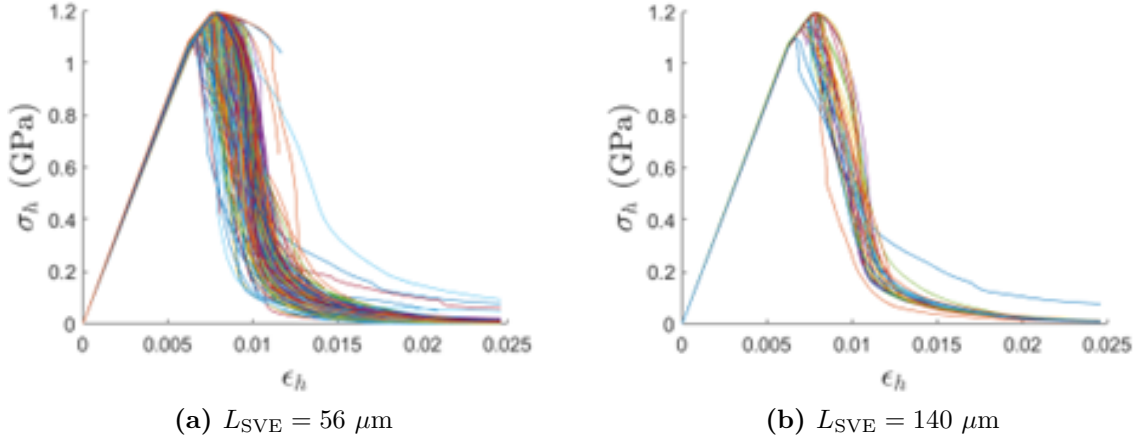
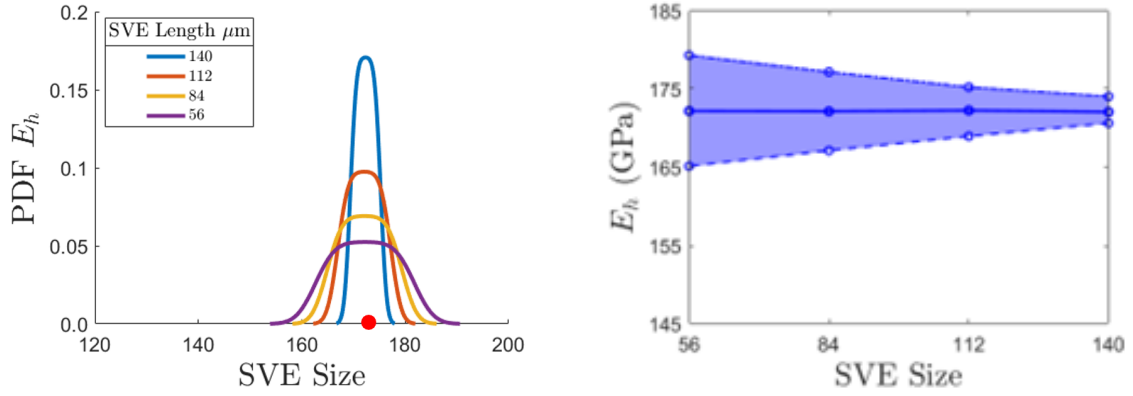


Figure 2.13: Horizontal stress vs strain overlay for (a) $L_{SVE} = 56 \mu\text{m}$; (b) $L_{SVE} = 140 \mu\text{m}$.

Figure 2.14 shows the PDF and size effect results for the horizontal stiffness. Referring to Figure 2.14b, stiffness for the horizontal load case is not as heavily affected by varying SVE size as the vertical stiffness in Figure 2.12b. Otherwise, both the vertical and horizontal stiffnesses show the same trends in the PDFs and sizes effects. That is, in both cases, the mean value stays relatively insensitive to the SVE size. The mean value for each SVE size also closely aligns with the publish value for E_h in Table 2.1. This is reflected by the red dot corresponding to the experimental results in Hanzl et al. (2015) for the RVE in Figure 2.2a.



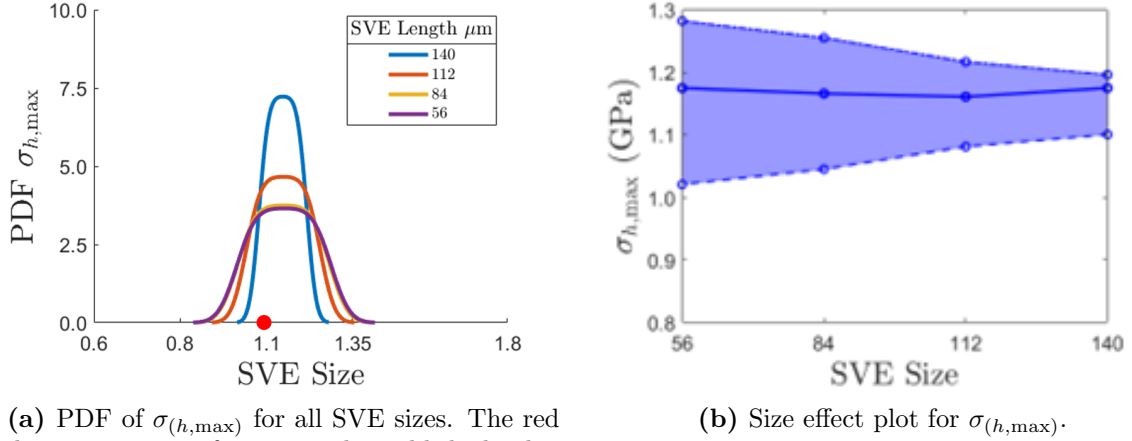
(a) PDF of E_h for all SVE sizes. The red dot serves as a reference to the published value from Hanzl et al. (2015).

(b) Size effect plot of E_h for all SVE sizes.

Figure 2.14: Horizontal results for E_h (a) PDF of E_h for all SVE sizes. The red dot serves as a reference to the published value from Hanzl et al. (2015); (b) Size effect plot of E_h for all SVE sizes.

Figure 2.15 shows the results for horizontal strength $\sigma_{(h,\max)}$. Referring to the PDFs in Figure 2.15a, the mean value for $\sigma_{(h,\max)}$ varies more dramatically, close to tenfold more, compared to the elastic modulus E_h . Again, the red dot corresponding to the experimental results in Hanzl et al. (2015) is provided for comparison with computational results of different SVE sizes. Figure 2.15b illustrates the increase in both the mean and minimum homogenized value of $\sigma_{(h,\max)}$ as SVE size increased. The reason for the increase to $\sigma_{(h,\max)}$ at larger SVE sizes and the difference between horizontal and vertical elastic moduli is explained by referring to the geometry of the melt pools in Figure 2.2a and Figure 2.5. For large SVEs, there is a higher likelihood of having a whole block of bulk material that runs across the entire SVE. Such blocks prevent the failure of the SVE through debonding across cohesive surfaces, as none will run across the layer. These stiff layers dictate the overall stiffness in the horizontal direction; the 3D printed layers in this case act as parallel springs, wherein the highest stiffness (the continuous layers) dictates the overall stiffness. For small SVEs, there is more likelihood of having certain melt pool lines cut through a layer. Accordingly, the overall horizontal strength becomes lower for such small SVEs. In contrast, for

all SVE sizes, the debonding in the vertical direction is easier and almost always possible, thus much less size sensitivity is observed in Figure 2.12 for $\sigma_{(v,\max)}$. The decrease of variations for E_h and $\sigma_{(h,\max)}$ is expected as both properties tend to their variation-based RVE size as the SVE size increases Ji et al. (2022).



(a) PDF of $\sigma_{(h,\max)}$ for all SVE sizes. The red dot serves as a reference to the published value from Hanzl et al. (2015).

(b) Size effect plot for $\sigma_{(h,\max)}$.

Figure 2.15: Horizontal results for $\sigma_{(h,\max)}$ (a) PDF of $\sigma_{(h,\max)}$ for all SVE sizes. The red dot serves as a reference to the published value from Hanzl et al. (2015); (b) Size effect plot for $\sigma_{(h,\max)}$.

2.4 Discussion

In this section, we summarize the results from the presented numerical results in the prior sections. First, we examine whether one can claim any of the four homogenized properties has reached its RVE size for $L_{\text{SVE}} = 140 \mu\text{m}$. In Abedi et al. (2022a) we have discussed mean-based, variation-based and boundary condition (BC)-based criteria to examine whether a homogenized properties has reached its RVE size limit. In the mean-based criterion, the RVE size is defined as the L_{SVE} , such that for all SVEs larger than that the relative variations of the mean value (e.g., the middle line in Figures 2.11b, 2.12b, 2.14b, and 2.15b) stays below a certain user-defined threshold ϵ across all larger SVE sizes. In the variation-based criterion, the RVE size corresponds

to the size beyond with the coefficient of variation (COV) stays below such threshold ϵ . The COV is defined as the ratio of standard deviation to the mean value of the quantity. Often the arbitrary threshold of $\epsilon = 0.01$ is used for both criteria [Pelissou et al. \(2009\)](#); [Kanit et al. \(2003\)](#). This variation-based criterion is the most common choice to determine the RVE size in literature, see for example [Kanit et al. \(2003\)](#); [Liu et al. \(2009\)](#). We refer the reader to [Abedi et al. \(2022a\)](#) for further discussion on these criteria and BC-based criterion not used in this work.

In [Abedi et al. \(2022a\)](#) we first obtain best fits to the means and COVs of a homogenized property versus L_{SVE} before determining when the normalized mean and COV fall below ϵ for the definition of mean- and variation-based RVEs. In this work, we adopt a simpler approach given the lower variation of homogenized properties discussed in section 3. For the mean-based criterion, we define the error in the mean values $e(\mu)$ as the largest difference between the mean values of all sizes divided by the largest mean value. That is, it is a relative error among all the mean-values of the given property. These values are reported in the first data row of Table 2.3. As evident, for all properties $e(\mu)$ is below or very close to $\epsilon = 0.01$. Thus, from this perspective, all homogenized properties can be claimed to have reached the mean-based RVE size below or around $L_{\text{SVE}} = 140 \mu\text{m}$.

Table 2.3: Summary of values used to examine mean- and variation-based RVE sizes for all four homogenized properties.

	Horizontal		Vertical	
	E_h	$\sigma_{(h,\text{max})}$	E_v	$\sigma_{(v,\text{max})}$
Mean-based: $e(\mu)$	0.000604	0.00766	0.00146	0.0166
Variation-based: COV ($L_{\text{SVE}} = 140 \mu\text{m}$)	0.00460	0.0230	0.00997	0.0162

The results for the variation-based criterion are shown in the second data line of Table 2.3. Herein, the COVs of the largest SVE size of $L_{\text{SVE}} = 140 \mu\text{m}$ are provided. For elastic properties and vertical strength, the COVs are below $\epsilon = 0.01$. Even for the homogenized strength the COV of 0.023 is close to the often-used threshold of

0.01. Thus, even for the variation-based criterion the properties are deemed to have reached their RVE size below or around $L_{\text{SVE}} = 140 \mu\text{m}$. This is an anticipated result, as Jiang et al. (2023) also obtained a similar finding pertaining to elastic properties.

Next, we examine the differences in the homogenized properties from two perspectives. First, for both criteria, elastic properties take smaller values, implying that they reach their RVE limit at a smaller size. This is consistent with our results in Abedi et al. (2022a) and Bahmani et al. (2019) for different two-phase composites. In Bahmani et al. (2019) stress contours demonstrate that minute local variations in the microstructure results in highly varied levels of stress concentration, thus the strength value assigned to an SVE. In contrast, the elastic properties reflect the average response of the SVE (as opposed to the weakest point type response for fracture properties) and are less sensitive to microstructural variations. This explains why the values for elastic properties are smaller in Table 2.3.

Second, we examine the difference between horizontal and vertical properties. From Table 2.3 we observe that the homogenized E_h not only has a more stable mean value (reflected in $e(\mu)$), but also has smaller normalized variations (reflected in COV). Both aspects are also graphically evident by comparing Figure 2.11b and Figure 2.14b. This can be attributed to whole regions spanning the RVE horizontally, acting as rather deterministic parallel springs for the horizontal loading case. For fracture properties, while a lower variation is observed for $\sigma_{(h,\text{max})}$ compared to $\sigma_{(v,\text{max})}$ in Figure 2.12b and Figure 2.15b and in Table 2.3, one needs to refer to the actual strain-stress responses in Figure 2.10 and Figure 2.13 to have a clearer understanding of the differences of the two loading beyond just the maximum stress. From the strain-stress responses we observe a lower variation of the elastic slope E_h compared to E_v (consistent with the COV values for $L_{\text{SVE}} = 140 \mu\text{m}$ in Table 2.3). In contrast, it is now the horizontal direction that has a higher variation in response post-elastic regime.

2.5 Conclusions

The SVE-based homogenization approach can be used to derive elastic and fracture properties for SLM material. The mean apparent values for vertical and horizontal QoIs resemble experimentally obtained values. Furthermore, increasing the SVE size reduces the variation of homogenized properties. The relative difference in mean values for E_v was more than twice that of E_h , indicating a heightened sensitivity to the effect of SVE size on vertical stiffness. The behavior in the horizontal and vertical directions appears to exhibit inverse tendencies, with the vertical direction displaying heightened sensitivity in linear components. In contrast, the horizontal direction demonstrates increased variability during fracture, indicating a divergent behavior between the two directions. The difference in behavior between horizontal and vertical results can be attributed to the microstructure of the SLM material. The likelihood of a melt pool boundary perpendicular to the applied load is greater for the vertical load case than the horizontal. The resulting over-stiffness phenomenon observed for the horizontal load case decreased for larger SVEs. As for fracture properties, we observe that they exhibit higher variations and less stable mean values when compared to elastic properties. In any case, for the SLM material considered, below or around the size of $140\text{ }\mu\text{m}$, all elastic and fracture properties have reached both the mean- and variation-based RVE size.

The results provide insight into how SLM material elastic and fracture properties tend to their macroscopic size-independent and homogeneous limit. While these RVE-based limits are suitable for many macroscopic problems, SVE-based homogenized properties are favorable for failure analysis as they maintain a sufficient level of material heterogeneity needed for such applications [Abedi et al. \(2022a\)](#); [Bahmani et al. \(2019\)](#). The heightened sensitivity of fracture properties to slight variations in SLM materials bears significant implications for material design and structural integrity. A more comprehensive understanding of the brittleness and fracture behavior becomes critical since even minor variations in these properties can

potentially lead to catastrophic brittle failures in real-world applications. We believe that these SVE-based elastic and fracture properties can be used for stochastic failure analysis of material as demonstrated in [Bažant and Planas \(1998\)](#).

Some other extensions of this work are as follows. First, we only had one set of experimental results to compare with our computational results. To accurately validate the results, we should have several experimental strain-stress responses of the SLM material for each SVE size considered. Second, subsequent mechanical analysis should include the temperature effects during manufacturing and ensuing residual stresses. These residual stresses are obtained from the thermomechanical analysis of the printing process [Luo and Zhao \(2018\)](#). Some examples of such analysis for a single laser path, multiple parallel paths, and an entire SLM part are provided in [Letenneur et al. \(2019\)](#); [Burkhardt et al. \(2020\)](#), and [Luo and Zhao \(2019\)](#), respectively. In future work, we aim to derive residual stresses resulting from simulating the manufacturing process and incorporating their effect on the nonlinear properties of the printed material, such as strength and fracture energy. Third, grain-level nonlinear material models such as crystal plasticity remove the restriction of crack propagation along melt pool boundaries and provide a more accurate overall representation of material failure. Fourth, SVE-based homogenization can be incorporated in multiscale linear and nonlinear analysis of SVEs. The lower computational cost of such multiscale analysis (compared to DNS) makes this approach a suitable forward solver in design problems, such as optimizing SLM-printing parameters [Letenneur et al. \(2019\)](#); [Sun et al. \(2016\)](#).

