



Computational micromechanics of ductile fracture in duplex periodic microstructures

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ARTICLE INFO

Keywords:

Ductile fracture
Constituent connectivity
Computational micromechanics
Duplex microstructures
Plasticity-induced damage
Finite element analysis

ABSTRACT

Controlling microstructural heterogeneity is a promising strategy for tailoring the mechanical properties of multi-constituent materials. In particular, constituent connectivity, including the continuity of stiff or high-strength constituents, has attracted considerable interest in computational micromechanics. Although recent advances have enabled detailed analyses of complex microstructures, the micromechanical mechanisms governing their nonlinear deformation and fracture behavior remain insufficiently understood. In this study, three-dimensional numerical material testing, combining finite element analysis with a plasticity-induced damage model, is employed to investigate the relationship between constituent morphology and ductile fracture in duplex periodic microstructures. The analyzed microstructures contain continuous or discrete high-strength constituents over a wide range of volume fractions. The results show that both constituent volume fraction and connectivity affect macroscopic yielding, whereas fracture behavior exhibits a particularly strong sensitivity to connectivity. Specifically, the continuity of the low-strength matrix substantially affects damage localization, tensile strength, and elongation. When the low-strength constituent forms a continuous matrix, plastic deformation and damage preferentially localize within that matrix. Consequently, macroscopic fracture can occur before the strengthening effect of a large volume fraction of the discrete high-strength constituent is fully realized. These results demonstrate that constituent volume fraction alone is insufficient to characterize the ductile fracture behavior of the periodic microstructures investigated in this study. The findings provide micromechanical insight into the distinct roles of constituent volume fraction, morphology, and connectivity and may contribute to the morphology-based design of heterogeneous materials with improved mechanical performance.

1. Introduction

Multi-constituent steels are highly valued for their favorable balance of strength and ductility. This combination of properties originates from microstructures comprising soft, ductile ferrite and high-strength constituents such as pearlite or martensite [1–3]. The mechanical contrast between these constituents enables such steels to undergo substantial deformation and absorb considerable energy before fracture, making them attractive for applications requiring both high load-bearing capacity and fracture resistance. The importance of constituent morphology is not limited to steels. Many structural metallic materials are strengthened by finely dispersed precipitates, with Ni-based superalloys being a prominent example. In these alloys, the γ' phase enhances high-temperature strength. Depending on the processing route, however, residual γ regions may remain within the γ' precipitates and adversely affect the

resulting mechanical properties [4,5]. Understanding how the morphology, distribution, and connectivity of multiple constituents affect the macroscopic mechanical response is therefore a fundamental issue in materials design.

The incorporation of microstructural heterogeneity into estimates of macroscopic mechanical properties is a classical subject in solid mechanics known as micromechanics [6,7]. Historically, this problem has been addressed using various theoretical frameworks. These include analytical mean-field approaches [8–14] and semi-analytical approaches derived from Eshelby's inclusion theory [15], such as the Mori–Tanaka method [16,17] and self-consistent models [18,19]. These classical approaches have provided a theoretical foundation for modern computational micromechanics. Advances in computational capabilities have established direct numerical simulation as a major tool in this field. Spatial discretization methods, particularly the finite element

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(FE) method, can explicitly represent the heterogeneous geometries of material microstructures [20–22]. These methods enable detailed calculations of local stress and strain fields and allow computational models to be constructed directly from three-dimensional image data obtained using techniques such as X-ray computed tomography (CT). Such image-based FE models have been used to analyze stress concentrations around defects and predict fatigue life [23]. Furthermore, combining FE analysis with mathematical optimization enables the inverse design of heterogeneous microstructures for targeted mechanical properties, as demonstrated in studies on the optimization of dual-phase metallic microstructures [24,25].

A fundamental theoretical concept in micromechanics is that of upper and lower bounds, which describe how constituent volume fraction and microstructural morphology affect macroscopic properties. For elastic materials, the classical Voigt [8] and Reuss bounds [9] are based on the assumptions of uniform strain and uniform stress, respectively. The Hashin–Shtrikman bounds [10,11] provide tighter estimates and are frequently used in the analysis and design of heterogeneous materials. Analogous models for the elastoplastic response of polycrystalline metals were established through the Taylor [26] and Sachs approaches [27]. The uniform-strain and uniform-stress assumptions underlying these models can be conceptually related to constituent continuity and the resulting load-transfer pathways. This connection allows related questions to be investigated using computational models that explicitly represent constituent morphology. For example, [24] demonstrated experimentally and numerically that the macroscopic elastoplastic responses of dual-constituent steels with various morphologies and volume fractions remain within bounds determined by the properties of their constituents. These findings illustrate how constituent volume fraction and morphology jointly influence the macroscopic response before fracture.

Ductile fracture is a critical failure mode in metallic materials and is generally accompanied by substantial plastic deformation before final separation [28,29]. It is commonly described as a sequence of void nucleation, growth, and coalescence. Void nucleation typically occurs at microstructural heterogeneities such as inclusions, grain boundaries, and constituent interfaces [30,31]. Strain incompatibility between neighboring constituents and the resulting local stress and strain concentrations can promote the formation of microscopic voids. Once nucleated, the voids grow in response to the local stress state and accumulated plastic deformation. Coalescence subsequently occurs when neighboring voids interact and localized deformation develops in the intervening ligaments [32]. This sequence eventually results in macroscopic crack formation and loss of load-carrying capacity. Understanding these mechanisms at the microstructural scale is therefore essential for predicting and mitigating fracture in engineering materials.

The FE simulation of ductile fracture remains challenging because material softening and damage localization produce highly localized deformation and may eventually result in a loss of numerical stability. One widely used framework is the Gurson–Tvergaard–Needleman (GTN) model [33,34], which describes the elastoplastic response of porous materials while accounting for void evolution. The GTN model captures the influence of stress triaxiality on void growth and has been extensively applied to the analysis of ductile fracture under various material and loading conditions [35–37]. Another established framework is continuum damage mechanics (CDM), in which the progressive deterioration of material properties is represented using internal damage variables [38,39]. Depending on its formulation, CDM can describe damage processes associated with ductile or brittle fracture and can therefore be applied to a broad range of material behaviors [40]. However, local constitutive models involving strain softening generally exhibit mesh dependency because the absence of an intrinsic material length scale permits damage to localize within a mesh-dependent region. Nonlocal and strain-gradient damage formulations have consequently been developed to regularize damage localization and reduce sensitivity to spatial discretization [41–44]. Phase-field fracture models provide another

approach to representing crack initiation and propagation within a continuous framework [45–48]. These advanced formulations incorporate nonlocal interactions or gradient terms to provide a more objective description of localized damage and fracture.

