A model for simulating the deterioration of structural-scale material responses of microheterogeneous solids

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Abstract

In this paper, we develop a model to characterize the deterioration of mechanical responses of microheterogeneous solids due to progressive microstructural failure with increased loading. In the approach, the effects of microscopic failure, so-called “relaxation”, are described by a variational boundary value problem with constraints on the microfields. The extent of the relaxation, which is induced by reducing the eigenvalues of the elasticity tensor at a point in the heterogeneous body, is dictated by the condition that the solution must satisfy the equations of equilibrium, and simultaneously the constraints at that point. Theoretical properties of the model are determined and a computational algorithm is developed to simulate the deterioration of the material microstructure. Numerical simulations involving the finite element method are given to illustrate various aspects of the model. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Many modern structural engineering materials contain two or more dissimilar component materials. A typical kind of heterogeneous material consists of a homogeneous matrix material binding together particulate matter of different mechanical properties (Fig. 1). Such inhomogeneities are common in carbide steels, concrete, metal matrix composites, etc. In general, the basic philosophy is to select material combinations to produce aggregate responses possessing desirable properties from each component. In many cases the particulate matter is harder than the matrix material, and is used as a stiffener. A drawback in the use of solid structures composed of heterogeneous media is the existence of highly distorted and intense microfields, which may cause a significant amount of microscale failure in the form of subcontinuum scale microfissures, interface separation, void nucleation, etc. As the loading progresses, these local failures increase in size and number and eventually merge to produce observed macroscopic failure. Therefore, the desirable aggregate response of the heterogeneous material may be lost. The usual structural-scale property of interest to an engineer is the relation between averages, $E^*, \langle \sigma \rangle_\Omega = E^* : \langle \epsilon \rangle_\Omega$. Here $\langle \cdot \rangle_\Omega \equiv (1/|\Omega|) \int_\Omega \cdot d\Omega$, and $\sigma$ and $\epsilon$ are the stress and strain tensor fields within a statistically representative volume element (RVE) of volume $|\Omega|$. In particular, knowledge of the deterioration of $E^*$ with progressive loading, or overloading, is an issue of importance. However, the mentioned subcontinuum failure mechanisms, which are the root cause for such structural-scale changes, are extraordinarily difficult to measure,

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and virtually impossible to directly incorporate in practical macrostructural level simulations. Therefore, the typical approach to describe the deterioration of the macroscopic response is to employ phenomenologically based macroscopic damage parameters, and corresponding evolution laws. These are applied directly on the macroscopic level in order to mimic the observed weakening (softening) responses of material samples with progressive loading. There are a variety of such approaches, loosely referred to as Continuum Damage Mechanics (CDM) models. For an overview of the field, see [1]. Common to such approaches is that the mentioned evolution law is based on, or operates solely upon, macroscopic quantities such as $\varepsilon^*$. Typically, the evolution law is a curve fit of observed laboratory behavior. Consequently, it is fair to state that such phenomenological models are not really predictive of responses that are unknown a priori.

The goal of this work is to develop a microscale model, amenable to direct numerical simulation, in order to describe the deterioration of aggregate responses of assemblages of heterogeneous material. Afterwards, if relations between volumetrically averaged quantities are desired, they can be post-processed from the microfield solution. The extent of deterioration, which is induced by reducing the eigenvalues of the elasticity tensor at a point in the heterogeneous body, is dictated by the condition that the solution must satisfy the equations of equilibrium, and simultaneously the constraints at that point. In a sense, the model is quite similar to plasticity formulations. However, the main difference is that the material properties change, as opposed to the generation of plastic strain. Here we concentrate only on the phenomena of microscopic deterioration, and exclude inelastic strains. However, the model is to be viewed as complementary to plasticity models, when they are applied on the microscale, and can be combined with them, although this will not be carried out in this work. For macroscopic approaches combining and comparing damage and plasticity models, we refer the reader to the representative articles of Carol et al., [2], Ju [3], Lemaître [4] and Yazdani and Schreyer [5]. Throughout the analysis the microscopic material is assumed to remain as a continuum. Therefore, to an extent, this model is also phenomenological, but on the microscale, since no attempts are made to geometrically describe the true subcontinuum fissuring mechanisms that cause the changes in microscopic properties.