Chapter 3

SVE-Based Homogenized Thermoelastic Coupling and Residual Stress–Driven Fracture in Multiphase Ceramics

3.1 Introduction

Structural ceramics are central to modern technological advances due to their ability to perform in extreme environments. Few materials can withstand the extremes of temperature, load, and chemical reactivity while maintaining high stiffness and stability in a lightweight design [Pelz et al. \(2021a\)](#); [Rubink et al. \(2021\)](#); [Pittari III et al. \(2015\)](#). As a result, they are deployed in critical sectors including ballistics, aerospace, and energy, with uses ranging from heat exchangers [Beall \(1992\)](#) and abrasives [Presser and Nickel \(2008\)](#) to nuclear systems [Koyanagi et al. \(2018\)](#); [Krstić et al. \(1996\)](#); [Katoh and Snead \(2019\)](#); [Koyanagi et al. \(2021\)](#) and armor [Medvedovski \(2005\)](#); [Vargas-Gonzalez et al. \(2010\)](#); [Medvedovski and Sarkar \(2004\)](#); [Silveira et al. \(2021\)](#).

Historically produced by powder-based consolidation (sintering, hot pressing/infiltration, HPHT), these routes establish mature baselines yet impose geometric limitations. Recent advances in ceramic AM, including stereolithography and direct-ink writing, overcome these constraints by enabling architected geometries and graded material layouts [Pelz et al. \(2021a\)](#); [Griffith and Halloran \(1996\)](#); [Peng et al. \(2018\)](#); [Oxman et al. \(2011\)](#); [Pelz et al. \(2021b\)](#).

The thermal histories and phase layouts enabled by AM set the stage for residual stresses. During cooling from fabrication temperatures, differences in thermal expansion between phases give rise to a mismatch in strains in each phase. [Watts et al. \(2011\)](#); [Matthey et al. \(2020\)](#); [Eshelby \(1957\)](#). The enforcement of compatibility brought about by these mismatched strains generates internal stresses that change apparent stiffness, strength, and fracture response [Pelz et al. \(2021a\)](#); [Shoulders et al. \(2024\)](#). Functionally graded and multimaterial builds can intentionally amplify or mitigate local CTE contrast, making residual stress a design variable and a processing outcome [Pelz et al. \(2021b\)](#).

Residual stresses are not only a processing artifact, but also a recognized toughening mechanism in brittle ceramics. Compressive residual states can delay crack initiation and elevate apparent fracture toughness, while tensile states often accelerate micro-cracking and premature failure [Taya et al. \(1990\)](#); [Sigl \(1996\)](#); [White and Dickey \(2011\)](#). Therefore, the ability to represent these stresses within constitutive models is critical for connecting processing history to macroscopic performance. From a constitutive standpoint, residual stress may be represented by defining a thermoelastic reference state that is not stress-free, embedding the initial stress/strain directly into the free energy in a thermodynamically consistent way. In this formulation, residual stresses enter directly into the elastic strain and thus into the driving energy for fracture, without violating balance or dissipation principles [Clayton et al. \(2022\)](#).

A central challenge is how fracture can be represented when residual stresses are already embedded in the material response. Traditional approaches to modeling

cracks, such as cohesive elements, discrete damage zones, or sharp interface criteria, require predefined paths or interface placements and can suffer mesh/enrichment bias, making them difficult to reconcile with evolving residual fields [Park and Paulino \(2011\)](#); [de Borst et al. \(2004\)](#). Extended finite element (XFEM) methods relax some of these restrictions but still rely on enrichment functions and crack tracking of the level set, which adds implementation overhead and complicates coupling to heterogeneous residual stress states [Moës et al. \(1999\)](#); [Yazid et al. \(2009\)](#); [Agathos et al. \(2018\)](#); [Feulvarch et al. \(2013\)](#).

For these reasons, the phase-field method offers a natural alternative. Originating in variational formulations of brittle fracture [Francfort and Marigo \(1998\)](#); [Bourdin et al. \(2000\)](#), it treats cracks as diffuse damage zones governed by energy minimization, eliminating the need for explicit surface tracking. Robust finite element implementations have demonstrated their ability to capture nucleation and branching in a single framework [Miehe et al. \(2010b\)](#); [Borden et al. \(2012\)](#). In ceramics, similar behavior has been reproduced in heterogeneous microcrystalline composites [Clayton et al. \(2019\)](#) and in diamond–SiC systems with tertiary phases [Clayton et al. \(2022\)](#), where crack branching, deflection, and interactions with residual stresses are central features. In this framework, residual stresses are embedded directly in the elastic strain energy, so the same function governs the mechanical response and damage evolution [Miehe et al. \(2010b\)](#); [Ambati et al. \(2015\)](#); [Clayton et al. \(2022\)](#). Thermo-mechanical extensions of the method have further shown its applicability to fracture under temperature gradients and thermal shock [Li et al. \(2022\)](#); [Wang et al. \(2023\)](#). As a result, crack initiation, crack paths, and the balance between normal and shear fracture emerge naturally from the microstructure rather than from user-imposed criteria [Miehe et al. \(2010a\)](#).

To introduce residual stresses in practice, an eigenstrain value can be prescribed for each phase, representing the free thermal expansion associated with cooling. In multi-phase systems, compatibility constraints prevent each phase from expanding independently, and the resulting mismatch produces a self-equilibrated residual

stress field, consistent with classical inclusion theory [Eshelby \(1957\)](#) and confirmed experimentally in multiphase ceramics [Watts et al. \(2011\)](#); [Matthey et al. \(2020\)](#); [Shoulders et al. \(2024\)](#). Such eigenstrain initializers have been adopted in modeling studies as a direct way to impose target stress patterns for controlled investigations of toughness and crack stability [Clayton et al. \(2022\)](#). The phase-field model is well suited for this approach, since eigenstrain-induced fields enter the same elastic strain energy that drives the evolution of the damage field [Clayton et al. \(2022\)](#); [Li et al. \(2022\)](#); [Wang et al. \(2023\)](#).

In micromechanics, residual stresses are described using effective stiffness and compliance, complemented by effective thermal expansion and specific thermal stress tensors [Böhm \(1998\)](#); [Benveniste and Dvorak \(1991\)](#); [Dvorak \(1992\)](#). At the phase level, localization and concentration tensors link overall fields to phase averages, preserving equilibrium and compatibility under thermal mismatch. From these relations, homogenized quantities that describe how residual stresses alter stiffness, expansion, and the distribution of elastic energy can be derived. Accurate use of these quantities requires careful treatment of the boundary state, since the end stress distribution can be susceptible to boundary condition assumptions [Bukanya et al. \(2021\)](#). To avoid artifacts associated with free or over-constrained configurations, affine displacements enforce the contraction implied by the residual field, avoiding artifacts of free or fully constrained boundaries. This type of boundary conditioning influences not only local stress distributions, but also the overall stress–strain response and energy dissipation observed in ceramics with heterogeneous thermal histories [Watts et al. \(2011\)](#); [Matthey et al. \(2020\)](#); [White and Dickey \(2011\)](#).

Residual stress effects are evaluated through homogenization in a statistical volume element (SVE) framework. Unlike a representative volume element (RVE), which assumes convergence to a single effective property, the SVE approach retains variability. Each window produces a different apparent response, and associated statistics provide both mean behavior and variability. Recent studies have emphasized that convergence must be assessed not only with respect to mean stability but also

with sensitivity to boundary conditions and window size [Abedi et al. \(2022b\)](#); [Acton et al. \(2022\)](#); [Abedi et al. \(2023\)](#).

The homogenized quantities of interest span multiple regimes. In the linear mechanical setting, the effective stiffness tensor characterizes elasticity under small strain. Thermoelastic coupling is captured through the effective coefficient of thermal expansion and the associated mapping tensors that link domain-average fields to phase-average stresses and strains under temperature change. In the nonlinear regime, effective strength and specific fracture energy (energy dissipated per unit volume) are extracted, directly informing fracture models. All quantities are reported under a consistent mixed-boundary condition, which balances displacement and traction constraints to avoid the extremes of purely kinematic or static assumptions.

3.2 Methods

The mechanical response of ceramics depends strongly on their underlying microstructure. Finite element models were created from segmented micrographs of B_4C/SiC composites [Shoulders et al. \(2024\)](#) using OOF2 [Reid et al. \(2009\)](#). These image-based meshes capture the main phase geometry and were used to simulate the composite’s linear and nonlinear thermoelastic response. All simulations were performed in ABAQUS [Manual \(2012\)](#), where phase-specific material properties, temperature-dependent boundary conditions, and load cases were implemented to extract the effective mechanical and thermomechanical properties. The elastic analyses define the baseline stiffness, and the thermomechanical simulations add temperature-dependent strains and nonlinear behavior to study residual stress formation and its effect on the nonlinear response.

3.2.1 Microstructure Partitioning

The analyzed microstructures consist of two phases: boron carbide (B_4C) inclusions embedded in a silicon carbide (SiC) matrix [Shoulders et al. \(2024\)](#). Boron carbide is stiffer and more brittle than the surrounding silicon carbide, creating a heterogeneous composite microstructure representative of high-temperature ceramic systems. A representative segmented micrograph and its corresponding finite element mesh are shown in Fig. 3.1.

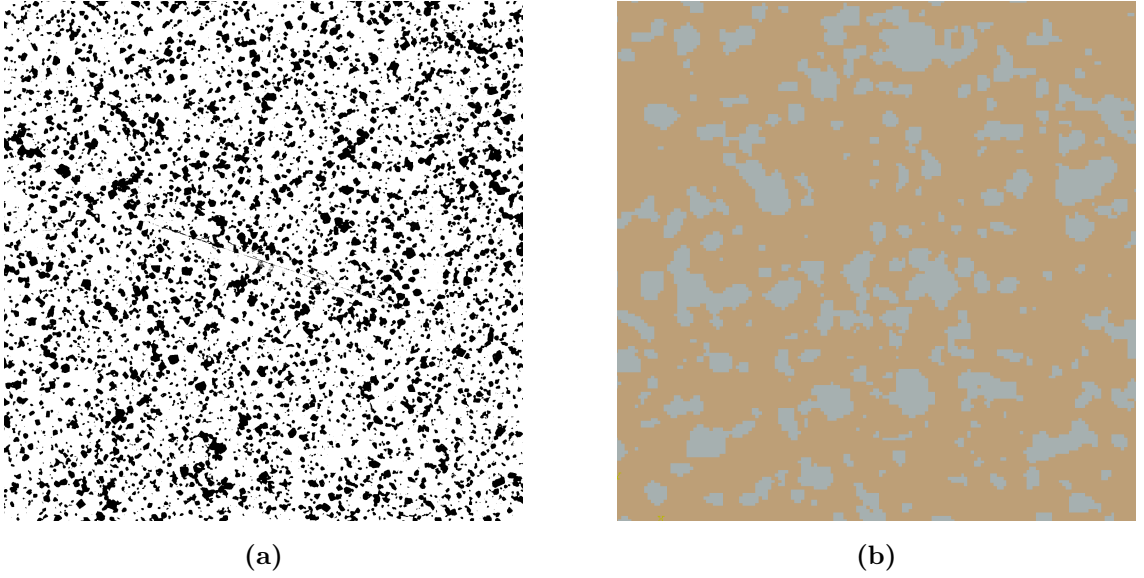


Figure 3.1: Segmented micrographs of B_4C /SiC composites [Shoulders et al. \(2024\)](#) (a) and corresponding microstructure using OOF2 [Reid et al. \(2009\)](#) (b).

The reconstructed microstructural domains were partitioned using SVE sizes of 0.014 mm, 0.028 mm, 0.056 mm, 0.112 mm, and 0.223 mm. We employed space-filling uniform square partitions, which ensure that each SVE occupies its designated area without overlap or gaps, adhering to the hierarchy of bounds described by Huet [Huet \(1990\)](#). SVEs of sizes $L_{SVE} = 0.014$ mm, 0.028 mm, 0.056 mm, 0.112 mm, and 0.223 mm fill the space of each microstructure with corresponding grids of , 256 (16×16), 64 (8×8), 16 (4×4), 4 (2×2) and 1 (1×1) SVEs, respectively. The moving-window framework [Baxter and Graham \(2000\)](#); [Graham and Baxter](#)

(2001); Baxter et al. (2005); Huet (1990) allows these partitions to be analyzed individually within OOF2, providing statistically meaningful measures of scale-dependent variability in the apparent elastic and thermomechanical response. This hierarchical decomposition is illustrated in Fig. 3.2, which shows how successive refinement proceeds by subdividing each subsequent partition into smaller SVEs.

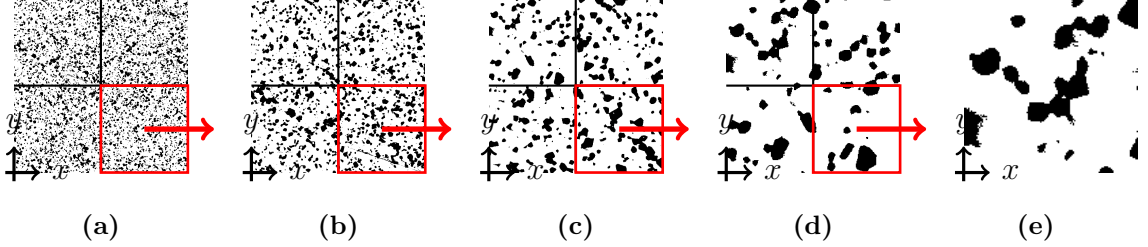


Figure 3.2: Hierarchical moving-window decomposition of the microstructure. Panels (a–e) show progressively refined SVE partitions ($L_{\text{SVE}} = 0.223, 0.112, 0.056, 0.028, 0.014$ mm). Each image, except the smallest, includes a 2×2 grid, with the bottom-right subregion (red box) indicating the window size used for the next refinement step.

3.2.2 Phase-Field Formulation and Material Parameters

Fracture was modeled using the variational phase-field UEL developed by Molnár *et al.* Molnár et al. (2020). This formulation follows the standard AT-2 phase-field model of brittle fracture Miehe et al. (2010b,a); Hu et al. (2021), in which cracks are represented by a diffused scalar variable $d \in [0, 1]$ that progressively reduces the material stiffness as damage evolves.

The total free energy is expressed as

$$\Gamma[d] = \int_{\Omega} \frac{G_c}{2\ell_c} (d^2 + \ell_c^2 |\nabla d|^2) \, d\Omega, \quad (1a)$$

and the elastic strain-energy density is degraded according to

$$\psi_{\text{el}}(u, d) = g(d) \psi_{\text{el}}^+(u) + \psi_{\text{el}}^-(u), \quad g(d) = (1 - d)^2 + k, \quad k \ll 1. \quad (1b)$$

Crack irreversibility is enforced through a stored history field

$$H = \max_t \psi_{\text{el}}^+(t), \quad (1c)$$

which ensures that previously formed damage does not heal upon unloading.

Here, G_c is the critical energy-release rate, ℓ_c is the regularization length that controls the width of the diffused crack, ψ_{el}^+ and ψ_{el}^- are the tensile and compressive energy components, and k is a small numerical parameter providing residual stiffness for stability. Following standard practice [Miehe et al. \(2010b\)](#), the characteristic length was related to the cohesive length used in mesh design as $\ell_c = l_{\text{coh}}/2$, ensuring sufficient resolution of the damage-process zone and mesh-independent energy dissipation.

Material parameters were selected from literature for boron carbide and silicon carbide composites [Shoulders et al. \(2024\)](#); [Rubink et al. \(2021\)](#); [Pittari III et al. \(2015\)](#). Elastic and thermal properties were taken from reported values of E , ν , G_c , and d (coefficients of thermal expansion), with the SiC matrix modulus adjusted to 45 GPa to amplify heterogeneity effects. The coefficients of thermal expansion for B_4C and SiC were 6.11 and 5.28 $\mu\text{m}/(\text{m}\cdot\text{K})$, respectively, and a uniform temperature change of $\Delta T = -1930$ K was applied to generate thermal residual stresses. The present study uses reduced stiffness values for SiC to increase mechanical contrast between the phases. This deviation from experimentally measured values [Shoulders et al. \(2024\)](#) should be regarded as a limitation, but it serves to highlight microstructural contrast and phase interaction effects more clearly (Table 3.1).

The number of elements per axis was determined from the characteristic length scale governing the damage process, where the effective strength is equal to $\sqrt{3EG_c/8l_{\text{coh}}}$ [Miehe et al. \(2010b\)](#). This relationship links the cohesive length to the material response and defines the minimum element size needed to resolve the diffused crack. Each mesh was refined so that several elements spanned this length,

ensuring accurate crack evolution and consistent energy dissipation across all domain sizes .