Because ductile fracture originates from local stress and strain concentrations under finite plastic deformation and subsequently propagates through the microstructure, conventional analytical approaches such as mean-field and Eshelby-based theories have limited ability to explicitly represent damage localization and the complete fracture process. As a result, classical micromechanical studies have primarily focused on elastic and elastoplastic properties, whereas damage localization and ductile fracture have received less systematic consideration. Constitutive models for ductile damage can, however, be incorporated directly into microstructure-resolved FE analyses. This approach enables the relationships among constituent morphology, local deformation, damage evolution, and macroscopic fracture properties to be investigated within a unified computational framework.

Although numerical models of ductile fracture continue to advance, the fundamental influence of heterogeneous microstructural geometry on fracture behavior remains insufficiently understood. Recent studies have often focused on complex microstructures, such as polycrystalline metals [49], or on coupled physical phenomena, such as the interaction between fracture and atomic diffusion [50,51]. In contrast, systematic studies using simple and well-defined microstructures remain important for benchmarking numerical methods and establishing fundamental design principles. Even in numerical studies examining the relationship between microstructure and ductility [25], fracture-related properties are often evaluated using Considère’s criterion based on the macroscopic stress–strain response. Such an approach does not explicitly resolve local damage evolution and may not fully capture the influence of constituent connectivity in three-dimensional periodic microstructures. Consequently, the respective roles of constituent volume fraction and connectivity in governing damage localization and macroscopic ductile fracture require further clarification.

The present study investigates the influence of constituent morphology and connectivity on the ductile fracture behavior of duplex periodic microstructures composed of constituents with different strengths. Three-dimensional numerical material testing (NMT) is performed on representative volume elements (RVEs) using FE analysis combined with a plasticity-induced damage model. Continuous and discrete distributions of the high-strength constituent are systematically compared over a range of constituent volume fractions. The objective is to clarify how constituent volume fraction and connectivity affect the macroscopic stress–strain response, yield strength, tensile strength, elongation, and local damage evolution. Particular attention is given to the relationship between the connectivity of each constituent and the localization of plastic deformation and damage. By relating the numerical results qualitatively to the classical concept of micromechanical bounds, this study provides insight into the distinct and complementary roles of constituent volume fraction, morphology, and connectivity in the ductile fracture behavior of duplex periodic microstructures. The results are intended to contribute to the morphology-based design of heterogeneous materials with improved mechanical performance.

2. Methods

2.1. Constitutive model

To represent plastic hardening followed by damage-induced softening, a constitutive model for ductile damage was implemented in the FE analysis. The model is based on rate-independent finite-strain elastoplasticity and employs the equivalent plastic strain, ξ , as the primary internal variable. Although more advanced frameworks, such as the GTN model and coupled elastoplastic-damage models discussed in the Introduction, can describe the effects of void evolution and stress state in greater detail, the simplified formulation adopted here allows the influence of constituent morphology to be examined without

introducing a large number of additional material parameters. The parameters of the present model can be calibrated from a uniaxial stress–strain response, whereas more elaborate models generally require additional experimental data obtained under different stress states and loading conditions. The present formulation is therefore adopted as a minimal model for investigating the relationships among constituent morphology, plastic-strain localization, and macroscopic softening.

Based on finite-strain elastoplasticity, the deformation gradient is multiplicatively decomposed into elastic and plastic parts:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p, \quad (1)$$

where $\mathbf{F}$ is the total deformation gradient, and $\mathbf{F}^e$ and $\mathbf{F}^p$ denote its elastic and plastic parts, respectively. This decomposition introduces the reference, intermediate, and current configurations. The elastic response is described using a St. Venant–Kirchhoff elastic model:

$$\hat{\mathbf{S}} = \mathbf{C}^e : \frac{1}{2} (\mathbf{C}^e - \mathbf{1}), \quad (2)$$

where $\hat{\mathbf{S}}$ is the second Piola–Kirchhoff stress tensor defined in the intermediate configuration, $\mathbf{C}^e$ is the fourth-order elastic stiffness tensor, and $\mathbf{C}^e = \mathbf{F}^{eT} \mathbf{F}^e$ is the elastic right Cauchy–Green deformation tensor. Isotropic elasticity is assumed, with Young's modulus E and Poisson's ratio ν as the elastic material parameters.

For the strain-rate-independent plastic response, the yield function is defined as

$$\phi = \Sigma - \Gamma \leq 0 \quad (3)$$

where Σ is the stress norm and Γ is the yield stress. The stress norm is defined using the von Mises stress:

$$\Sigma := \sqrt{\frac{3}{2} \text{dev}[\hat{\mathbf{T}}] : \text{dev}[\hat{\mathbf{T}}]^T} \quad (4)$$

where $\hat{\mathbf{T}} = \mathbf{C}^e \hat{\mathbf{S}}$ is the Mandel stress tensor in the intermediate configuration. The yield stress is expressed as

$$\Gamma(\xi) := q(\xi) r(\xi) \quad (5)$$

where q defines the plastic hardening behavior and r is a degradation function representing damage-induced softening. Specifically, q is defined by a Voce-type nonlinear hardening law with an additional linear term [52]:

$$q := \tau_Y + H\xi + (\tau_{\text{sat}} - \tau_Y)(1 - \exp[-h\xi]) \quad (6)$$

where τ_Y represents the initial yield stress of the master curve, H is the linear hardening coefficient, τ_{sat} denotes the saturated yield stress in the nonlinear term when the plastic history variable ξ becomes sufficiently large, and h is the sensitivity coefficient governing nonlinear work hardening. The degradation function r is defined as an asymptotic function transitioning from 1 (undamaged) to 0 (fully damaged), with the critical plastic strain ξ_{cr} acting as the inflection point:

$$r := \frac{1}{2} + \frac{1}{\pi} \text{ArcTan}[\alpha(\xi_{\text{cr}} - \xi)] \quad (7)$$

where α governs the sensitivity of the asymptotic function. The value of α should be set relatively high, and its increase directly corresponds to a more rapid progression of fracture. Because the degradation function begins to decrease gradually before ξ reaches ξ_{cr} , the present formulation does not contain a distinct threshold for damage initiation. The plastic evolution is governed by an associated flow rule, and the constitutive equations are integrated using an implicit stress-integration algorithm.