The outline of the paper is as follows. In Section 2 a model is formulated to describe the phenomena of interest. Various properties of the model are discussed. In Section 3 a computational algorithm is developed to determine the deterioration of the microstructure. In Section 4 three-dimensional numerical experiments are then carried out, and the results are discussed. In Section 5 some concluding remarks are given.
2. A micromechanical relaxation model

We consider a structure which occupies an open bounded domain in $\Omega \subset \mathbb{R}^3$. Its boundary is denoted $\partial \Omega$. The body is in static equilibrium under the action of body forces, $f$, and surface tractions, $t$. The boundary $\partial \Omega = \Gamma_u \cup \Gamma_t$ consists of a part $\Gamma_u$ and a part $\Gamma_t$ on which displacements and tractions are, respectively, prescribed. The virgin mechanical properties of the heterogeneous material are characterized by a spatially varying elasticity tensor $E \in \mathbb{R}^{3 \times 3 \times 3}$ which is assumed to satisfy $a_1 \epsilon : \epsilon \geq \epsilon : \epsilon \geq 0 \forall x \in \Omega$, where $E_{ijkl}(x) = E_{ijkl}(x) = E_{ijkl}(x) = E_{ijkl}(x)$, $1 \leq i, j, k, l \leq 3$, $E_{ijkl}(x)$ being the Cartesian components of $E$ at point $x$. A frequent notation used throughout this work, when we compare two microscopic elasticity tensor functions, for example $E_{(I)}$ and $E_{(II)}$, is $E_{(I)} \leq E_{(II)}$, which means that the eigenvalues of $(E_{(II)} - E_{(I)})$ are nonnegative. Following standard notation, we denote $H^1(\Omega)$ as the usual space of functions with generalized partial derivatives of order $\leq 1$ in $L^2(\Omega)$. We define $H^1(\Omega) \equiv [H^1(\Omega)]^3$ as the space of vector-valued functions whose components have generalized partial derivatives of order $\leq 1$ in $L^2(\Omega)$ $\equiv [L^2(\Omega)]^3$. We shall use the symbol “$u_{\mid_{\partial \Omega}}$” for boundary values. The data are assumed to be such that $f \in L^2(\Omega)$ and $t \in L^2(\Gamma_t)$, but less smooth data can be considered without complications.

2.1. Undeteriorated (unrelaxed) formulation

We denote $u$ as the undeteriorated “unrelaxed” solution field of the following variational boundary value problem:

\[
\begin{align*}
\text{Find } u \in H^1(\Omega), u \mid_{\Gamma_u} &= d \text{ such that } \forall v \in H^1(\Omega), \quad v \mid_{\Gamma_u} = 0 \cdot \\
\int_{\Omega} \nabla v : E : \nabla u \, d\Omega &= \int_{\Omega} f : v \, d\Omega + \int_{\Gamma_t} t : v \, dA.
\end{align*}
\]

This formulation contains no description of microscopic deterioration, which we refer to in this work as “relaxation”. We now construct a model for a relaxing microstructure, by enforcing two physically motivated requirements for a weakening material undergoing irreversible changes: (1) under pure displacement boundary loading control, $\Gamma_u = \partial \Omega$, the body should exhibit energy dissipation and (2) for pure traction loading control, $\Gamma_t = \partial \Omega$, an energy increase.

2.1.1. Energetic restrictions on microstructural relaxation

Consider two symmetric positive definite material property (elasticity tensor) distributions, the unrelaxed material, $E$, and a deteriorated or relaxed material $E_{\text{rel}}$. Both are separately used to generate solutions to two boundary value problems, with different material coefficients, but having the same exterior geometry and loading. The corresponding displacement $(u)$, stress $(\sigma)$ and strain $(\epsilon = (1/2)(\nabla u + (\nabla u)^T))$ states produced when using these materials are denoted $(u, \sigma, \epsilon)$ and $(u_{\text{rel}}, \sigma_{\text{rel}}, \epsilon_{\text{rel}})$, respectively. Consider their respective strain energies:

\[
\begin{align*}
I & \equiv \int_{\Omega} \epsilon : E : \epsilon \, d\Omega \\
I_{\text{rel}} & \equiv \int_{\Omega} \epsilon_{\text{rel}} : E_{\text{rel}} : \epsilon_{\text{rel}} \, d\Omega.
\end{align*}
\]