The timestep was determined from the characteristic response times of each phase to maintain quasi-static loading. Wave speeds derived from the elastic stiffness and mass density properties defined how quickly stresses could propagate, while the phase-field formulation introduced a slower timescale for damage evolution. The smaller of these governed the timestep (listed in Table 3.2).

Table 3.1: Elastic and thermal properties of SiC and B₄C used in the simulations compared with experimental values from Shoulders et al. (2024).

		Model inputs		Shoulders et al. (2024)	
		SiC	B ₄ C	SiC	B ₄ C
E	GPa	45	455	434	454
ν	–	0.18	0.18	0.20	0.19
d	MK ^{−1}	5.28	6.11	5.28	6.11

Table 3.2: Numerical parameters used in the phase-field simulations. Fracture toughness values G_c are taken from Beaudet et al. (2015) for B₄C and Clayton et al. (2022) for SiC.

Parameter	Units	Value
G_c	mJ/mm ²	2.33 / 3.27
ρ	g/cm ³	3.20 / 2.50
l_{coh}	μm	1.0
h	μm	$l_{\text{coh}}/4$
Δt	μs	2.0
ΔT	K	−1930

3.2.3 Thermomechanical Response

The local thermoelastic relation between stress, strain, and temperature change can be expressed in either stiffness or compliance form:

$$\boldsymbol{\sigma} = \mathbf{C}\boldsymbol{\varepsilon} + \mathbf{c}\Delta T \quad \Longleftrightarrow \quad \boldsymbol{\varepsilon} = \mathbf{D}\boldsymbol{\sigma} + \mathbf{d}\Delta T, \quad (3.1)$$

where $\mathbf{C}$ and $\mathbf{D}$ are the stiffness and compliance tensors, and $\mathbf{c}$ and $\mathbf{d}$ are the corresponding thermal coupling tensors.

Both representations are thermodynamically equivalent and must satisfy the reciprocity (or coupling) conditions:

$$\mathbf{C}\mathbf{D} = \mathbb{I}, \quad \mathbf{c} + \mathbf{C}\mathbf{d} = \mathbf{0}. \quad (3.2)$$

The first ensures that the stiffness and compliance tensors are exact inverses, while the second enforces compatibility between the thermal coupling tensors in the stiffness and compliance formulations.

Isotropic and Multiphase Cases

For an isotropic material, the elastic response depends on only two independent constants, such as the Young's modulus E and Poisson's ratio ν , or equivalently the bulk modulus K and shear modulus μ . Under isotropy, the thermal coupling reduces to a single scalar parameter d , *i.e.*, the *coefficient of thermal expansion* (CTE) defined earlier. This represents the volumetric thermal strain per unit temperature change, so that $\mathbf{d} = d\mathbf{I}$. For a composite composed of n_p isotropic phases, indexed by $j \in \{1, \dots, n_p\}$, each phase is characterized by its own stiffness tensor $\mathbf{C}^j$ and thermal coupling tensor $\mathbf{d}^j$, obtained from the corresponding elastic moduli and thermal expansion behavior. A schematic representation of an n_p -phase microstructure is shown in Fig. 3.3, where each labeled region j occupies a known volume fraction v_{f}^j .

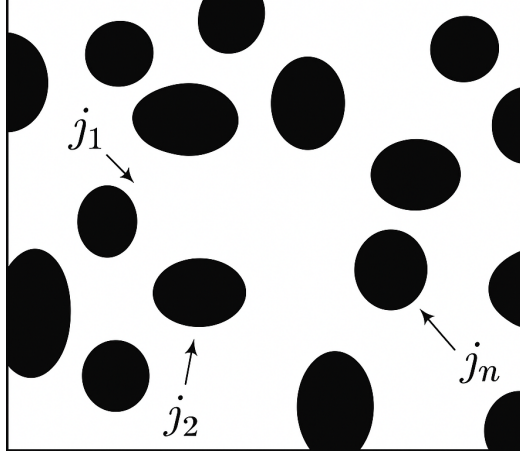


Figure 3.3: Representative n_p -phase microstructure used to define phase-wise thermoelastic tensors $\mathbf{C}^j$ and $\mathbf{d}^j$.

For the two-phase case relevant here, the composite consists of a matrix phase (m) and an inclusion phase (i), with $v_f^m + v_f^i = 1$. Each phase is therefore fully defined by its $\mathbf{C}^{(m,i)}$, $\mathbf{d}^{(m,i)}$.

Mean-Field Framework

The objective is to determine an equivalent homogeneous relation that represents the overall thermoelastic response of the composite. This macroscopic behavior is written as

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{C}^* \langle \boldsymbol{\varepsilon} \rangle + \mathbf{c}^* \Delta T \quad \Longleftrightarrow \quad \langle \boldsymbol{\varepsilon} \rangle = \mathbf{D}^* \langle \boldsymbol{\sigma} \rangle + \mathbf{d}^* \Delta T, \quad (3.3)$$

where the starred quantities denote the effective stiffness, compliance, and thermal coupling tensors of the homogenized material.

Because the composite consists of multiple phases, the average fields (denoted by $\langle \cdot \rangle$) Within each phase j must also be defined:

$$\langle \boldsymbol{\varepsilon}^j \rangle = \mathbf{A}^j \langle \boldsymbol{\varepsilon} \rangle + \mathbf{a}^j \Delta T, \quad \boldsymbol{\sigma}^j = \mathbf{B}^j \langle \boldsymbol{\sigma} \rangle + \mathbf{b}^j \Delta T, \quad (3.4)$$

where $\mathbf{A}^j$ and $\mathbf{B}^j$ are the mechanical localization tensors and $\mathbf{a}^j$ and $\mathbf{b}^j$ are the corresponding thermal localization terms. These quantities describe how the global

fields distribute within each phase. The localization tensors $\mathbf{A}^j$ and $\mathbf{B}^j$, as well as tensors $\mathbf{a}^j$ and $\mathbf{b}^j$ are not independent; similar to 3.2 they satisfy reciprocal relations, not provided for brevity (see Böhm (1998)).

For reference, analytical mean-field estimates were also computed using the Mori–Tanaka scheme Böhm (1998); Hu and Weng (1998); Shoulders et al. (2024); Caliskan et al. (2025). This approach uses the Eshelby inclusion solution to relate phase moduli and volume fractions through the strain-concentration tensor, providing closed-form effective stiffness and thermal expansion estimates. These values represent the RVE-limit predictions that bound and contextualize the finite-element homogenization results. A detailed comparison with the FEM-based estimates is provided later to assess their consistency and scale dependence.

Numerical Homogenization via Finite Element Analysis

The effective stiffness and thermal coupling tensors ($\mathbf{C}^*$, $\mathbf{c}$) are obtained numerically by applying a set of representative load cases to each microstructural realization. In Voigt notation, the constitutive relation takes the form,

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \end{bmatrix} + \begin{bmatrix} c_{11} \\ c_{22} \\ c_{12} \end{bmatrix} \Delta T, \quad (3.5)$$

which corresponds to the tensor form in eq 3.3. All tensors are expressed in Voigt notation under plane strain conditions, with the shear component written as $2\varepsilon_{12}$ corresponding to the engineering shear strain $\gamma_{12} = 2\varepsilon_{12}$.

To determine each column of $\mathbf{C}^*$ and the thermal vector $\mathbf{c}$, four finite element load cases (LCs) are performed. During mechanical loading (LC1–LC3), the macroscopic strains are prescribed while $\Delta T = 0$, allowing the average stresses to yield the columns of $\mathbf{C}^*$ directly. Three boundary condition schemes are considered—pure displacement (DBC), pure traction (TBC), and mixed (MBC)—which together bound the response

and enable comparison across constraint levels. Representative boundary condition setups for the three mechanical loading modes (LC1–LC3) are described here. Under DBC, macroscopic strains are imposed on the model boundaries while nodal tractions remain free. Under TBC, macroscopic tractions are applied on the boundary while nodal displacements remain free part from minimal constraints to suppress rigid-body motion. With MBC, one boundary degree of freedom is prescribed through a displacement constraint, while the orthogonal component is applied through a traction condition. The resulting deformation and stress distributions for the three boundary condition types (DBC, TBC, MBC) are shown in Figs. 3.4–3.6, corresponding to the three mechanical load cases (LC1–LC3).

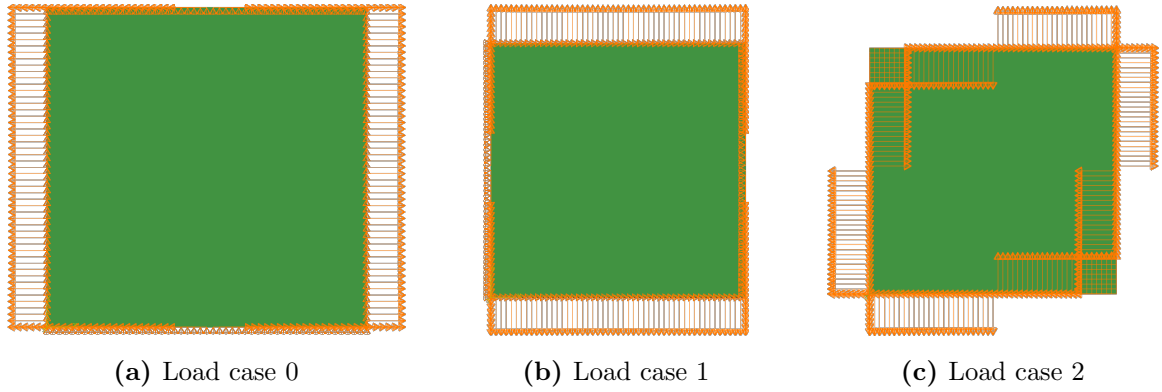


Figure 3.4: Displacement boundary condition (DBC) configuration for (a) loading in XX (LC1), (b) loading in YY (LC2), and (c) simple shear in XY (LC3). Orange arrows indicate prescribed displacements, and triangles denote fixed degrees of freedom. No tractions are applied under DBC.

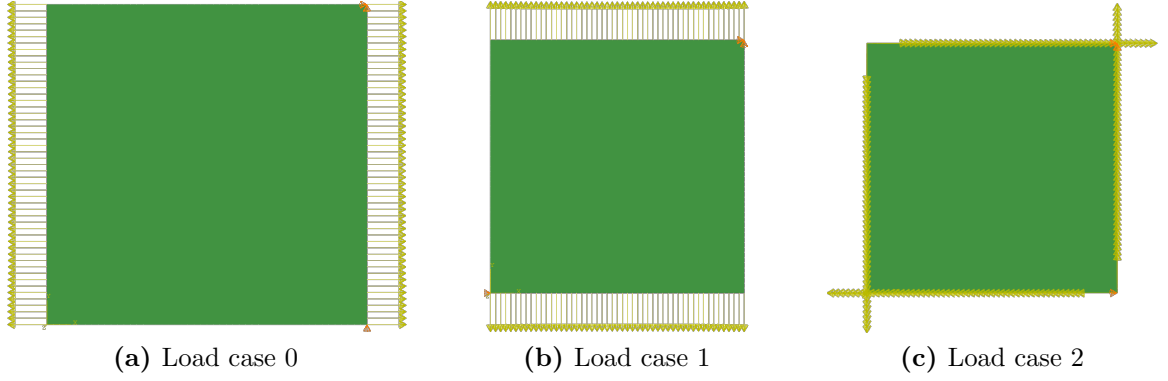


Figure 3.5: Traction boundary condition (TBC) configuration for (a) loading in XX (LC1), (b) loading in YY (LC2), and (c) simple shear in XY (LC3). Green arrows indicate applied surface tractions, and triangles denote minimal constraints used only to suppress rigid-body motion. No other displacements are prescribed on the loaded edges under TBC.

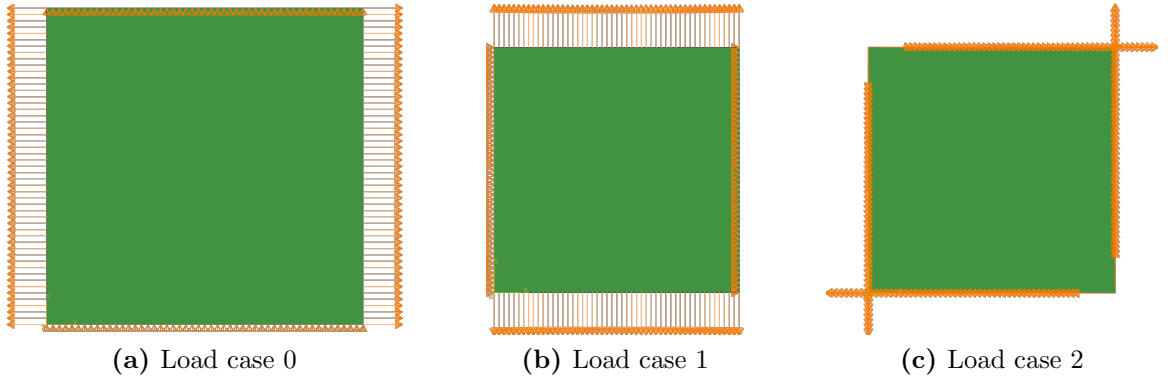


Figure 3.6: Mixed boundary condition (MBC) configuration for (a) loading in XX (LC1), (b) loading in YY (LC2), and (c) simple shear in XY (LC3). Orange arrows indicate prescribed displacements, yellow arrows denote applied tractions, and triangles indicate fixed degrees of freedom. Under MBC, one direction of boundary motion is displacement-controlled while the orthogonal direction is traction-controlled.

Homogenized Thermal Coupling

In the thermal case (LC4), a uniform temperature change $\Delta T \neq 0$ is applied while mechanical constraints depend on the selected boundary condition. For DBC, the deformation is fixed ($\boldsymbol{\varepsilon} = \mathbf{0}$); for TBC, external tractions are set to zero (free expansion); and for MBC, a combination of zero displacement and traction components is prescribed. The homogenized thermal coupling tensor is obtained from the macroscopic stress and strain responses to an imposed temperature change ΔT as

$$\mathbf{c}^* = \frac{1}{\Delta T} (\langle \boldsymbol{\sigma} \rangle - \mathbf{C}^* \langle \boldsymbol{\varepsilon} \rangle), \quad (3.6)$$

where $\langle \boldsymbol{\sigma} \rangle$ and $\langle \boldsymbol{\varepsilon} \rangle$ denote the volume-averaged stress and strain fields under thermal loading. Here, a positive temperature change $\Delta T > 0$ induces tensile thermal stress in a constrained body when $\mathbf{c}^*$ is negative, consistent with the conventional relation $\mathbf{c} = -\mathbf{C}\mathbf{d}$, where $\mathbf{d}$ is the thermal expansion tensor.

The corresponding compliance-side representation follows:

$$\mathbf{d}^* = -(\mathbf{C}^*)^{-1} \mathbf{c}^*, \quad (3.7)$$

providing the complete macroscopic thermoelastic coupling in stiffness and compliance form.

Each component of $\mathbf{c}^*$ represents the macroscopic stress developed per unit temperature change under zero-strain conditions, whereas the components of $\mathbf{d}^*$ describe the corresponding macroscopic thermal strain generated under stress-free conditions. Together, they quantify the effective thermal expansion behavior of the heterogeneous composite.

For completeness, the macroscopic and phase-wise thermal coefficients can be expressed in a compact form that couples the mechanical localization tensors and phase responses:

$$\mathbf{a}^{(j)} = \frac{1}{\Delta T} \left(\langle \boldsymbol{\varepsilon} \rangle^{(j)} - \mathbf{A}^{(j)} \langle \boldsymbol{\varepsilon} \rangle \right), \quad \mathbf{b}^{(j)} = \frac{1}{\Delta T} \left(\langle \boldsymbol{\sigma} \rangle^{(j)} - \mathbf{B}^{(j)} \langle \boldsymbol{\sigma} \rangle \right), \quad (3.8)$$

Nonlinear Thermomechanical Loading

During the cooldown stage, the homogenized thermal strain tensor $\mathbf{d}^*$ obtained from LC4 defines the imposed macroscopic contraction. For a uniform temperature change $\Delta T < 0$, the effective thermal strain:

$$\bar{\boldsymbol{\varepsilon}} = \mathbf{d}^* \Delta T,$$

which represents the free thermal deformation of the homogenized domain. This strain is applied as affine normal displacements on the domain boundaries, producing a uniform contraction consistent with the effective thermoelastic response. The edges can slide freely, so the MBC applies the shrinkage only in the normal direction, allowing in-plane relaxation. This approach is analogous to the flat or periodic boundary treatments used in [Bukenya et al. \(2021\)](#). This thermal contraction defines the almost stress-free configuration to which the subsequent mechanical and phase-field loading stages are applied. After the thermal contraction stage, the domain is loaded dynamically under a spatially affine biaxial velocity field. The inclusion is drawn into tension from the thermally relaxed configuration, while the surrounding matrix develops compression due to its elastic and thermal mismatch.