The present model uses the equivalent plastic strain as the sole damage-driving variable and does not explicitly account for stress triaxiality, the Lode parameter, or tension–compression asymmetry. This is

an intentional simplification adopted to isolate the effects of constituent morphology and connectivity under the monotonic loading conditions considered here. Nevertheless, local stress states within heterogeneous microstructures may vary considerably, even under macroscopically uniaxial tension. Consequently, the predicted locations and evolution of damage may depend on the selected degradation law. The use of simple and well-defined periodic microstructures reduces the number of interacting microstructural factors and enables a fundamental micromechanical analysis using the present simplified constitutive model. However, the robustness of the predicted damage-localization behavior with respect to alternative damage formulations has not been established in the present study. A stress-state-dependent damage criterion could be introduced in future work to account for the effects of void growth and microcracking.

2.2. Finite element analysis method for periodic microstructures

Let Ω_Y denote the domain of a periodic representative volume element (RVE), with material coordinates $\mathbf{Y}$. In the absence of body forces, the microscopic mechanical equilibrium problem is expressed in weak form as

$$\int_{\Omega_Y} \mathbf{P} : \nabla_Y \boldsymbol{\eta} d\Omega_Y = 0 \quad \forall \boldsymbol{\eta} \in W_{\text{periodic}}, \quad (8)$$

where $\boldsymbol{\eta}$ denotes the variation of the microscopic periodic displacement $\tilde{\mathbf{u}}$. Here, $\mathbf{P}$ is the first Piola–Kirchhoff stress and W_{periodic} signifies the Sobolev space of periodic functions. Based on the principle of two-scale kinematics [53], the microscopic displacement field is decomposed into a macroscopically homogeneous component and a periodic fluctuation:

$$\mathbf{u} = \bar{\mathbf{H}} \mathbf{Y} + \tilde{\mathbf{u}}, \quad (9)$$

where $\bar{\mathbf{H}}$ represents the macroscopic displacement gradient. The fluctuation field satisfies

$$\tilde{\mathbf{u}}(\mathbf{Y}^+) = \tilde{\mathbf{u}}(\mathbf{Y}^-) \quad (10)$$

at corresponding points $\mathbf{Y}^+$ and $\mathbf{Y}^-$ on opposite boundaries of the RVE. The arbitrary rigid-body translation of the fluctuation field is eliminated by imposing an appropriate constraint. Accordingly, the microscopic displacement gradient $\mathbf{H}$ is formulated as follows:

$$\mathbf{H} = \nabla_Y \mathbf{u} = \bar{\mathbf{H}} + \nabla_Y \tilde{\mathbf{u}}. \quad (11)$$

A macroscopic variable $\bar{\bullet}$ is defined as the volume average of its microscopic counterpart $\bullet$ over the domain:

$$\bar{\bullet} = \frac{1}{|\Omega_Y|} \int_{\Omega_Y} \bullet d\Omega_Y, \quad (12)$$

where $|\Omega_Y|$ denotes the volume of the RVE. In the FE analysis, the macroscopic displacement gradient $\bar{\mathbf{H}}$ is prescribed as the primary boundary condition [54].

Periodic boundary conditions provide a consistent framework for evaluating the effective response of a periodically repeated microstructure. By enforcing compatible displacements at corresponding points on opposite boundaries, they preserve the intended constituent connectivity across the RVE boundaries and reduce artificial boundary effects. They also allow localized deformation patterns to develop within the RVE while maintaining compatibility with its periodic replicas. The calculated response should therefore be interpreted as that of an infinitely repeated periodic microstructure subjected to the prescribed macroscopic deformation, rather than that of a finite tensile specimen. In particular, free-surface effects and specimen-scale necking are not explicitly represented. This distinction allows the present study to focus on plastic-deformation and damage localization associated with constituent morphology and connectivity. However, periodic boundary conditions do not eliminate localization arising from the constitutive formulation or spatial discretization. Because the local damage model does not contain an intrinsic length scale, the post-localization response remains mesh dependent, as discussed in Section 2.3.

2.3. Finite element models and analyses

The FE models were discretized using eight-node hexahedral elements incorporating the *F*-bar method [55] to alleviate volumetric locking. Four periodic microstructures were constructed with spherical inclusions arranged in a body-centered cubic (BCC) lattice. The investigated inclusion volume fractions were 12.5%, 37.5%, 50.0%, and 62.5%, all of which are below the maximum packing fraction of approximately 68.0% for the adopted BCC geometry. Periodic boundary conditions preserve the intended constituent connectivity across opposite boundaries of the RVE. The constructed FE models are shown in Fig. 1, where one-eighth of each RVE is rendered transparent to display its internal morphology. Perfect bonding was assumed at all constituent interfaces; therefore, interfacial separation and debonding were not considered in the present analyses. For each geometrical partition, two complementary constituent assignments were considered. In one assignment, the high-strength constituent occupied the spherical inclusions, while the low-strength constituent formed the continuous matrix. In the complementary assignment, the material assignments were interchanged, such that the high-strength constituent formed the continuous matrix and the low-strength constituent occupied the spherical inclusions. This procedure enables the effects of constituent volume fraction and connectivity to be systematically examined using complementary material assignments on the same underlying geometrical partition.

The same elastic properties were assigned to both constituents: Young's modulus $E = 210$ GPa and Poisson's ratio $\nu = 0.3$. Therefore, the mechanical contrast between the constituents arises solely from their plastic behaviors including damage-induced softening. Two sets of constitutive parameters were considered, representing a low-strength, high-ductility constituent and a high-strength, low-ductility constituent. The corresponding parameters are summarized in Table 1. The critical plastic strain of the high-strength constituent was selected such that the plastic work accumulated up to the inflection point of its degradation function was comparable to that accumulated by the low-strength constituent up to its prescribed critical plastic strain. The accumulated

Table 1

Constitutive parameters assigned to the high-strength and low-strength constituents.