We have the following result for $\Gamma_u = \partial \Omega$:

\[
\begin{align*}
(E - E_{\text{rel}}) \geq 0 & \Rightarrow \int_{\Omega} \epsilon : E : \epsilon \, d\Omega - \int_{\Omega} \epsilon_{\text{rel}} : E_{\text{rel}} : \epsilon_{\text{rel}} \, d\Omega \geq 0.
\end{align*}
\]
Similarly, defining
\[
I_1 \overset{\text{def}}{=} \int_{\Omega} \sigma : E^{-1} : \sigma \ d\Omega \quad \text{and} \quad I_{\text{rel}} \overset{\text{def}}{=} \int_{\Omega} \sigma_{\text{rel}} : E_{\text{rel}}^{-1} : \sigma_{\text{rel}} \ d\Omega,
\]
we have \( \delta\sigma = \sigma_{\text{rel}} - \sigma \), if \( \Gamma_i = \partial\Omega \)
\[(E^{-1} - E_{\text{rel}}^{-1}) \leq 0 \implies \int_{\Omega} \sigma : E^{-1} : \sigma \ d\Omega - \int_{\Omega} \sigma_{\text{rel}} : E_{\text{rel}}^{-1} : \sigma_{\text{rel}} \ d\Omega \leq 0.\]

The relations in Boxes (3) and (5) provide sufficient restrictions on the properties of a relaxed microstructure, such that physically realistic macroscopic responses can be insured. For the sake of completeness, we prove such results. The proofs are constructive, and we believe add extra insight to the analysis to follow later.

2.2. Proof of energetic relaxation restrictions

Consider two symmetric positive definite material property (elasticity tensor) distributions, \( E_{(1)} \) and \( E_{(II)} \) used in same boundary value problem, for example Box (1). The corresponding stress and strain states using these materials are denoted \((e^{(1)}, \sigma^{(1)})\) and \((e^{(II)}, \sigma^{(II)})\), respectively. Consider their respective strain energies:
\[
I_1 = \int_{\Omega} e^{(1)} : E_{(1)} : e^{(1)} \ d\Omega \quad \text{and} \quad I_{\text{II}} = \int_{\Omega} (e^{(1)} + \delta e) : E_{(II)} : (e^{(1)} + \delta e) \ d\Omega.
\]

We have, denoting \( \delta e = e^{(II)} - e^{(1)} \),
\[
I_1 - I_{\text{II}} = \int_{\Omega} e^{(1)} : E_{(1)} : e^{(1)} \ d\Omega - \int_{\Omega} e^{(1)} : E_{(II)} : (e^{(1)} + \delta e) \ d\Omega - \int_{\Omega} \delta e : E_{(II)} : (e^{(1)} + \delta e) \ d\Omega
\]
\[
= \int_{\Omega} e^{(1)} : (E_{(1)} - E_{(II)}) : e^{(1)} \ d\Omega
\]

\[
= \int_{\Omega} e^{(1)} : (E_{(1)} - E_{(II)}) : e^{(1)} \ d\Omega - \int_{\Omega} (e^{(1)} + \delta e) : E_{(II)} : \delta e \ d\Omega
\]
\[
= \int_{\Omega} e^{(1)} : (E_{(1)} - E_{(II)}) : e^{(1)} \ d\Omega + \int_{\Omega} \delta e : E_{(II)} : \delta e \ d\Omega.
\]

The vanishing terms in the preceding analysis terms are due to a direct application of the principle of virtual work. The end result is that \( (E_{(1)} - E_{(II)}) \geq 0 \) implies
\[
\int_{\Omega} e^{(1)} : E_{(1)} : e^{(1)} \ d\Omega - \int_{\Omega} (e^{(1)} + \delta e) : E_{(II)} : (e^{(1)} + \delta e) \ d\Omega \geq 0.
\]
and

\[
II_1 - II_1 = \int_{\Omega} \sigma^{(1)} : E^{-1}_{(I)} : \sigma^{(1)} \, d\Omega - \int_{\Omega} \sigma^{(1)} : E^{-1}_{(I)} : (\sigma^{(1)} + \delta \sigma) \, d\Omega + \int_{\Omega} \delta \sigma : E^{-1}_{(I)} : (\sigma^{(1)} - \delta \sigma) \, d\Omega \leq 0 \text{ if } r_x = \varepsilon \varepsilon
\]