3.3 Linear Results

Linear analyses under DBC, MBC, and TBC quantify the elastic response to the imposed eigenstrain, directly measuring how boundary constraints govern the strain and stress distribution in the cooled residual state. At each SVE size, the influence of boundary conditions on the apparent response is examined to quantify constraint

sensitivity and to identify the scale at which the response becomes effectively boundary-independent.

This approach follows the SVE-based homogenization framework of Abedi *et al.* [Abedi et al. \(2022b, 2023\)](#), which demonstrated how boundary conditions and domain size govern the apparent elastic response of two-phase composites. To facilitate comparison across boundary conditions and SVE sizes, directional responses are averaged to obtain a single representative measure for each apparent property.

For any apparent property evaluated in the x and y directions, the mean response is defined as

$$f := \frac{f_x + f_y}{2}, \quad (3.9)$$

where f_x and f_y represent the corresponding directional components [Abedi et al. \(2022b\)](#). The following sections consistently apply this definition to elastic and thermomechanical quantities.

3.3.1 Geometry

Figure [3.7](#) shows the mean value of v_f and its variation among realizations. The overlap of the boundary-condition curves indicates that the partitioning preserves a consistent inclusion distribution across cases. Although individual small SVEs may exhibit greater variation in local volume fraction due to microstructural heterogeneity, their mean converges to the same global value as larger domains, consistent with the variance scaling reported by [Kanit et al. \(2003\)](#). Across all conditions, $v_f \approx 0.23$, confirming that differences in the following elastic and thermal responses arise from boundary and size effects rather than geometric variation.

3.3.2 Elastic Response

The apparent bulk modulus κ , shear modulus G , and Young's modulus E follow the expected boundary-condition hierarchy: DBC gives the upper bound, TBC the lower, and MBC lies between them (assuming the Hill-Mandel Energy equivalency

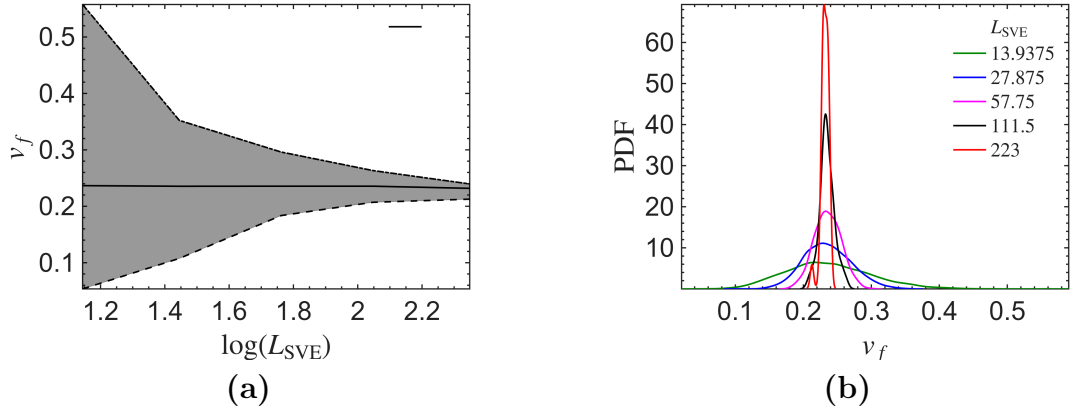


Figure 3.7: (a) Mean inclusion volume fraction v_f as a function of SVE size, with shaded regions indicating the range between minimum and maximum values across realizations. (b) Probability density functions (PDFs) of v_f for each SVE size.

condition is satisfied). These differences are most pronounced at the smallest SVE sizes, where boundary constraints dominate the local response. With increasing L_{SVE} , all three moduli converge rapidly toward a standard value, indicating a transition to boundary-independent behavior as seen in Figure 3.8. The apparent Poisson's ratio ν does not hold to the same boundary condition hierarchy, as it is not bounded by the upper and lower limits and can vary non-monotonically at small SVE sizes.

Probability density functions (PDFs) for the apparent moduli corroborate the size-effect trends (Figure 3.9). For each boundary condition, the densities contract rapidly with increasing L_{SVE} , indicating a reduction in inhomogeneity and an approach to a unique effective value. Across boundary conditions, the primary difference is a shift in the mean (DBC upper, TBC lower, MBC between), while the distribution shapes remain similar. The values in Table 3.3 show the elastic behavior at the largest SVE size, where boundary effects are minimal. DBC and TBC remain the upper and lower bounds for all moduli, while MBC stays close to the middle, showing that the response has effectively converged.

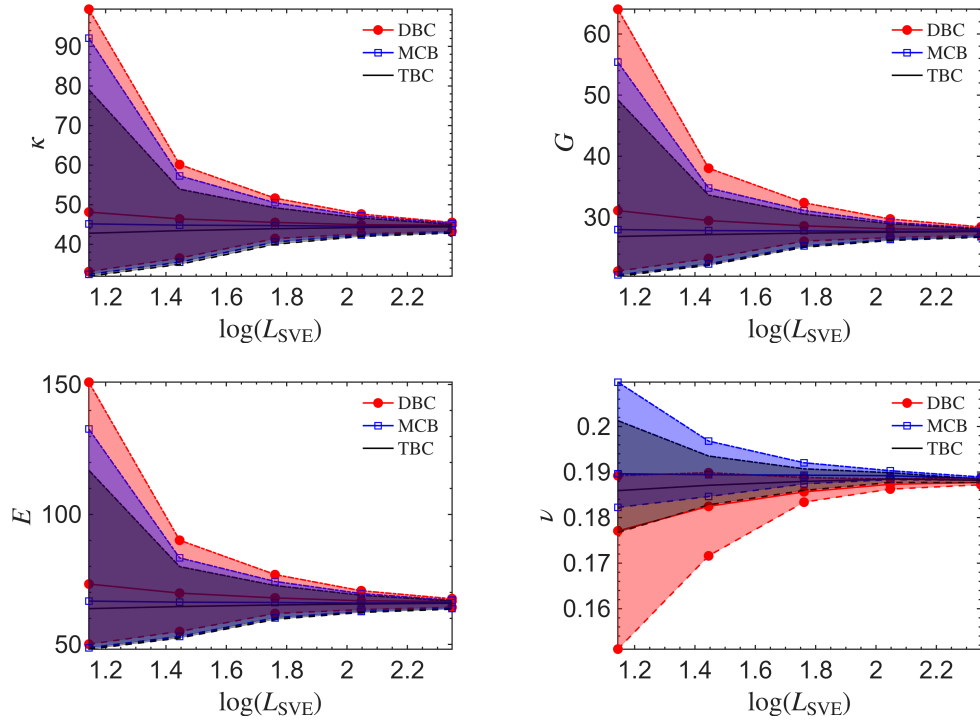


Figure 3.8: Apparent elastic moduli as functions of SVE size for displacement (DBC), mixed (MCB), and traction (TBC) boundary conditions. (a) Bulk modulus κ , (b) shear modulus G , (c) Young's modulus E , and (d) Poisson's ratio ν .

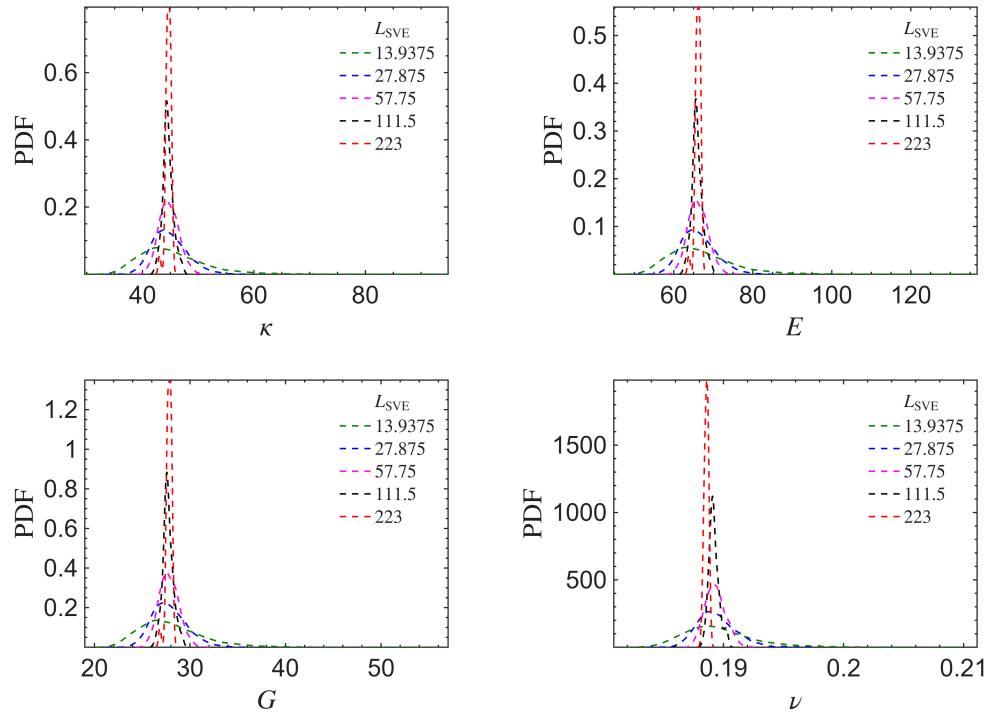


Figure 3.9: Probability density functions of apparent moduli under mixed boundary conditions (MBC). (a) Bulk modulus κ , (b) Young's modulus E , (c) Shear modulus G , and (d) Poisson's ratio ν .

Table 3.3: Homogenized elastic moduli and ν at the largest SVE size for displacement (DBC), mixed (MBC), and traction (TBC) boundary conditions.

Field					RVE size			p		
	DBC	MBC	TBC	MFM	DBC	MBC	TBC	DBC	MBC	TBC
v_f	0.2318				650.9	633.9	635.2	0.856	0.864	0.864
κ	44.81	44.65	44.42	41.74	245.9	240.1	247.0	0.921	0.906	0.844
μ	27.59	27.40	27.34	25.93	236.8	228.5	233.3	0.937	0.896	0.845
E	65.77	65.38	65.18	63.98	239.0	231.5	236.8	0.933	0.899	0.844
ν	0.1922	0.1932	0.1923	0.2335	27.61	23.37	20.82	0.901	1.030	0.969

At the largest SVE size, the apparent moduli in Table 3.3 show minimal sensitivity to boundary condition. DBC and TBC remain the theoretical bounds, yet their separation is small, and MBC aligns closely between them. This agreement indicates that constraint effects have largely diminished and that the response has reached a representative, boundary-independent state as demonstrated in Figures 3.8, and 3.9. This table includes the earlier comparison between the FEM and MFM estimates, which show consistent agreement with the converged FEM results. The RVE size represents the characteristic length at which the apparent property becomes effectively size-independent. The exponent p quantifies the rate of statistical convergence, describing how the coefficient of variation (COV) decreases with increasing SVE size, $\text{COV} \sim L_{\text{SVE}}^p$. When the COV reaches a prescribed threshold (*e.g.*, 0.01), the corresponding SVE dimension is taken as the RVE size.

3.3.3 Thermal Response

Mismatch in thermal expansion between phases generates internal stresses that drive the redistribution of stresses in each phase during cooling. Both (b_i and b_m) follow the expected boundary-condition hierarchy, with DBC giving the largest magnitudes,

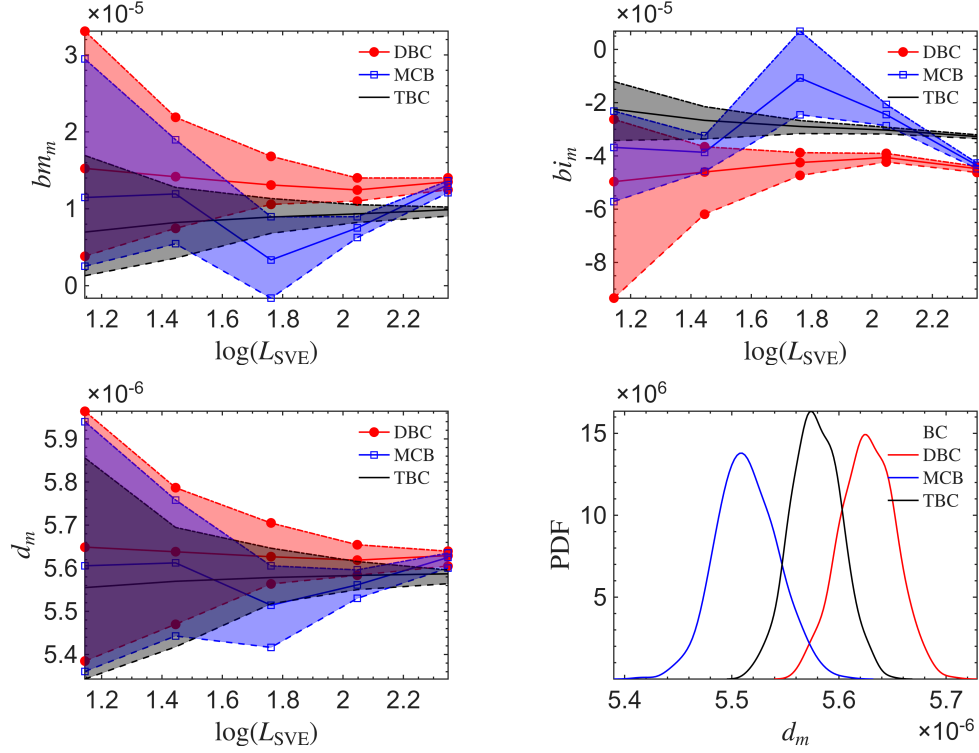


Figure 3.10: Thermal coupling behavior across SVE sizes and boundary conditions. (a) Matrix coefficient d_m , (b) inclusion correction b_i , and (c) matrix correction b_m as functions of L_{SVE} for DBC, MBC, and TBC. (d) Probability density functions of d_m at $L_{\text{SVE}} = 0.25$ illustrate boundary-condition-dependent mean shifts.

TBC the smallest, and MBC lying between. The effective thermal strain (d^*) shows similar convergence trends. DBC and TBC responses define the upper and lower bounds of the apparent properties, respectively, though the MBC response does not always lie between them. The roles of these boundary conditions are reversed for the stiffness-based quantities (Fig. 3.10).

The signs remain consistent with $b_i < 0$ and $b_m > 0$, indicating tensile inclusions and a compressive matrix under cooling. The effective thermal strain d^* varies little with size, confirming that the macroscopic free contraction of the composite is matrix-dominated. At larger L_{SVE} , fluctuations in inclusion and matrix thermal stresses diminish, suggesting that stress exchange and cancellation between phases increasingly govern the effective response.

TBC yields the most consistent trends among the three boundary conditions. DBC performs similarly overall but exhibits noticeably higher variation at intermediate and small L_{SVE} . MBC shows irregular behavior for b_i and b_m at intermediate sizes, where the mean values fluctuate rather than decay smoothly. A contributing factor is that MBC does not fully satisfy the Hill–Mandel energy equivalence condition Böhm (1998), which can introduce residual bias in intermediate SVE sizes.

The values in Table 3.4 summarize the thermal behavior at the largest SVE size. This table also provides the previously noted comparison between the FEM and MFM results, showing that the analytical estimates remain consistent with the converged numerical response. The effective CTE (d^*) shows minimal variation across boundary conditions, indicating that the macroscopic free contraction of the composite is stable and largely matrix controlled. The overall thermal stress offset (c^*) becomes slightly less compressive from DBC to TBC, showing that traction boundaries permit greater relaxation during cooling. The inclusion and matrix coefficients (a_i and a_m) maintain opposite signs, consistent with the thermal expansion mismatch that drives tensile inclusions and a compressive matrix.