Constituent	τ_y [GPa]	H [GPa]	τ_{sat} [GPa]	h	ξ_{cr}	α
High-strength	0.8	0.5	1.1	20	0.3	50
Low-strength	0.2	0.2	0.3	10	0.9	50

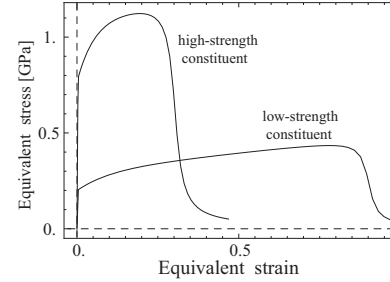


Fig. 2. Equivalent stress–strain responses of the high-strength and low-strength constituents.

plastic work was evaluated as

$$W_p(\xi) = \int_0^\xi \Gamma(\zeta) d\zeta. \quad (13)$$

where ζ is an integration variable. This procedure provides a consistent basis for defining two virtual constituents with different strength and ductility levels. Experimental identification of the intrinsic mechanical properties of individual microstructural constituents, particularly the parameters governing damage at large plastic strains, remains challenging. Although tensile tests can be performed on corresponding single-constituent materials, highly ductile specimens may undergo specimen-scale necking before their material response at large homogeneous strains can be identified. The parameter sets adopted here should therefore be interpreted as those of idealized virtual constituents rather than as direct calibrations for specific materials. This idealization enables the influence of constituent morphology and connectivity to be investigated under consistently defined constitutive conditions.

The equivalent stress–strain responses generated using the two constitutive parameter sets are shown in Fig. 2. The equivalent stress is defined as the von Mises stress. The equivalent strain ϵ^* is calculated from the deviatoric part of the logarithmic strain $\epsilon = \frac{1}{2} \ln [F F^T]$ in the current configuration:

$$\epsilon^* = \sqrt{\frac{2}{3} \text{dev}[\epsilon] : \text{dev}[\epsilon]}. \quad (14)$$

The simulations were performed using an implicit quasi-static scheme by prescribing the macroscopic displacement gradient $\bar{H}$. Following the formulation described in Section 2.2, three macroscopic loading conditions were considered:

$$(a) \bar{H}_a = \begin{bmatrix} u & 0 & 0 \\ 0 & * & 0 \\ 0 & 0 & * \end{bmatrix}, \quad (b) \bar{H}_b = \begin{bmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & * \end{bmatrix}, \quad (c) \bar{H}_c = \begin{bmatrix} 2u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & * \end{bmatrix}, \quad (15)$$

where u denotes a prescribed component of the macroscopic displacement gradient. The components denoted by $*$ were not prescribed directly but were determined such that the corresponding macroscopic normal stress components vanished. Condition $\bar{H}_a$ represents macroscopic uniaxial tension along the Y_1 direction, with the transverse deformation determined under zero macroscopic transverse stress. Condition $\bar{H}_b$ represents equibiaxial tension in the Y_1 – Y_2 plane, with

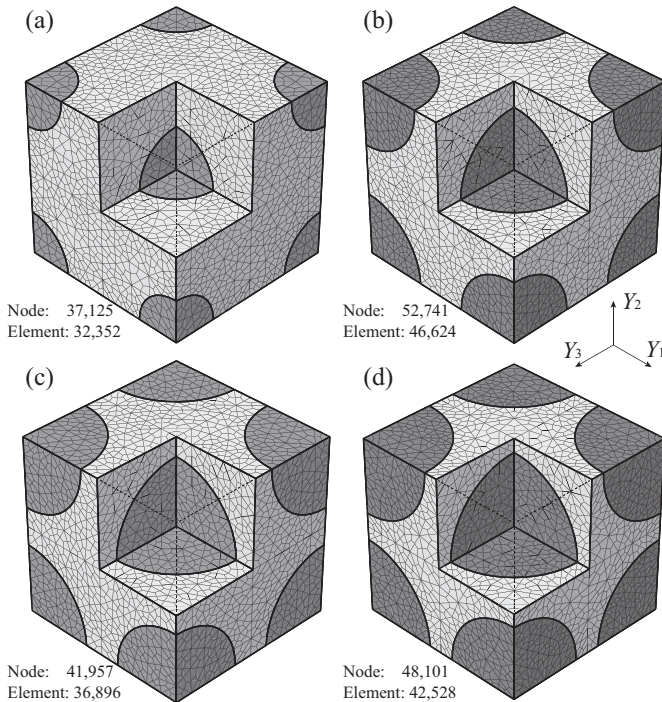


Fig. 1. Finite element models of periodic duplex microstructures with inclusion volume fractions of (a) 12.5%, (b) 37.5%, (c) 50.0%, and (d) 62.5%. One-eighth of each RVE is rendered transparent to show the internal morphology.

the out-of-plane deformation determined under zero macroscopic normal stress in the Y_3 direction. Condition $\bar{H}_c$ represents proportional nonequibiaxial tension in the Y_1 – Y_2 plane, with a prescribed in-plane displacement-gradient ratio of 2 : 1 and zero macroscopic normal stress in the Y_3 direction. These loading conditions were selected to examine the responses of the periodic microstructures under different tensile deformation modes.

The macroscopic equivalent stress was then calculated as the von Mises stress associated with the macroscopic Cauchy stress tensor evaluated by volume averaging the microscopic Cauchy stress over the current RVE domain. Similarly, the macroscopic equivalent strain was calculated from the logarithmic strain tensor obtained using the macroscopic deformation gradient.

Each simulation was continued into the post-peak regime until the iterative solution procedure failed to converge. Convergence loss occurred after pronounced damage-induced softening and strain localization had developed. The resulting severe element distortion was identified as the primary cause preventing further continuation of the calculation. Although the termination of the analysis is a numerical event, the reported tensile strength and elongation were evaluated at the peak of the macroscopic equivalent stress–strain response and therefore preceded the loss of solver convergence. Additional analyses performed using different increment settings reproduced essentially the same macroscopic response and yielded consistent peak-based properties.