\[
= \int_{\Omega} \sigma^{(1)} : (E^{-1}_{(I)} - E^{-1}_{(II)}) : \sigma^{(1)} \, d\Omega - \int_{\Omega} \sigma^{(1)} : E^{-1}_{(II)} : \delta \sigma \, d\Omega
\]

\[
= \int_{\Omega} \sigma^{(1)} : (E^{-1}_{(I)} - E^{-1}_{(II)}) : \sigma^{(1)} \, d\Omega - \int_{\Omega} (\sigma^{(1)} + \delta \sigma) : E^{-1}_{(II)} : \delta \sigma \, d\Omega - \int_{\Omega} \delta \sigma : E^{-1}_{(II)} : \delta \sigma \, d\Omega
\]

\[
= \int_{\Omega} \sigma^{(1)} : (E^{-1}_{(I)} - E^{-1}_{(II)}) : \sigma^{(1)} \, d\Omega - \int_{\Omega} \delta \sigma : E^{-1}_{(II)} : \delta \sigma \, d\Omega
\]

Therefore \((E^{-1}_{(I)} - E^{-1}_{(II)}) \leq 0\) implies

\[
\int_{\Omega} \sigma^{(1)} : E^{-1}_{(I)} : \sigma^{(1)} \, d\Omega - \int_{\Omega} (\sigma^{(1)} + \delta \sigma) : E^{-1}_{(II)} : (\sigma^{(1)} + \delta \sigma) \, d\Omega \leq 0.
\]

Similar results, however for more restrictive (uniform) loading cases, and not in the context of a micro-failure analysis, can be found in [6].

The above results assert that a sufficient condition to meet our physical restrictions is to force the eigenvalues of \(E_{rel}\) to decrease at a location where failure occurs, and to remain unchanged otherwise. It is therefore convenient to define a spatially varying tensorial relaxation function, \(\alpha\), which operates on the eigenvalues of an otherwise unrelaxed elasticity tensor:

\[
E_{rel} = \alpha \Delta E \Rightarrow \delta \mathcal{E} \mathcal{G}(E_{rel}) = \{ A_{rel/1}, A_{rel/2}, A_{rel/3}, A_{rel/4}, A_{rel/5}, A_{rel/6} \} = \{ x_1 A_1, x_2 A_2, x_3 A_3, x_4 A_4, x_5 A_5, x_6 A_6 \},
\]

where \(0 < x_1 \cdots x_6 \leq 1\). The simplest representation, which is the one we employ in this work is

\[
E_{rel} = \alpha \Delta E \quad \text{with } 0 < \alpha \leq 1.
\]

The scalar relaxation function \(\alpha\) takes on different values throughout the body, which are dictated by the solution to a so-called relaxed boundary value problem introduced next.

**Remark.** When the material is directionally independent (two free constants), we have

\[
E = \begin{bmatrix}
\kappa + \frac{4}{3} \mu & \kappa - \frac{1}{3} \mu & \kappa - \frac{2}{3} \mu & 0 & 0 & 0 \\
\kappa - \frac{1}{3} \mu & \kappa + \frac{4}{3} \mu & \kappa - \frac{2}{3} \mu & 0 & 0 & 0 \\
\kappa - \frac{1}{3} \mu & \frac{1}{3} \mu & \kappa + \frac{4}{3} \mu & 0 & 0 & 0 \\
0 & 0 & 0 & \mu & 0 & 0 \\
0 & 0 & 0 & 0 & \mu & 0 \\
0 & 0 & 0 & 0 & 0 & \mu
\end{bmatrix}
\]
and correspondingly $\mathbb{E} : \varepsilon = 3\kappa (\text{tr } \varepsilon / 3) I + 2\mu \varepsilon'$, where $\text{tr } \varepsilon = \varepsilon_{ii}$ and $\varepsilon' = \varepsilon - 1/3(\text{tr } \varepsilon) I$. The eigenvalues of an isotropic elasticity tensor are $(3\kappa, 2\mu, 2\mu, \mu, \mu, \mu)$. Therefore, we must have $\kappa > 0$ and $\mu > 0$ to retain positive definiteness of $\mathbb{E}$, and consequently $\varkappa > 0$ and $\varkappa > 0$ for $\mathbb{E}_{\text{rel}}$.