Table 3.4: Homogenized thermal coupling quantities at the largest SVE size for displacement (DBC), mixed (MBC), and traction (TBC) boundary conditions. All values in the first four columns are scaled by 10^{-6} .

Field	$(\times 10^{-6})$				RVE size			Exponent p		
	DBC	MBC	TBC	MFM	DBC	MBC	TBC	DBC	MBC	TBC
d^*	5.634	5.625	5.587	5.544	21.36	21.92	18.21	0.862	0.856	0.839
b_i	-46.05	-43.55	-32.71	-20.31	220.6	1319	198.1	0.953	0.619	0.941
b_m	15.251	11.466	6.970	6.195	674.1	1518	629.9	0.845	0.798	0.888
c^*	-505.1	-502.3	-496.4	-462.8	273.6	273.3	279.5	0.923	0.902	0.846
a_i	4.688	4.710	4.757	5.024	60.12	53.84	43.53	1.035	0.946	0.810
a_m	-1.415	-1.422	-1.436	-1.516	809.5	778.8	763.6	0.854	0.866	0.879

Table 3.4 shows that although the thermal coupling quantities approach convergence with increasing SVE size, boundary conditions continue to exert a measurable influence even at the largest L_{SVE} . The corresponding RVE sizes and p values show

that select quantities have stabilized with respect to SVE size within a given boundary condition scheme. However, small differences among boundary conditions persist, suggesting that complete boundary-independence has not yet been reached even at the largest L_{SVE} . Most notably, b_i shows the most significant discrepancy in both RVE size and p when comparing MBC with DBC and TBC.

3.4 Nonlinear Results

Two loading conditions are considered to evaluate the influence of residual thermal fields: a mechanical-only case without eigenstrain and a thermomechanical case incorporating the cooled residual state. Each realization follows the same sequence of loading stages, beginning with elastic deformation, followed by damage initiation, peak stress σ_m , post-peak softening, stress relaxation to zero, and the final equilibrium state. Key quantities such as σ_m , the corresponding strain ε_m , and the strain at stress relaxation ε_0 provide a consistent basis for comparing mechanical and thermomechanical responses.

3.4.1 Mechanical

The mechanical-only simulations, without residual thermal effects, serve as the reference for subsequent comparisons. The progression through each representative stage is illustrated for a single realization at $L_{\text{SVE}} = 0.223$ mm (Img 15, Sub 1) in Figures 3.11–3.13.

Figure 3.11 reports the corresponding macroscopic stress–strain trace with numbered markers (1)–(6) that index consistent points along the loading path: (1) initial undamaged state, (2) damage onset, (3) peak stress, (4) intermediate softening, (5) stress relaxation, and (6) final failure configuration. The initial damaged, maximum, and stress-relaxed (zero-stress) stages are particularly important and are decorated with subscripts i , m , and o in subsequent discussions. These indices

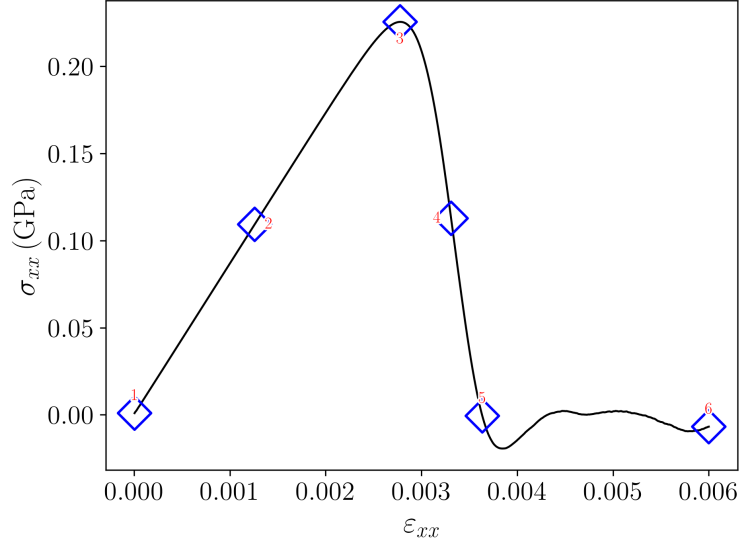


Figure 3.11: Macroscopic σ_{xx} – ϵ_{xx} trace for one realization at $L_{\text{SVE}} = 0.223$ mm with markers (1)–(6) defining the stages of loading evolution.

are reused in Figures 3.12 and 3.13 for the same domain to show the evolution of the damage field and the corresponding hydrostatic stress distributions along the loading path.

For the largest SVE size ($L_{\text{SVE}} = 0.223$ mm), 3.12 illustrates the evolution of damage under mechanical loading. At the start of loading (1), the microstructure is undeformed and stress-free. With increasing strain (2–3), damage initiates within the matrix as small, isolated nuclei form at local stress concentrations between inclusions. Beyond the peak load (4–6), diffuse cracks branch and merge throughout the matrix, producing a connected damage pattern and gradual stiffness degradation. The local hydrostatic-stress maps in Figure 3.13 remain tensile at all stages. The field is spatially heterogeneous, with higher magnitudes in the inclusions and lower in the matrix. Magnitudes increase with applied strain up to the peak load and decrease during softening. The macroscopic stress–strain overlays for both loading directions and SVE sizes are shown in Figure 3.14.

Smaller SVEs show higher apparent peak stresses with greater variability. Many realizations display oscillatory post-peak drops, reflecting progressive fragmentation

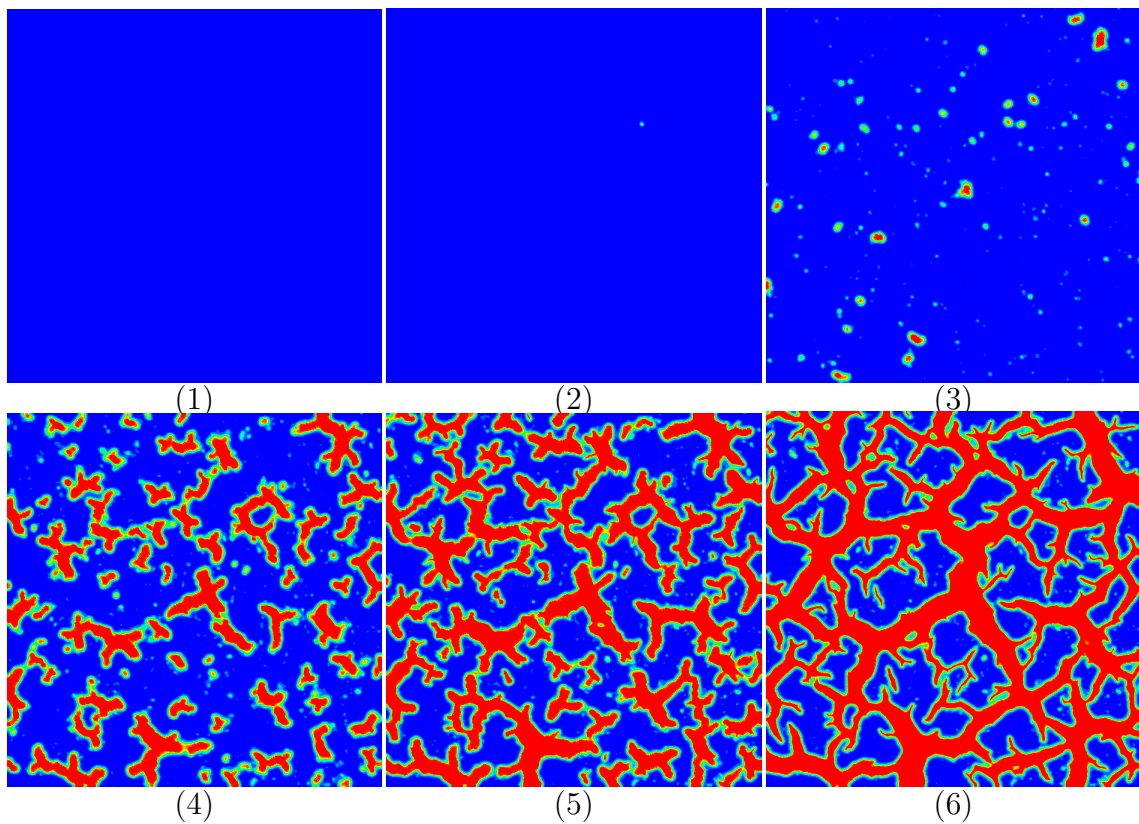


Figure 3.12: Damage evolution at stages (1)–(6) under mechanical loading only (thermal effects omitted). Red is fully damaged, blue undamaged.

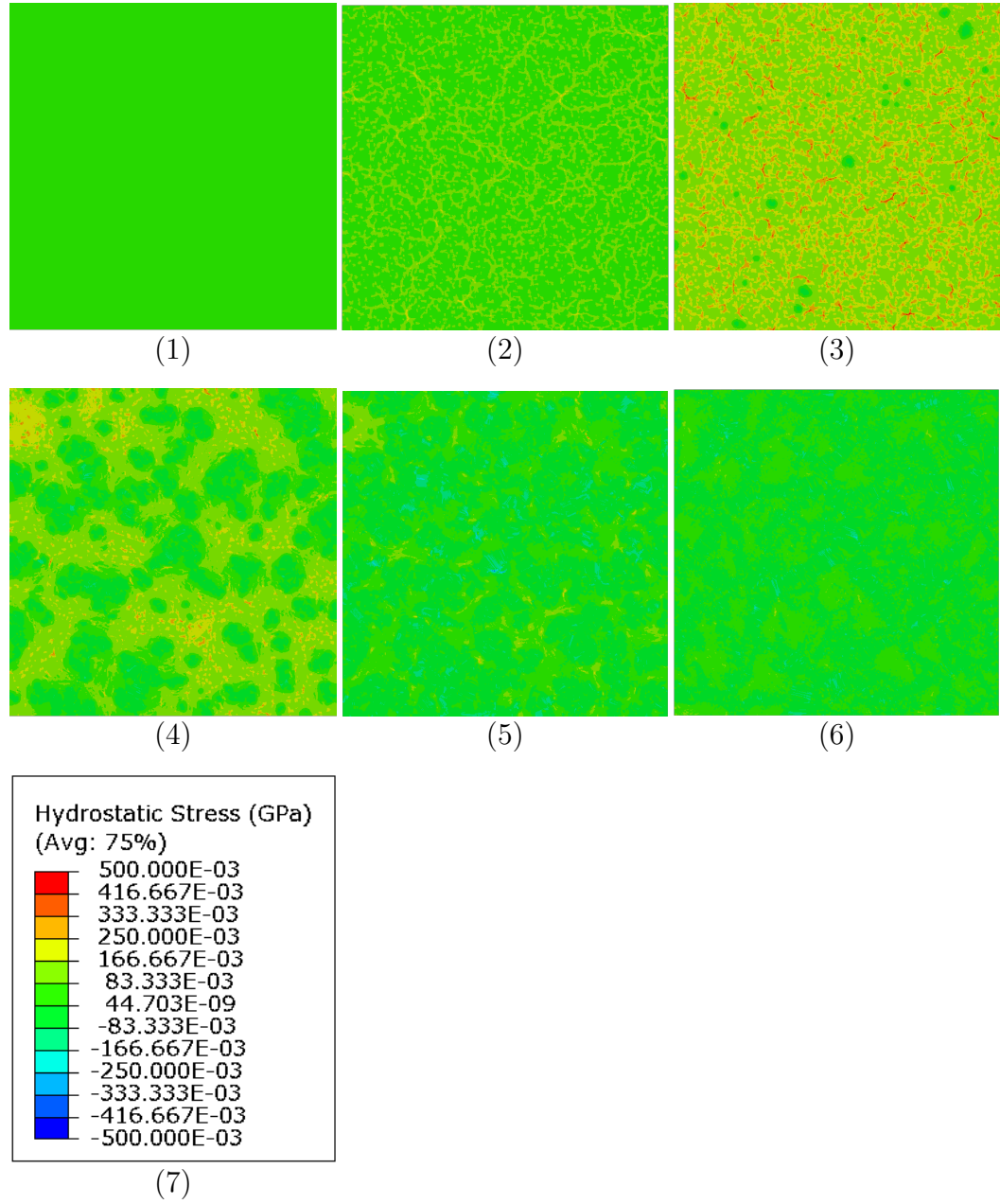


Figure 3.13: Evolution of hydrostatic stress (GPa) at stages (1)–(6) under mechanical loading only (thermal effects omitted). The shared legend (7) provides the corresponding hydrostatic stress scale in GPa.

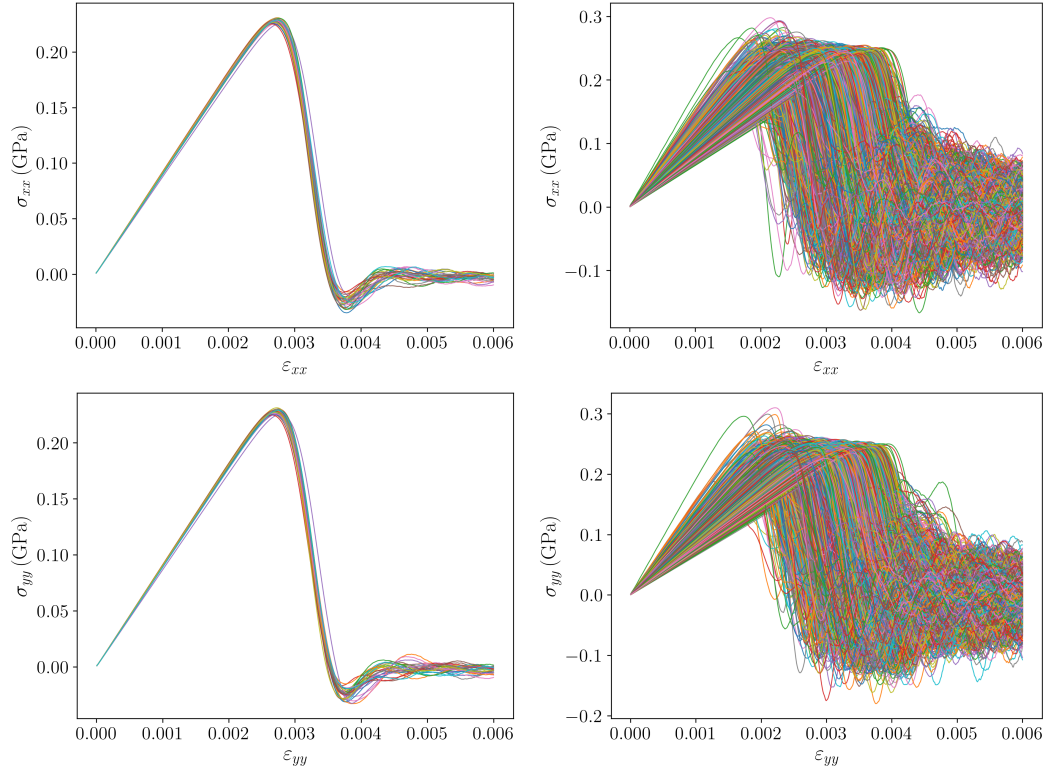


Figure 3.14: Non-thermal stress-strain overlays. Top: σ_{xx} ; bottom: σ_{yy} . Left: $L_{\text{SVE}} = 0.223$ mm; right: $L_{\text{SVE}} = 0.0139$ mm.

as isolated cracking events dominate the response. Larger SVEs exhibit tightly clustered curves with smoother softening. This result is consistent with statistical size effects, as larger SVEs sample more defects, averaging discrete failure events and smoothing the overall response. This size dependence aligns with previous SVE homogenization studies [Abedi et al. \(2022b\)](#); [Acton et al. \(2022\)](#), where stress-based quantities converge more slowly than strain-based ones.

No systematic differences are visible between the xx and yy loading directions, suggesting a close to isotropic response at the homogenized scale. The corresponding averaged quantities are summarized in Table 3.5, providing the reference state against which the influence of thermal fields will be interpreted. The anisotropy of nonlinear properties, reflected by the differences between the x - and y -direction values, will be further discussed in Section 3.5.