The tensile strength was defined as the maximum equivalent stress in the macroscopic equivalent stress–strain response, and the corresponding equivalent strain was defined as the elongation. The 0.2% offset yield strength was evaluated using the effective elastic stiffness, $E^* = \frac{3E}{2(1+\nu)}$, which relates the von Mises equivalent stress to the equivalent strain under infinitesimal uniaxial elastic loading. For consistency among the different multiaxial loading conditions, the offset line was shifted by $\bar{\epsilon}^* = 0.002$ along the macroscopic equivalent-strain axis. Because these macroscopic properties were evaluated from periodically repeated RVEs, free-surface effects and specimen-scale necking were not explicitly represented. The reported elongation should therefore be interpreted as the equivalent strain at the peak macroscopic stress of the periodic microstructure, rather than as the total elongation of a finite tensile specimen.

Because the local damage formulation does not contain an intrinsic material length scale, the response after damage localization is mesh dependent. Accordingly, the comparative simulations were performed using comparable characteristic element sizes and mesh resolutions across all RVEs. To illustrate the influence of spatial discretization, an additional mesh-sensitivity analysis was conducted for both complementary constituent assignments based on the geometrical partition with

an inclusion volume fraction of 50.0%. At an inclusion volume fraction of 50.0%, the two constituents have equal volume fractions in both complementary assignments, allowing the influence of constituent connectivity to be examined without changing the constituent volume fractions. The responses obtained using the reference and substantially coarser meshes under loading condition (a) are compared in Fig. 3. For both constituent assignments, mesh refinement reduced the predicted tensile strength, the post-peak macroscopic stress level, and the equivalent strain at peak stress. The influence of mesh refinement was more pronounced when the high-strength constituent occupied the spherical inclusions and the low-strength constituent formed the continuous matrix. In this configuration, damage and plastic deformation localized within the continuous low-strength matrix, and the predicted softening response exhibited greater sensitivity to spatial discretization. These results illustrate the sensitivity of the damage-localization and post-peak responses to mesh discretization and demonstrate the importance of maintaining consistent discretization conditions when comparing different microstructures. This analysis is not intended to establish strict mesh convergence or mesh objectivity. Rather, the quantitative results presented in this study should be interpreted as comparative results obtained under controlled mesh conditions.

3. Results and discussion

3.1. Macroscopic perspective

The macroscopic equivalent stress–strain responses of the complementary microstructures under loading condition (a) are shown in Fig. 4. The geometrical partitions considered in this comparison have spherical-inclusion volume fractions of 37.5%, 50.0%, and 62.5%. The results reveal systematic differences in yield strength, tensile strength, and elongation depending on both constituent volume fraction and constituent connectivity.

The highest macroscopic strength among the cases shown in Fig. 4 is obtained when the high-strength constituent forms the continuous matrix at a high-strength-constituent volume fraction of 62.5%. For the same continuous configuration, reducing the volume fraction of the high-strength constituent to 37.5% decreases both the yield strength and tensile strength. In contrast, the elongation varies only moderately over the investigated range of volume fractions. This relatively small variation is associated with the tendency of plastic deformation and damage to localize within the continuous high-strength constituent, whose critical plastic strain $\bar{\epsilon}_{cr}$ is lower than that of the low-strength constituent. When the high-strength constituent occupies the discrete spherical inclusions, increasing its volume fraction to 62.5% produces only a moderate increase in tensile strength but substantially reduces the elongation. Conversely, the case with a high-strength-constituent volume fraction of 37.5% exhibits greater elongation, accompanied by a moderate reduction in tensile strength. Within each connectivity class, the case with a high-strength-constituent volume fraction of 50.0% exhibits an intermediate response between the corresponding 37.5% and 62.5% cases.

To summarize the overall trends, the yield strength, tensile strength, and elongation are plotted against the volume fraction of the high-strength constituent in Fig. 5. The corresponding values under loading condition (a) are listed in Table 2. The dataset also includes the two complementary assignments based on a spherical-inclusion volume fraction of 12.5%, corresponding to high-strength-constituent volume fractions of 12.5% and 87.5%. The yield strengths obtained under the three loading conditions show relatively small quantitative differences, whereas greater differences are observed in tensile strength and elongation. Nevertheless, the effects of constituent volume fraction and connectivity follow qualitatively similar trends under all investigated loading conditions.

The observed responses can be interpreted qualitatively in relation to classical micromechanical bounds. When the high-strength constituent forms the continuous matrix, load transfer through the high-strength

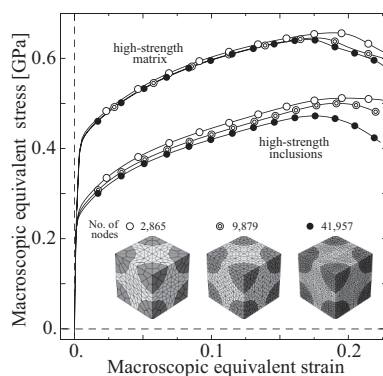


Fig. 3. Influence of mesh discretization on the macroscopic equivalent stress–strain responses under loading condition (a) for the two complementary constituent assignments based on the geometrical partition with a spherical-inclusion volume fraction of 50.0%.

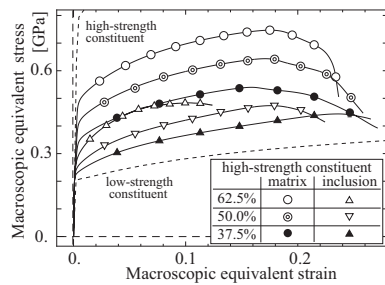


Fig. 4. Macroscopic equivalent stress–strain responses under loading condition (a) for the complementary constituent assignments based on geometrical partitions with spherical-inclusion volume fractions of 37.5%, 50.0%, and 62.5%.

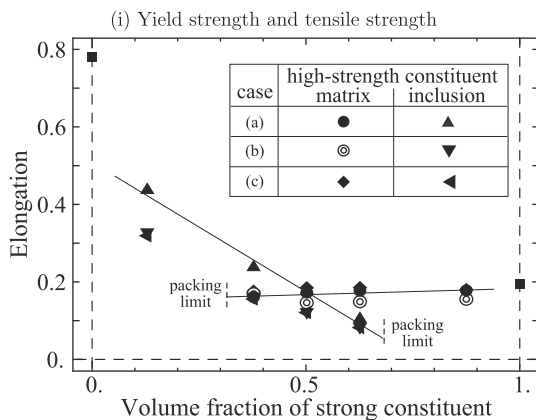
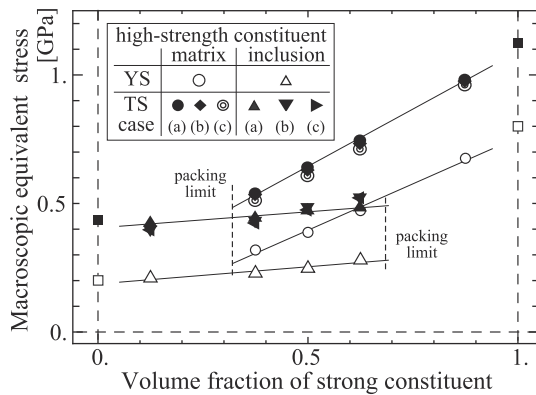


Fig. 5. Dependence of (i) yield strength and tensile strength and (ii) elongation on the volume fraction and connectivity of the high-strength constituent. Regression lines are shown for loading condition (a).

network results in a pronounced increase in macroscopic strength with increasing high-strength-constituent volume fraction. This trend qualitatively resembles the behavior associated with the uniform-strain assumption underlying the Voigt model. In contrast, when the high-strength constituent is distributed as discrete inclusions within a continuous low-strength matrix, the tensile strength exhibits a weaker dependence on the high-strength-constituent volume fraction. In this configuration, the continuous low-strength matrix accommodates a substantial portion of the deformation, producing a trend qualitatively closer to that associated with the uniform-stress assumption underlying the Reuss model. These comparisons provide a conceptual interpretation of the observed trends and do not imply that the nonlinear fracture responses satisfy the classical Voigt or Reuss bounds exactly.

Table 2

Macroscopic mechanical properties under loading condition (a): yield strength (YS), tensile strength (TS), and elongation (EL).

High-strength constituent		Macroscopic properties		
Volume fraction	Connectivity	YS [GPa]	TS [GPa]	EL [-]
87.5%	continuous (matrix)	0.6757	0.9841	0.1761
62.5%		0.4724	0.7468	0.1753
50.0%		0.3877	0.6417	0.1704
37.5%		0.3191	0.5400	0.1587
62.5%	discrete (inclusions)	0.2796	0.4839	0.1020
50.0%		0.2474	0.4724	0.1755
37.5%		0.2286	0.4437	0.2361
12.5%		0.2096	0.4236	0.4359

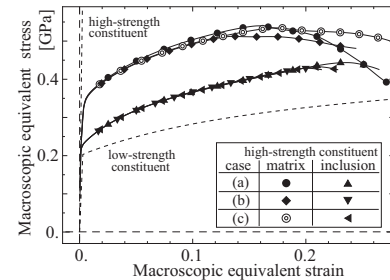


Fig. 6. Macroscopic equivalent stress–strain responses under loading conditions (a), (b), and (c) for the complementary constituent assignments based on a spherical-inclusion volume fraction of 37.5%.

These results also provide insight into the relationship between strength, ductility, and constituent morphology. The mechanical response of duplex materials containing constituents with contrasting strength and ductility is generally expected to lie between the responses of the individual constituents, producing the conventional strength–ductility trade-off sometimes represented by a “banana curve.” In conventional random microstructures, the constituent with the lower volume fraction typically tends to form the dispersed constituent, although its actual connectivity depends on the microstructural topology. The idealized periodic microstructures considered here enable constituent connectivity to be varied systematically over a wide range of volume fractions. The resulting responses include cases that depart substantially from the conventional strength–ductility trend typically associated with random microstructures. In particular, increasing the volume fraction of discrete high-strength inclusions does not necessarily produce a proportional increase in macroscopic tensile strength because deformation and damage can remain concentrated within the continuous low-strength matrix.

Within the range examined, the dependencies of yield strength, tensile strength, and elongation on the high-strength-constituent volume fraction can be approximated by linear regression for each connectivity class. These regressions are empirical descriptions of the analyzed data and should not be interpreted as general mixture laws. In particular, the fitted regression lines do not pass through the corresponding single-constituent responses at volume fractions of zero and unity. The actual relationships must therefore deviate from the fitted linear trends as the microstructures approach the single-constituent limits. The spherical-inclusion morphology arranged in a BCC lattice is also subject to a maximum packing fraction of approximately 68.0%. This geometrical constraint limits the range of spherical-inclusion volume fractions that can be represented while preserving the adopted morphology. Space-filling geometries, such as truncated-octahedral structures [24], could avoid this packing limitation. However, generating such models while maintaining geometrical similarity and systematically controlling constituent volume fraction would require a more elaborate model-construction procedure.

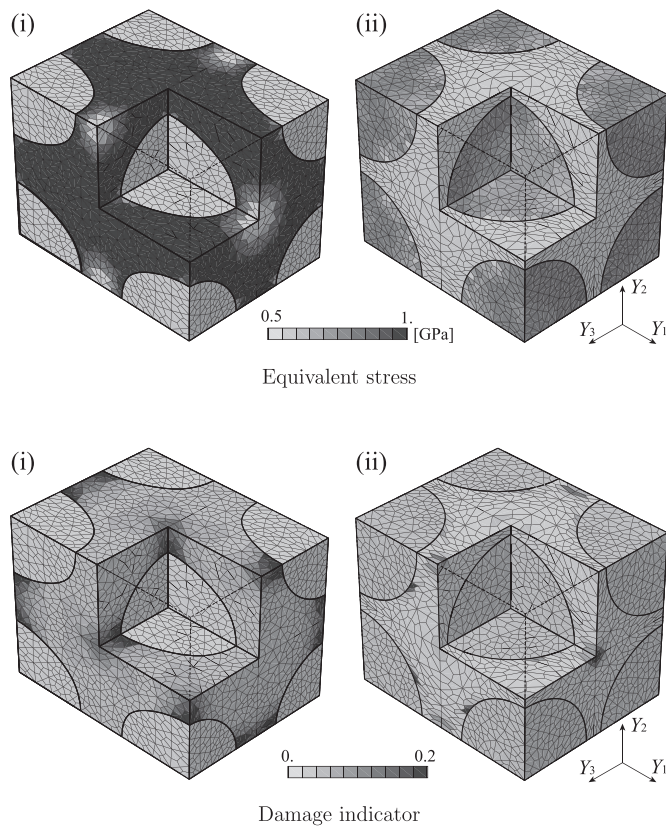


Fig. 7. Distributions of equivalent stress and the damage indicator $D = 1 - r$ at the peak macroscopic stress under loading condition (a) for microstructures with a high-strength-constituent volume fraction of 62.5%. The high-strength constituent is distributed as (i) a continuous matrix and (ii) discrete spherical inclusions. Higher values of D indicate more advanced damage-induced degradation.