Table 3.5: Baseline results without thermal effects. Mean (μ) and standard deviation (σ) of peak stress σ_m , strain at peak ε_m , and first-zero strain ε_0 for the 11 and 22 tensor components at two SVE sizes.

L_{SVE} (mm)	Comp.	σ_m (GPa)		ε_m		ε_0	
		μ	σ	μ	σ	μ	σ
0.223	11	0.228	0.002	0.002 71	0.000 03	0.003 53	0.000 03
	22	0.228	0.002	0.002 72	0.000 03	0.003 54	0.000 03
0.0139	11	0.235	0.013	0.002 81	0.000 36	0.003 73	0.000 49
	22	0.235	0.013	0.002 81	0.000 36	0.003 74	0.000 49

3.4.2 Thermomechanical

The coupled thermo-mechanical case introduces residual thermal fields prior to mechanical loading. Deformation again proceeds through six representative stages that capture the evolution from the initial undamaged configuration to complete

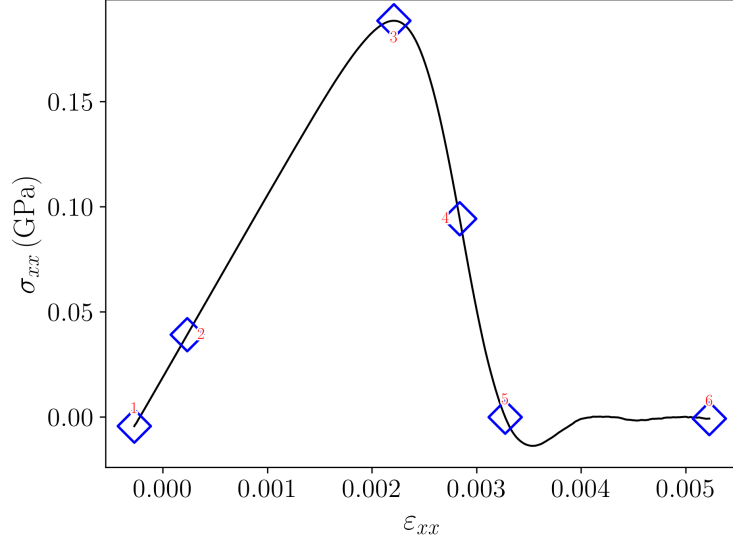


Figure 3.15: Macroscopic σ_{xx} - ε_{xx} trace for one realization at $L_{\text{SVE}} = 0.223$ mm with markers (1)–(6) defining the stages of loading evolution with thermal effects

failure. These stages are illustrated for a single realization at $L_{\text{SVE}} = 0.223$ mm (Img 15, Sub 1) in Figures 3.15–3.17.

Figure 3.15 reports the corresponding macroscopic stress–strain trace with numbered markers (1)–(6) that index consistent points along the same loading path above. These indices are reused in Figures 3.16 and 3.17 for the same domain to link the evolving microstructure and local responses to the overall stress–strain behavior. Figure 3.16 presents the spatial evolution of the damage field, while Figure 3.17 shows the corresponding hydrostatic stress distributions at each stage.

For the largest SVE size, the thermomechanical case begins from the cooled, pre-stressed state in Figure 3.15: at the onset (1) faint compressive patterns are already present in the matrix around inclusions. With continued loading (2–3), the first nonzero damage appears at similar sites as in the mechanical case. In the later stages (4–6), damage coalesces into a connected network as before, but the branches appear finer and the final damaged area is somewhat reduced.

Referring to Figure 3.17, the effects of residual thermal stress are visible in the initial stage (1): the matrix in compression and the inclusions in tension. As external

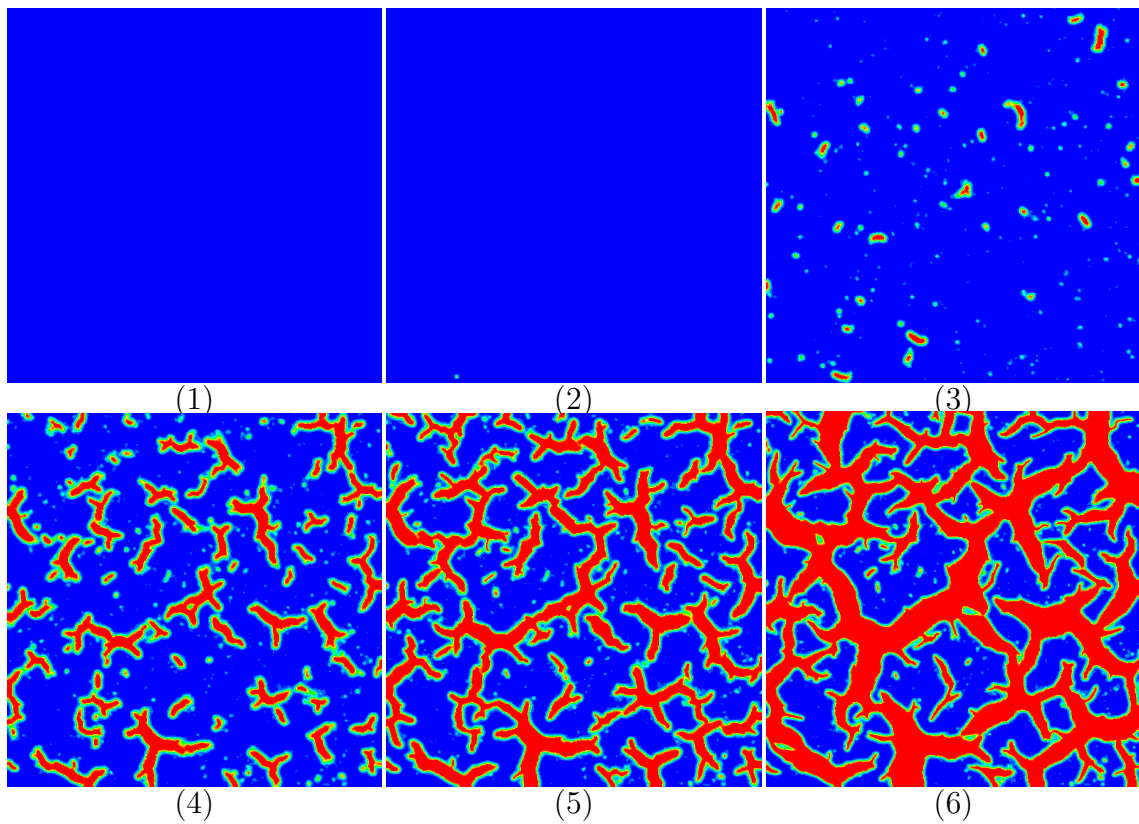


Figure 3.16: Damage evolution at stages (1)–(6) with thermal effects. Red is fully damaged, blue undamaged.

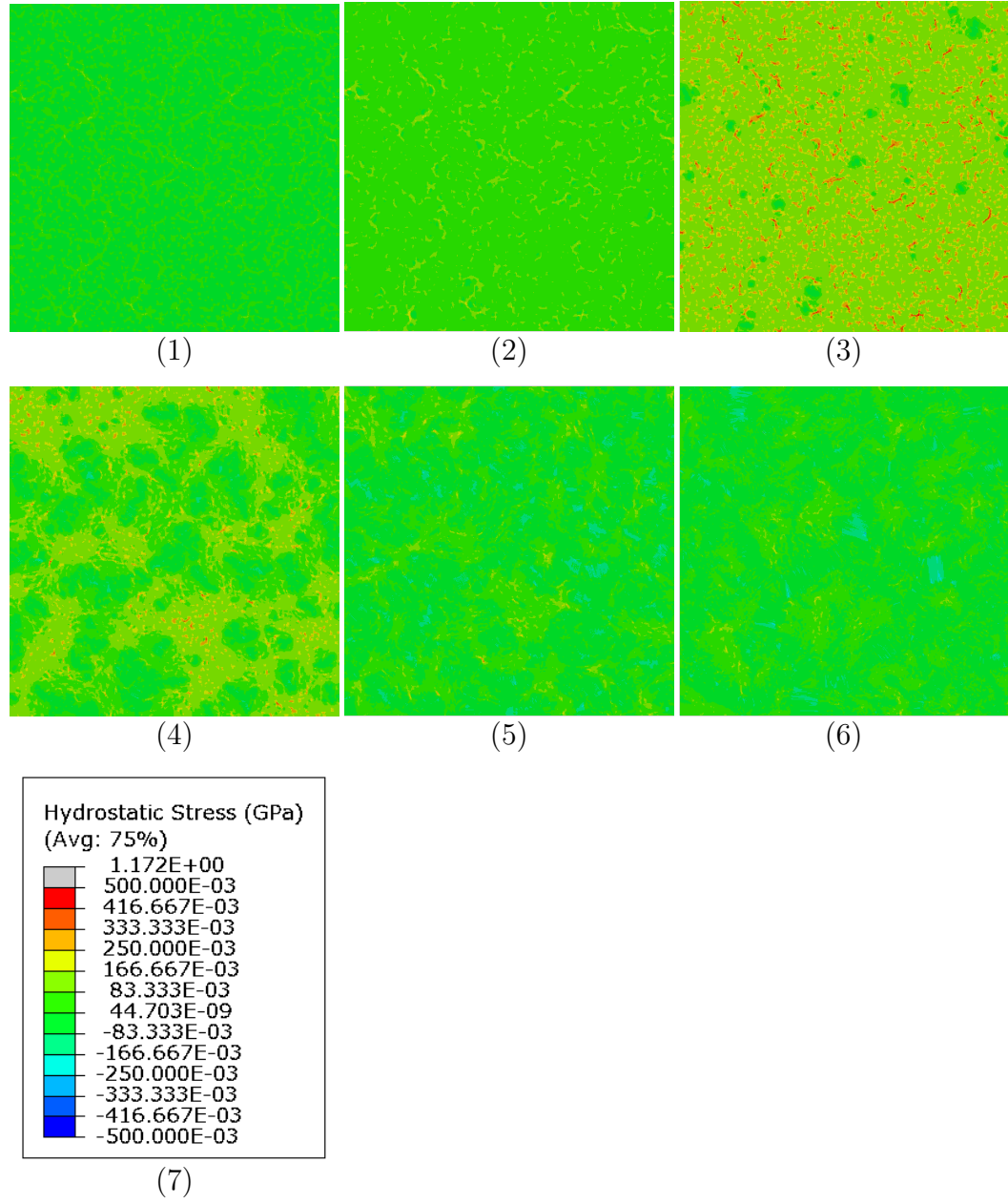


Figure 3.17: Hydrostatic stress evolution (units: GPa) at stages (1)–(6) including thermal effects. The shared color legend (7) reports the hydrostatic stress magnitude in GPa.

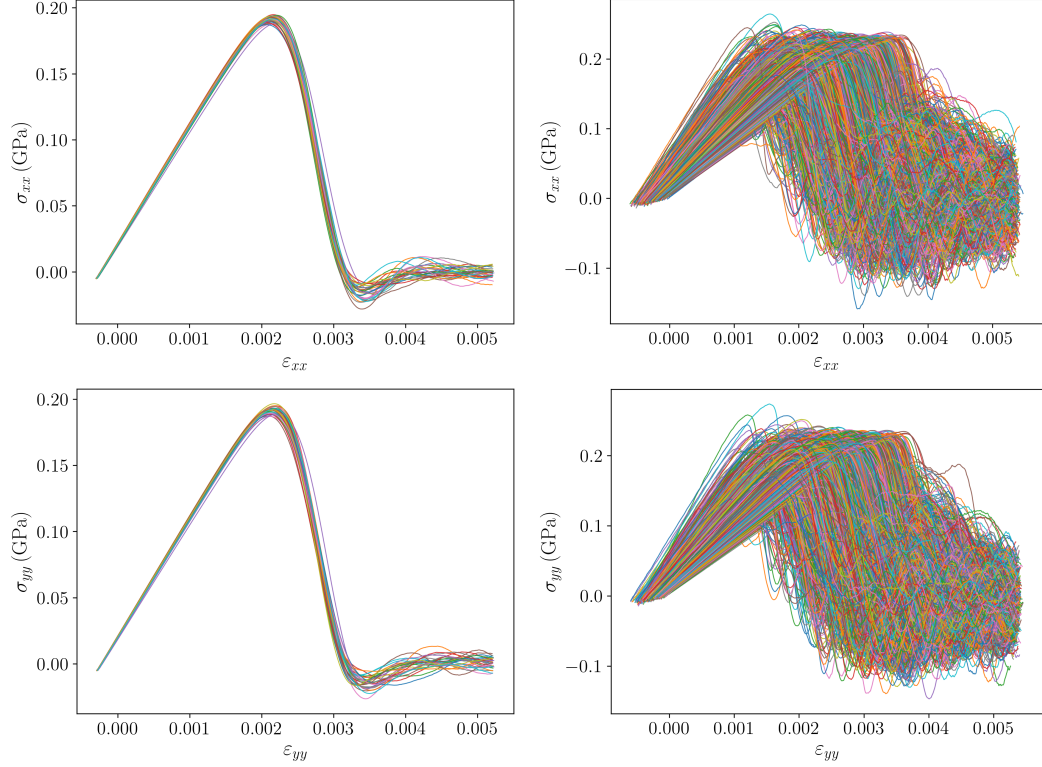


Figure 3.18: Thermal stress–strain overlays. Top: σ_{xx} ; bottom: σ_{yy} . Left: $L_{\text{SVE}} = 0.223$ mm; right: $L_{\text{SVE}} = 0.0139$ mm.

loading is applied (2–3), the overall tension increases and the initial compressive regions begin to be pulled into tension. As in the mechanical-only case, stresses relax after stage (3)

Macroscopic stress–strain overlays for both loading directions and SVE sizes are shown in Figure 3.18. For the larger SVE, the curves remain closely grouped, showing nearly identical loading and softening paths across realizations, though the overall peak stress is reduced relative to the no thermal case. The overlays display a wider range of curve shapes at the smaller SVE size. Some realizations show gradual, extended softening before complete relaxation, while others exhibit sharp post-peak drops. This increased scatter reflects the influence of residual thermal stresses, which interact with local heterogeneity to alter both the strength and the sequence of microscopic failure events.

As in the mechanical-only case, no systematic differences appear between the xx and yy responses, again close to an isotropic response at the homogenized scale. The reduction in peak stress, together with the broader post-peak variability observed in Figure 3.18, is reflected quantitatively in the averaged metrics of Table 3.6.

Table 3.6: Results with thermal effects. Each value pair gives the mean (μ) and standard deviation (σ) of the peak stress σ_m , strain at peak ε_m , and first-zero strain ε_0 for the 11 and 22 tensor components at two SVE sizes.

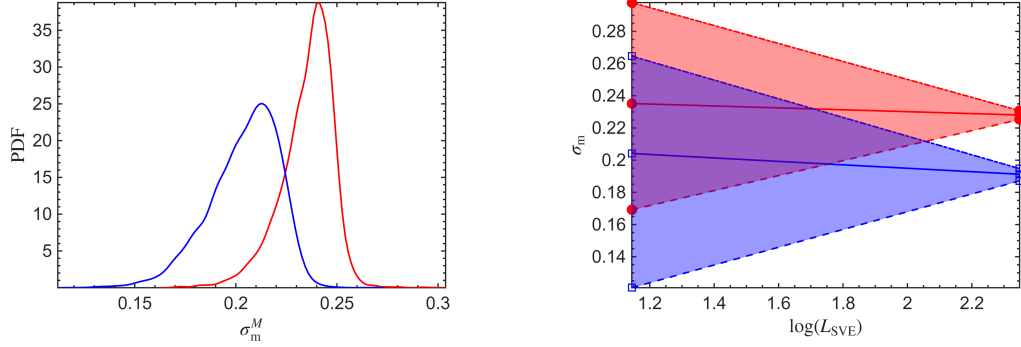
L_{SVE} (mm)	Comp.	σ_m (GPa)		ε_m		ε_0	
		μ	σ	μ	σ	μ	σ
0.223	11	0.191	0.002	0.002 14	0.000 03	0.003 15	0.000 04
	22	0.191	0.002	0.002 15	0.000 03	0.003 17	0.000 05
0.0139	11	0.204	0.017	0.002 31	0.000 41	0.003 52	0.000 57
	22	0.204	0.017	0.002 32	0.000 41	0.003 54	0.000 57

3.4.3 Comparison of Mechanical and Thermomechanical

The following comparison examines the thermomechanical response at two representative loading stages: peak stress (3) and stress relaxation (5). The analysis considers the macroscopic stress σ_m and phase-averaged damage $\bar{\phi}_I, \bar{\phi}_M$ at the first stage, and the residual strain ε_0 , phase-averaged damage, and dissipated energy ψ_d^0 at the second stage.