The macroscopic equivalent stress–strain responses under all three loading conditions are shown in Fig. 6 for the two complementary assignments based on a spherical-inclusion volume fraction of 37.5%. The responses remain similar during the initial elastic and elastoplastic regimes. Differences become more evident near and beyond the peak stress, where localized plastic deformation and damage evolution become increasingly dependent on the macroscopic loading condition and constituent assignment.

Overall, a continuous distribution of the high-strength constituent produces a pronounced increase in macroscopic yield and tensile strengths. Its influence on elongation is more nuanced and depends on both the high-strength-constituent volume fraction and the connectivity of the low-strength constituent. In particular, at high volume fractions of the high-strength constituent, the continuous high-strength configuration retains greater elongation than the configuration in which the high-strength constituent remains discrete within a continuous low-strength matrix. The micromechanical mechanisms underlying these macroscopic trends are examined in Section 3.2.

3.2. Microscopic perspective

For loading condition (a), the distributions of equivalent stress and the damage indicator $D := 1 - r$ at the peak macroscopic stress are shown in Figs. 7 and 8 for high-strength-constituent volume fractions of 62.5% and 37.5%, respectively. As defined in Section 2.1, the degradation function r decreases from a value close to unity toward zero as damage-induced degradation progresses. Accordingly, the damage indicator D increases from a value close to zero toward unity, with higher

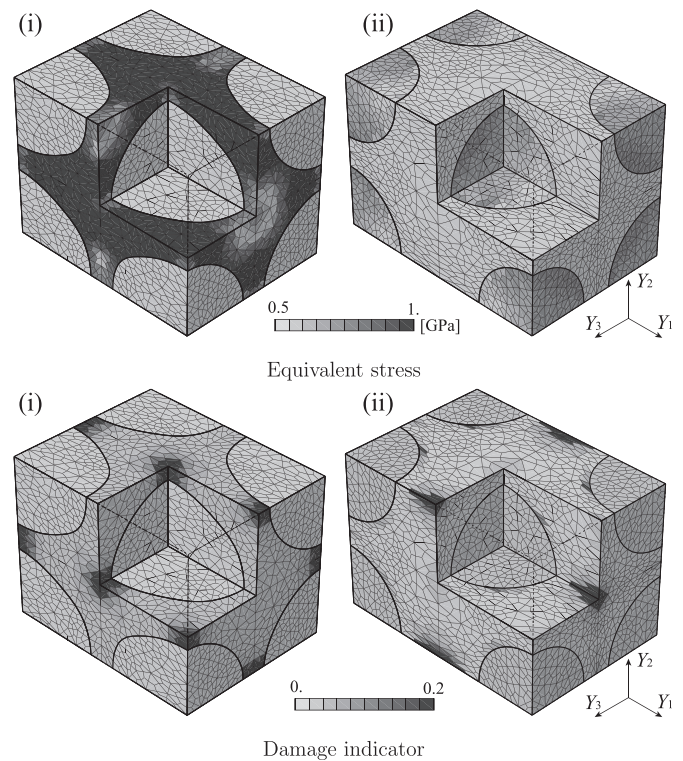


Fig. 8. Distributions of equivalent stress and the damage indicator $D = 1 - r$ at the peak macroscopic stress under loading condition (a) for microstructures with a high-strength-constituent volume fraction of 37.5%. The high-strength constituent is distributed as (i) a continuous matrix and (ii) discrete spherical inclusions. Higher values of D indicate more advanced damage-induced degradation.

values indicating more advanced degradation. To facilitate visualization of the internal fields, one-eighth of each RVE is rendered transparent.

A central observation of the microscopic analysis is that pronounced plastic deformation and damage-induced degradation develop predominantly within the continuous constituent. This result indicates that constituent connectivity plays an important role in determining the localization pattern and the onset of macroscopic softening, in addition to the effect of constituent volume fraction. When the high-strength constituent forms the continuous matrix, plastic deformation and degradation develop mainly within that continuous constituent, although their spatial distributions are affected by the embedded low-strength inclusions. Conversely, when the high-strength constituent occupies the discrete spherical inclusions and the low-strength constituent forms the continuous matrix, plastic deformation is concentrated predominantly within the continuous low-strength constituent. Consequently, even at a relatively high volume fraction of the discrete high-strength constituent, the continuous low-strength matrix can reach an advanced state of degradation before the strengthening effect of the high-strength constituent is fully realized. This localization behavior provides a micromechanical explanation for why increasing the volume fraction of discrete high-strength inclusions produces only a moderate increase in tensile strength while potentially reducing elongation.

The spatial distributions of stress and degradation also depend strongly on constituent morphology. Regions of pronounced degradation develop near constituent interfaces, where differences in the deformation of the high-strength and low-strength constituents produce localized plastic-strain concentrations. Interchanging the constituent assignments changes the locations and connectivity of these highly deformed regions. Thus, constituent morphology affects not only the magnitude of the macroscopic response but also the spatial pathways along which plastic

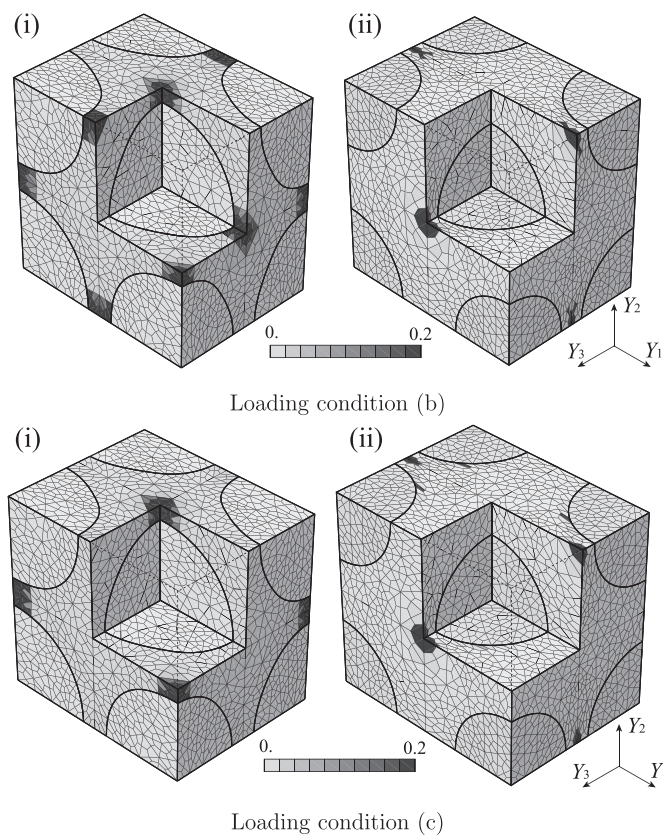


Fig. 9. Distributions of the damage indicator $D = 1 - r$ at the peak macroscopic stress under loading conditions (b) and (c) for microstructures with a high-strength-constituent volume fraction of 37.5%. The high-strength constituent is distributed as (i) a continuous matrix and (ii) discrete spherical inclusions. Higher values of D indicate more advanced damage-induced degradation.

deformation and damage evolve. The present observations do not imply that constituent volume fraction is unimportant. Rather, constituent volume fraction affects the overall stress and strain levels, whereas constituent connectivity strongly influences the spatial locations and connected pathways of deformation and damage localization. The combined effects of these two microstructural characteristics govern the predicted fracture response of the periodic microstructures considered here.

The distributions of the damage indicator D at the peak macroscopic stress under loading conditions (b) and (c) are shown in Fig. 9 for microstructures with a high-strength-constituent volume fraction of 37.5%. The detailed degradation patterns vary with the imposed macroscopic deformation because the local stress and strain states depend on the loading condition. Nevertheless, pronounced degradation remains concentrated predominantly within the continuous constituent under all three loading conditions. The connectivity of this constituent therefore provides persistent pathways for plastic-strain and damage localization, although the precise locations and extents of the degraded regions vary with the macroscopic loading condition.

A similar tendency was observed in additional analyses using a lower initial yield stress of $\tau_Y = 0.3$ GPa for the high-strength constituent. This observation indicates that the relationship between constituent connectivity and damage localization persists for this additional parameter set. However, its generality over a wider range of strength contrasts and constitutive parameters has not been established in the present study. Additional analyses would be required to determine how the localization behavior changes with constituent strength contrast. The conclusions drawn from the present results should also be interpreted within the limitations of the adopted constitutive model. Because the

equivalent plastic strain is used as the sole damage-driving variable, the model does not explicitly account for stress triaxiality, the Lode parameter, tension–compression asymmetry, or interfacial debonding. Alternative stress-state-dependent damage criteria could modify the locations and sequence of damage initiation and its subsequent evolution. Therefore, although the present results associate damage localization with the deformation patterns induced by constituent morphology and connectivity, the robustness of the predicted localization behavior with respect to alternative damage formulations remains to be established. Furthermore, the present conclusions apply to ductile damage accompanied by substantial plastic deformation and should not be directly extended to brittle materials, in which fracture may occur with little or no plastic deformation. Within the scope of the idealized periodic microstructures and constitutive assumptions considered here, the results clarify how constituent volume fraction and connectivity jointly affect plastic-deformation pathways, damage localization, and macroscopic softening.

4. Conclusion

This study investigated the influence of constituent morphology and connectivity on ductile fracture using FE simulations of periodic matrix–inclusion microstructures combined with a simplified plasticity-induced damage model. The results demonstrate that, in addition to constituent volume fraction, constituent connectivity strongly influences macroscopic fracture behavior by affecting the spatial pathways of plastic deformation and damage localization. When the high-strength constituent forms a continuous matrix, load transfer through the high-strength network produces pronounced increases in macroscopic yield and tensile strengths. In contrast, when the high-strength constituent is distributed as discrete inclusions within a continuous low-strength matrix, plastic deformation and damage remain concentrated predominantly within the low-strength matrix. Consequently, increasing the volume fraction of the discrete high-strength constituent produces only a moderate increase in tensile strength and may substantially reduce elongation. These results indicate that constituent volume fraction alone is insufficient to characterize the ductile fracture behavior of the periodic microstructures investigated in this study. The contrasting responses of the continuous and discrete configurations can be interpreted qualitatively in relation to the uniform-strain and uniform-stress assumptions underlying the Voigt and Reuss models, respectively. However, this interpretation does not imply that the nonlinear fracture responses satisfy these classical bounds exactly. Rather, the results clarify how constituent connectivity modifies load-transfer and damage-localization pathways, thereby producing strength–ductility relationships that may differ substantially from those typically associated with random microstructures.

The present conclusions are limited to the idealized periodic microstructures and constitutive assumptions considered in this study. The adopted model does not explicitly account for stress triaxiality, the Lode parameter, tension–compression asymmetry, or interfacial debonding. Moreover, because the local damage formulation does not contain an intrinsic material length scale, the predicted post-localization response remains mesh dependent. The quantitative results should therefore be interpreted as comparative predictions obtained under controlled discretization conditions. Future work should examine the robustness of the observed trends using stress-state-dependent and regularized damage formulations. Further extensions should incorporate interfacial debonding, history-dependent constitutive behavior under non-monotonic loading, and more complex microstructures. These developments could support the morphology-based inverse design of heterogeneous materials with improved strength–ductility combinations.

CRediT authorship contribution statement

Ikumu Watanabe: Writing – original draft, Visualization, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization,

Supervision, Validation, Writing – review & editing. **Tianwen Tan:** Methodology, Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This work was partially supported by the Japan Science and Technology Agency (JST) through the CREST program under Grant Number JPMJCR1995 and the 35th Iron and Steel Institute of Japan (ISIJ) Research Promotion Grant. We also thank Ms. Yuki Yamamoto and Dr. Sachiko Taniguchi of the National Institute for Materials Science for their invaluable technical assistance in developing the numerical model.

Data availability

Data will be made available upon request.

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