Peak Stress

At this stage, the macroscopic response shows that when thermal residual fields are present, the overall strength σ_m decreases and occurs at smaller strains relative to the mechanical-only case. At the smaller SVE ($L_{\text{SVE}} = 0.0139$ mm), the thermomechanical case exhibits a lower mean stress σ_m and a broader distribution, indicating greater variability among realizations (Fig. 3.19a). At the larger SVE



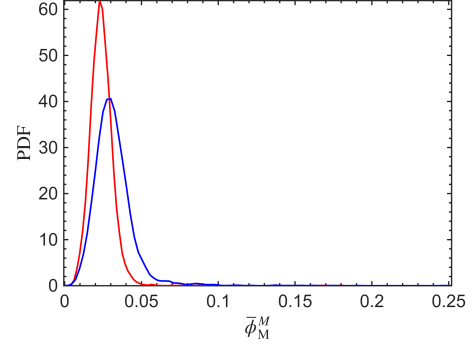
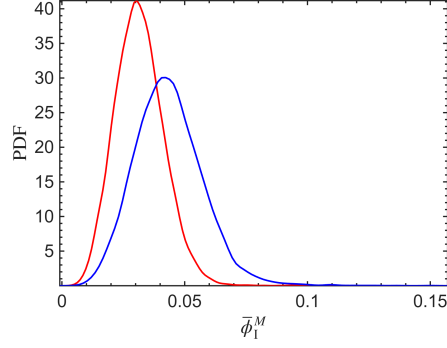
(a) σ_{xx} probability density at $L_{SVE} = 0.0139$ mm (b) σ_{yy} size-effect envelope across L_{SVE}

Figure 3.19: Peak-stress stage comparison between thermomechanical (blue) and mechanical-only (red) cases. (a) Probability density of σ_{xx} at $L_{SVE} = 0.0139$ mm. (b) Size-effect envelope of σ_{yy} across L_{SVE} , showing the evolution of effective strength with domain size.

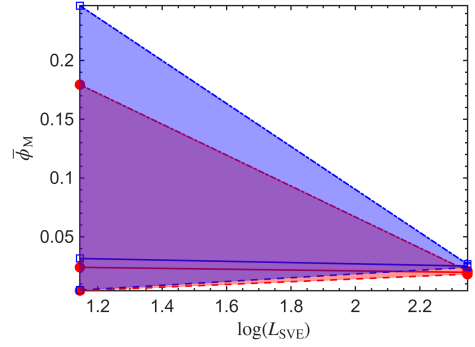
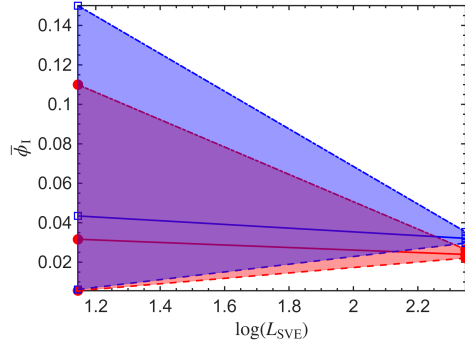
($L_{SVE} = 0.223$ mm), the size-effect envelope of σ_m shows a comparable reduction in mean values and narrower overall spread (Fig. 3.19b). The stress responses in both directions follow the same trend, with the reduction in mean values under thermal loading remaining consistent across SVE sizes.

Although the macroscopic response remains isotropic, the underlying phase stresses need not be. Thermal eigenstrains create initial tensile stresses in the inclusions and compressive stresses in the matrix, which change how each phase develops damage during loading. As shown in Figures 3.20a–b, both phase-averaged damage measures, $\bar{\phi}_I$ and $\bar{\phi}_M$, are higher under thermomechanical loading. For the smaller SVE, the PDFs show greater damage values and broader spreads, meaning that more realizations experience higher levels of damage. The corresponding size-effect envelopes in Figures 3.20c–d show that this difference between thermal and mechanical cases remains across all L_{SVE} . These higher values of $\bar{\phi}_I$ and $\bar{\phi}_M$ at maximum applied stress are observed when residual stresses are present before loading.

Variability with SVE size was quantified using the coefficients of variation (COV) and fitted scaling $COV = AL_{SVE}^{-p}$; the results and corresponding L_{RVE} are listed



(a) $\bar{\phi}_I$ probability density at $L_{SVE} = 0.0139$ mm (b) $\bar{\phi}_M$ probability density at $L_{SVE} = 0.0139$ mm



(c) $\bar{\phi}_I$ size-effect envelope across L_{SVE}

(d) $\bar{\phi}_M$ size-effect envelope across L_{SVE}

Figure 3.20: Peak-stress stage comparison between thermomechanical (blue) and mechanical-only (red) cases. (a,b) Probability density distributions of the phase-averaged damage measures $\bar{\phi}_I$ and $\bar{\phi}_M$ at $L_{SVE} = 0.0139$ mm. (c,d)

in Table 3.7. For macrostresses, variability decreases with increasing SVE size in both loading cases, but the thermomechanical case maintains a higher COV at all sizes. At the largest SVE, COV values of about 0.011–0.013 indicate that statistical convergence has not yet been fully achieved, with L_{RVE} roughly twice that of the mechanical case. The fitted exponents $p \approx 0.7$ –0.72 are consistent across cases, showing a relatively slow convergence of homogenized properties. For phase-averaged damage, both phases follow similar trends with $p \approx 0.8$ –0.85, indicating comparable decay rates with size. The matrix shows a larger prefactor (A) and higher small-SVE dispersion under thermal loading, reflecting more local heterogeneity. Despite contraction with size, neither phase reaches a plateau in variability, suggesting that a fully representative volume has not yet been attained.

Table 3.7: COV ranges at small and large SVE, fitted scaling parameters in $\text{COV} = A L_{\text{SVE}}^{-p}$, and normalized RVE length reported as L_{RVE}^* .

Quantity	COV		Scaling (A, p)		L_{RVE}^*	
	Mech.	Therm.	A	p	Mech.	Therm.
σ_{xx}^{M}	0.0547–0.0075	0.0841–0.0113	6×10^{-6}	0.72	10.5	19.4
σ_{yy}^{M}	0.0550–0.0078	0.0845–0.0126	7×10^{-6}	0.70	10.5	19.4
$\bar{\phi}_{\text{I}}$	0.312–0.035	0.317–0.033	1.1×10^{-4}	0.80	47.1	57.9
$\bar{\phi}_{\text{M}}$	0.337–0.032	0.419–0.028	8.2×10^{-5}	0.85	48.0	49.1

Stress relaxation

The subsequent stage in the load evolution marks the onset of stress relaxation and captures the residual strain retained after unloading. The probability density functions in Figs. 3.21a–b quantify this residual strain across realizations. For the smaller SVE ($L_{\text{SVE}} = 0.0139$ mm), the mechanical and thermomechanical curves nearly coincide, showing similar recovery and minimal local variability. At the larger SVE ($L_{\text{SVE}} = 0.223$ mm), the distributions separate, suggesting that thermal residual fields introduce greater spatial contrast. This difference reflects the persistence of

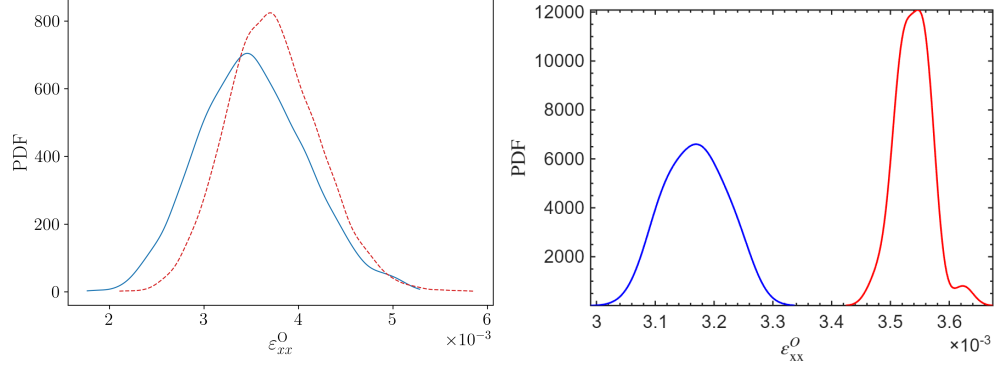


Figure 3.21: Residual strain distributions ε_{xx}^O ($L_{\text{SVE}} = 0.0139$ mm) and ε_{xx}^O ($L_{\text{SVE}} = 0.223$ mm) at the stress-relaxation stage (5). Blue curves correspond to thermomechanical cases, and red curves to mechanical-only cases.

internal mismatch strains formed during cooling. As a result, larger domains retain a more uneven and heterogeneous residual strain field.

We again examine the phase-averaged damage in the inclusion ($\bar{\phi}_I$) and matrix ($\bar{\phi}_M$) at the stress-relaxation stage. The thermomechanical case shows reduced damage compared with peak load (Stage 3), most notably in the matrix phase. At the smaller SVE ($L_{\text{SVE}} = 0.0139$ mm), the thermal and mechanical distributions are nearly coincident. At the larger SVE ($L_{\text{SVE}} = 0.223$ mm), the thermomechanical case exhibits lower $\bar{\phi}_M$ and a smaller decrease in $\bar{\phi}_I$.

This behavior contrasts with the increase observed at peak load. The residual field that previously enhanced local tension now acts oppositely, as the matrix remains under compression during unloading. This compressive state makes the matrix more resistant to further damage. The dissipated energy ψ_d^O provides a global measure of how much irreversible deformation remains once macroscopic stresses have relaxed. The lower dissipation in energy is best reflected in 3.23b the largest ($L_{\text{SVE}} = 0.223$ mm).

Variability trends at the stress-relaxation stage show how unloading alters the statistical response across SVE sizes. COV is fit in the form $\text{COV} = A, L_{\text{SVE}}^{-p}$, with the corresponding L_{RVE} , are summarized in Table 3.8. Compared with peak load, overall variability decreases, indicating that residual compression suppresses much

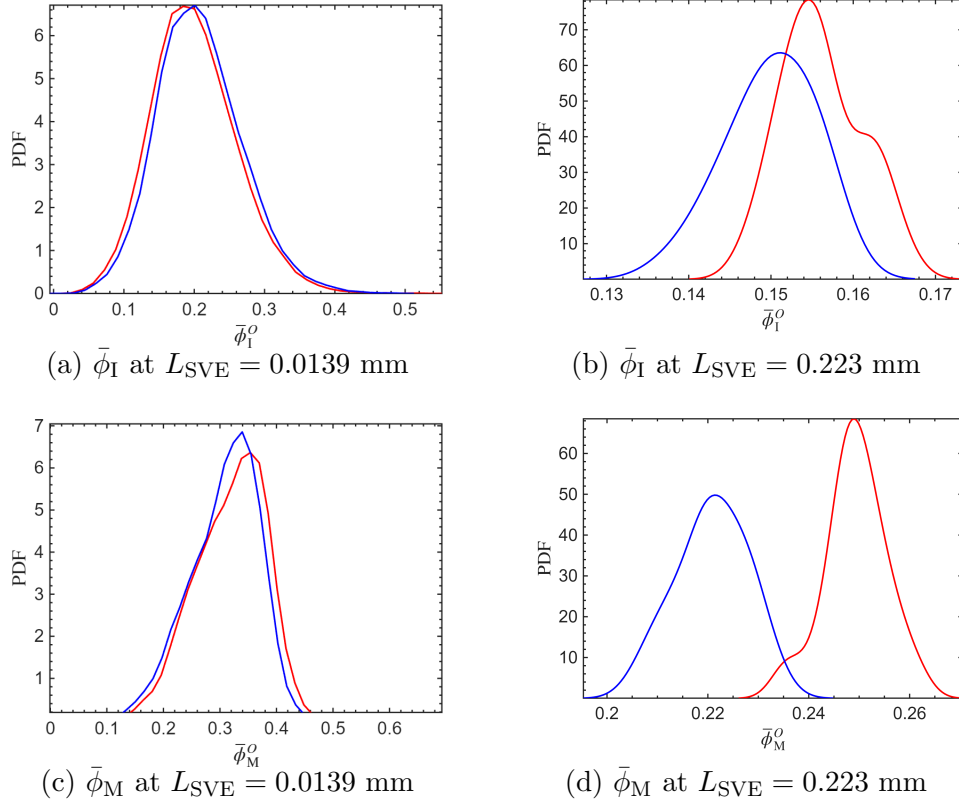


Figure 3.22: Phase-averaged damage probability distributions at the stress-relaxation stage (5). Blue curves correspond to thermomechanical cases, and red curves to mechanical-only cases. Panels (a,b) show inclusion-averaged damage ($\bar{\phi}_I$), while panels (c,d) show matrix-averaged damage ($\bar{\phi}_M$). Results are shown for small ($L_{\text{SVE}} = 0.0139$ mm) and large ($L_{\text{SVE}} = 0.223$ mm) SVEs, respectively.

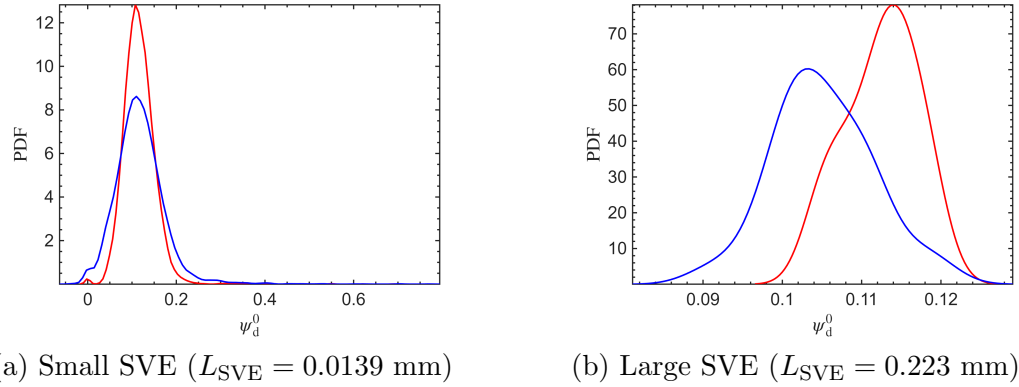


Figure 3.23: Dissipated energy density ψ_d^0 at the stress-relaxation stage (5). Blue: thermomechanical case; red: mechanical-only case. Probability density distributions are shown for small and large SVEs.

of the earlier scatter. Thermal loading, however, maintains a higher baseline COV, particularly for quantities sensitive to local relaxation such as phase damage and dissipated energy. For $\bar{\phi}_I$ and $\bar{\phi}_M$, small-SVE COVs rise under thermal conditions (from ~ 0.02 – 0.03 to ~ 0.03 – 0.04), with L_{RVE} increasing from about 2.5–3 to roughly 3.5–4. The fitted exponents ($p \approx 0.9$) remain similar between cases, while larger (A) under thermal loading indicate stronger local heterogeneity. The dissipated energy ψ_d follows the same trend, showing slightly higher variability and marginally larger L_{RVE} in the thermomechanical case.

Table 3.8: COV ranges at small and large SVE, fitted scaling parameters in $\text{COV} = A L_{\text{SVE}}^{-p}$, and normalized RVE length reported as L_{RVE}^* for the stress-relaxation stage.

Quantity	COV (small $\rightarrow$ large)		Scaling (A, p)		L_{RVE}^*	
	Mech.	Therm.	A	p	Mech.	Therm.
σ_m	0.021–0.018	0.029–0.020	2×10^{-6}	2.0	1.37	1.70
$\bar{\phi}_I$	0.029–0.036	0.034–0.049	6×10^{-5}	0.96	3.22	3.53
$\bar{\phi}_M$	0.021–0.020	0.028–0.032	4×10^{-5}	0.89	2.58	3.15
ψ_d	0.045–0.090	0.044–0.073	8.9×10^{-3}	1.02	7.49	9.06

3.5 Anisotropy Results

Directional anisotropy quantifies differences in the composite’s response along orthogonal axes. Following [Abedi et al. \(2023\)](#), for each apparent property f evaluated in the x and y directions, the mean and normalized anisotropy measures are defined as

$$A^f := \left| \frac{f_x - f_y}{f} \right|, \quad (3.10)$$

where f represents the mean of the two directional components. An isotropic response corresponds to $A^f = 0$, while finite values indicate the magnitude of directional bias for the property f .

For elastic fields, the Ranganathan–Ostoja–Starzewski index A_{RO} [Abedi et al. \(2022b\)](#) provides another measure of anisotropy derived from the bulk and shear moduli, derived from the stiffness and compliance tensors. The variation of A^f and A_{RO} with L_{SVE} is used to evaluate how directional bias evolves and whether the response tends toward isotropy at larger scales.

3.5.1 Elastic Anisotropy

Figure 3.24 shows the evolution of elastic anisotropy with SVE size under DBC, MBC, and TBC. The in-plane stiffness anisotropy (a) $A^{C_{xy}}$, based on the directional difference between C_{11} and C_{22} . The Ranganathan–Ostoja–Starzewski index (b) A_{RO} , as explained above.

Both measures follow the same general trend. Anisotropy is largest at the smallest L_{SVE} , with MBC giving the highest values, followed by DBC and TBC. The differences between boundary conditions decrease steadily as L_{SVE} increases, and by $L_{\text{SVE}} \approx 0.125$ – 0.25 , the curves approach zero. At these sizes, the effective stiffness becomes nearly isotropic.

The magnitudes of $A^{C_{xy}}$ are higher than those of A_{RO} , as expected. $A^{C_{xy}}$ isolates direct contrasts between stiffness components, while A_{RO} represents the overall tensor-level anisotropy. This behavior is consistent with the thermal results, where fixed-axis or component-wise measures yield larger anisotropy values than tensor quantities, as discussed in subsequent sections.

3.5.2 Thermal Anisotropy

Thermal mismatch between phases introduces directional bias in the local eigenstrain field. At small SVE sizes, clustered inclusions constrain matrix expansion unevenly, producing anisotropic strain and stress patterns that depend on the boundary condition. Anisotropy is highest at the smallest L_{SVE} , with DBC giving the most significant values, TBC the lowest, and MBC falling in between. Both measures

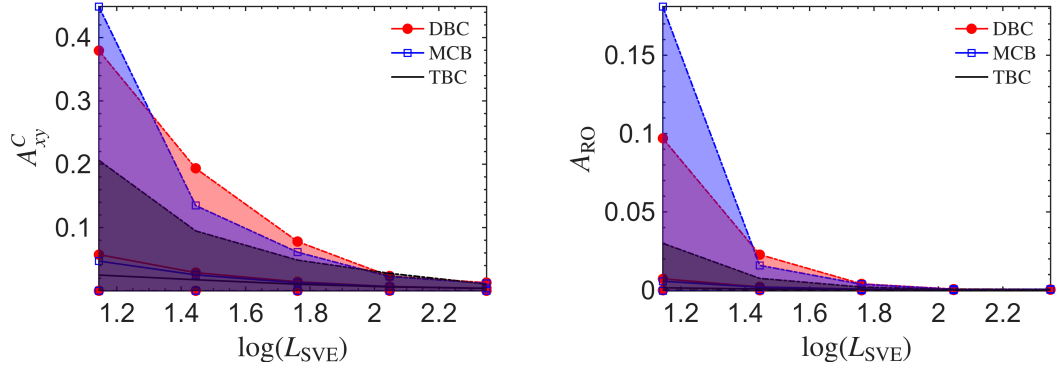


Figure 3.24: Elastic anisotropy versus SVE size under DBC, MCB, and TBC. (a) In-plane stiffness anisotropy $A^{C_{xy}}$ based on the directional difference between C_{11} and C_{22} . (b) Ranganathan–Ostoja–Starzewski index A_{RO} derived from the compliance tensor.

decrease rapidly as L_{SVE} increases, showing that the thermal response becomes more isotropic as local heterogeneities are averaged. The slightly higher A^{d*} values compared to A^{d*}_{xy} follow intuition: fixed-axis comparisons highlight the strongest directional contrasts, while the rotational measure smooths these variations over all orientations.

3.5.3 Fracture Anisotropy

Fracture anisotropy characterizes how directional stress response depends on microstructural variability and the presence of thermal residual fields. Figure 3.26 shows the anisotropy measure A^{σ_m} of phase-averaged stress at the peak-stress stage (3) for mechanical-only (red) and thermomechanical (blue) loading.

At small L_{SVE} , anisotropy is significantly higher in the thermomechanical case ($A^{\sigma_m} \approx 0.5$) than in the mechanical-only case ($A^{\sigma_m} \approx 0.3$). This increase reflects the influence of residual tension in the inclusions and compression in the matrix, which enhances directional stress differences. As L_{SVE} increases, the two curves converge rapidly toward zero, indicating that both loading conditions approach isotropic

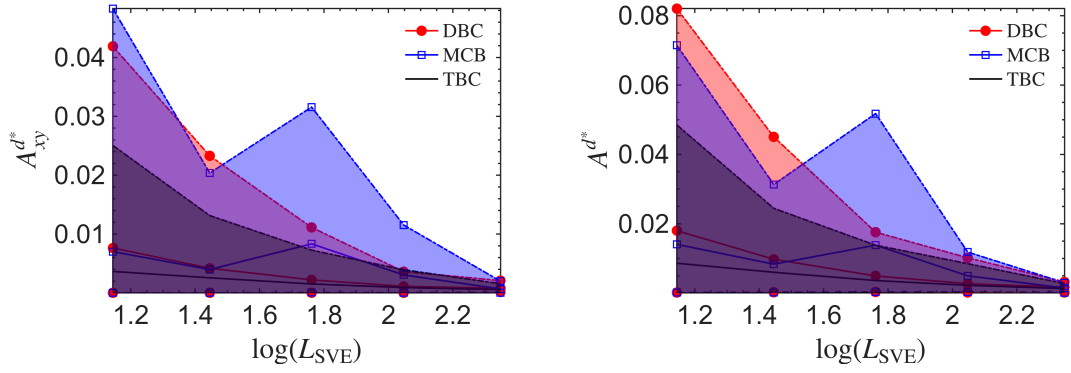


Figure 3.25: Thermal anisotropy versus SVE size. (a) Rotational anisotropy A_{xy}^f in the effective thermal strain d^* . (b) Directional anisotropy A_d^f along the principal x and y axes.

behavior at larger scales. The trend mirrors that of the elastic and thermal results, where boundary effects and local heterogeneity dominate at small scales but average out with increasing size.

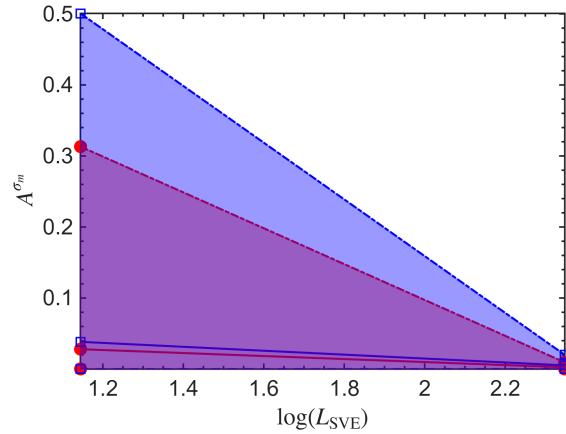


Figure 3.26: Fracture anisotropy at the peak-stress stage (3) under mechanical-only (red) and thermomechanical (blue) loading.

$A^{C_{xy}}$ shows the largest magnitudes across all L_{SVE} , followed by $A_{xy}^{d^*}$ and A^{d^*} , while A^{σ_m} remains smallest. The higher $A^{C_{xy}}$ values reflect the stronger directional response of the stiffness tensor to phase contrast and constraint. The effective thermal strain and maximum stress fields are less sensitive to these local variations,

giving lower anisotropy levels. At small L_{SVE} , microstructural variations increase these differences, while larger volumes lead to more uniform behavior. All indices decrease with increasing L_{SVE} , showing that anisotropy in stiffness, thermal, and stress responses weakens as the volume size grows.

Directional stresses corresponding to these stages are shown in Figure 3.27. For the mechanical-only case (Fig. 3.27a), σ_{xx} (black) and σ_{yy} (green) evolve nearly in parallel at all sizes, showing slight directional bias in the absence of thermal mismatch. When thermal fields are included (Fig. 3.27b), both components exhibit slightly lower peaks and a small offset between directions, most evident at the smallest L_{SVE} . This separation mirrors the anisotropy trends in Figure 3.26, confirming that residual stresses introduce a modest directional preference that fades with increasing size.

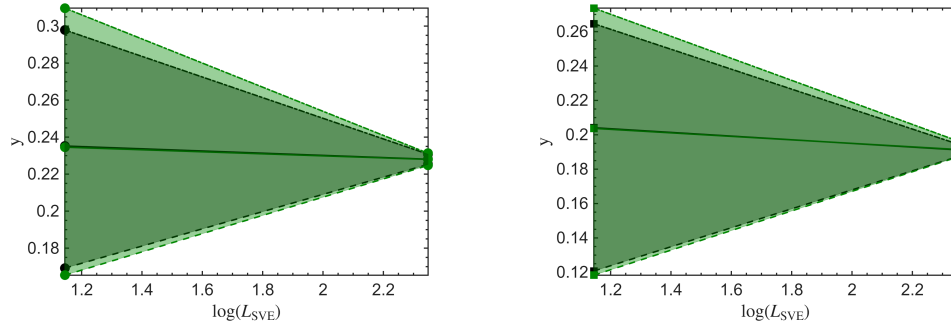


Figure 3.27: Directional stress components σ_{xx} (black) and σ_{yy} (green) at peak load. (a) Mechanical-only case. (b) Thermomechanical case.

3.6 Conclusion

The linear analyses show that boundary conditions and SVE size strongly influence the apparent elastic and thermal responses. Elastic moduli follow the expected hierarchy and converge toward boundary-independent values as domain size increases (Fig. 3.8; Table 3.3). Thermal coupling terms exhibit similar trends, with DBC producing the largest magnitudes and TBC the most stable (Fig. 3.10; Table 3.4). Among the thermal quantities, b_i converges most slowly, underscoring that inclusion

stress corrections remain sensitive to boundary effects even at large L_{SVE} . Although TBC provides the smoothest convergence, it idealizes a traction-free BC and may not fully capture the constraint of an interior SVE subjected to cooling. For this reason, MBC were selected for subsequent dynamic loading, as they better represent the mixed constraints experienced by interior domains despite minor irregularities at intermediate sizes.

The corresponding anisotropy measures confirm that this convergence reflects stabilization of the mean response and a reduction in directional bias. The Ranganathan–Ostoja–Starzewski index A_{RO} and the normalized anisotropy measure A_f decrease steadily with L_{SVE} , showing that apparent isotropy emerges alongside modulus convergence and boundary-condition independence. At larger SVE sizes, the absence of systematic xx/yy differences in the macroscopic overlays (Figs. 3.14 and 3.18) further supports this isotropic limit.

Building on the linear trends, the nonlinear analyses show how residual thermal fields alter strength, damage, and variability. Relative to the mechanical-only baseline (Table 3.5, Fig. 3.14), the thermomechanical case exhibits lower overall strength (Table 3.6; Fig. 3.18) but higher phase-averaged damage at comparable stages (Fig. 3.20). These differences arise from the residual stresses established during cooling, which compress the matrix and tension the inclusions. The pre-compressed matrix is therefore better prepared to accommodate subsequent tensile loading, weakening the peak response but improving resilience (Fig. 3.20).

The influence of this residual stress state extends to the energy response. Matrix compression offsets part of the stored elastic energy, reducing the work done by fracture (Fig. 3.23). As a result, less energy is irreversibly consumed through crack growth, leading to a more efficient release of strain energy during unloading. These observations connect the thermal-induced pre-stress directly to the apparent macroscopic dissipation behavior.

Directional effects remain visible at small scales. Thermal and fracture anisotropy both peak at the smallest L_{SVE} , reflecting how clustered inclusions and residual fields

create preferential stress paths. These contrasts diminish rapidly with increasing size, indicating that microstructural averaging and residual stress redistribution promote isotropy in both stiffness and damage evolution (Figs. 3.26–3.27).

Size effects remain important: smaller SVEs display greater variation, while larger SVEs show more uniform softening and reduced fragmentation (Figs. 3.14, 3.18, 3.19). This behavior reflects the increasing statistical representativeness of larger domains, where many microscopic cracking events average out to a smoother macroscopic response. Despite these phase-level asymmetries, the overall behavior remains effectively isotropic for mid to large SVEs. The simultaneous reduction in anisotropy and variability with increasing L_{SVE} underscores that both statistical and directional heterogeneity converge toward macroscale homogeneity.

Variability follows the same scaling law in both loading cases, $\text{COV} = A L_{\text{SVE}}^{-p}$, but thermal loading increases the baseline A without changing (p) (Tables 3.7 and 3.8), implying that larger L_{RVE}^* or additional realizations are required to achieve statistical convergence in strength and damage. For macrostress, this translates to roughly twice the representative length compared with the mechanical case, while phase damage and dissipated energy show similar exponents but higher small-SVE scatter under thermal conditions.

Taken together, the response at this scale remains highly complex, governed by local stress redistribution and microstructural heterogeneity. The absence of a fully converged RVE highlights that the observed variability and size dependence stem from intrinsic heterogeneity. Capturing this behavior requires linking local mechanisms to global averages, since microscale stress patterns ultimately shape the apparent macroscopic behavior.

At a broader level, these findings point toward a multiscale interpretation of residual effects. The material response is shaped by thermal contrast and the spatial scale at which interactions are resolved. The local heterogeneity dominates at fine resolution, revealing how stress redistributions and microcrack patterns emerge from inclusion–matrix mismatch. These local effects blend as the representative

domain grows, capturing the cumulative relaxation behavior that governs the apparent macroscopic response. In this sense, both material contrast and observation scale govern the balance between strength and resilience. Understanding this relationship requires a framework that connects local interactions to their macroscopic consequences, allowing scale to emerge naturally from the underlying physics.

Chapter 4

Conclusions

A statistical homogenization framework was developed to connect microstructure, residual stress, and apparent mechanical response in two systems: a metallic SLM microstructure and a multiphase ceramic composite. The results show how mechanical behavior evolves with microstructural heterogeneity and thermomechanical factors across length scales.

In the SLM case, statistical homogenization captured how melt pool geometry governs the transition from local variability to stable, direction-dependent behavior as scale increases. Elastic moduli converged rapidly, while fracture strength remained sensitive to local topology. This suggests that apparent stability and directional consistency emerge only after sufficient statistical averaging of the underlying heterogeneity.

In the ceramic system, eigenstrain-induced residual stresses illustrated how thermal mismatch modifies apparent stiffness, strength, and damage evolution. Matrix compression reduced peak response but enhanced post-peak stability, indicating that strength and resilience are linked through the redistribution of stored energy.

Across both systems, anisotropy and variability diminished with increasing SVE size, reflecting a shared mechanism through which macroscale homogeneity arises from microstructural disorder. The findings demonstrate that the effective properties of

heterogeneous materials are not fixed constants but scale-dependent outcomes shaped by geometry and processing history.

The framework connects microstructural statistics to apparent response, allowing fine-scale behavior to inform higher scales without losing essential physics. It shows that local variability can be systematically up-scaled into stable, continuum-level descriptions, bridging the space between microscale fidelity and macroscale efficiency. The framework approximated thermal effects through prescribed eigenstrains rather than direct process simulation. Future extensions should use coupled thermal mechanical modeling to capture process-induced stresses and better link fabrication, microstructure, and effective response. Such developments enable models that naturally translate microstructural effects across scales.

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Vita

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