### 2.3. Relaxed formulation

Consistent with the previous results, to describe losses of stiffness in the material on the microscopic level, we construct a relaxed solution, $u_{\text{rel}}$, that is generated by a weakened material modulus, $\mathbb{E}_{\text{rel}} \leq \mathbb{E}$. The corresponding variational boundary value problem governing the relaxed solution is

\begin{align}
\text{Find } u_{\text{rel}} \in H^1(\Omega), u_{\text{rel}}|_{\Gamma_0} = d & \text{ such that } \forall v \in H^1(\Omega), v|_{\Gamma_0} = 0,
\int_\Omega \nabla v : \mathbb{E}_{\text{rel}} : \nabla u_{\text{rel}} \, d\Omega = \int_\Omega f \cdot v \, d\Omega + \int_{\Gamma_i} t \cdot v \, dA, \\
\text{If } \mathcal{M} < \mathcal{K} & \text{ then } \mathbb{E}_{\text{rel}} = \mathbb{E}, \text{ (no relaxation)},
\text{If } \mathcal{M} = \mathcal{K} & \text{ then } 0 < \mathbb{E}_{\text{rel}} = \varkappa \mathbb{E} \leq \mathbb{E}, \text{ (relaxation).}
\end{align}

The functions $\mathcal{M} = \mathcal{M}(\mathbb{E}_{\text{rel}}, u_{\text{rel}}, \varkappa)$ and $\mathcal{K} = \mathcal{K}(\mathbb{E}_{\text{rel}}, u_{\text{rel}}, \varkappa)$, respectively serve as a measure of, and constraint on, selected internal fields of interest to the analyst. The functions $\mathcal{M}$ and $\mathcal{K}$ could be scalar, vector, or tensor valued. In this work we consider only scalar constraints, of which specific forms are introduced later. The values of $\varkappa$ are dictated by the fact that the solution $u_{\text{rel}}$ must satisfy the equations of equilibrium, and simultaneously the constraints.

### 2.4. One-dimensional examples

Consider a simple one-dimensional bar composed of a material that is initially linearly elastic. For a displacement tension test load: $u_{\text{rel}}(0) = 0$ and $u_{\text{rel}}(x = L) = \varepsilon \times L$, where $\varepsilon$ is an arbitrary constant that represents “applied strain”, the corresponding boundary value problem is

\begin{align}
\frac{d}{dx} \left( E_{\text{rel}} \frac{du_{\text{rel}}}{dx} \right) = 0 \Rightarrow \frac{du_{\text{rel}}}{dx} = \varepsilon \Rightarrow \sigma_{\text{rel}} = E_{\text{rel}} \varepsilon,
\end{align}

where $E_{\text{rel}} = \varkappa E$ is a material which may relax (Fig. 4). To satisfy a fixed stress constraint, such as $\sigma_{\text{rel}} \leq \sigma^{\text{crit}}$, the material must adjust to (Fig. 2)

\begin{align}
\sigma_{\text{rel}} > \sigma^{\text{crit}} \Rightarrow E_{\text{rel}} \varepsilon = \sigma^{\text{crit}} \Rightarrow E_{\text{rel}} = \frac{\sigma^{\text{crit}}}{\varepsilon} \quad \text{or} \quad \sigma_{\text{rel}} \leq \sigma^{\text{crit}} \Rightarrow E_{\text{rel}} = E.
\end{align}

![Fig. 2. A characterization of the solution behavior.](image-url)
In this case, the relaxation function ($\alpha$) is

$$\text{if } \sigma_{\text{rel}} > \sigma_{\text{crit}} \Rightarrow \alpha = \frac{\sigma_{\text{crit}}}{\sigma_{\text{rel}}} \quad \text{or} \quad \text{if } \sigma_{\text{rel}} \leq \sigma_{\text{crit}} \Rightarrow \alpha = 1.$$  \hfill (19)

A relatively general constraint equation, for the case when the constraint surface is dependent on the deformation, is (see Fig. 3)

$$\sigma_{\text{crit}} = \sigma_{\text{lim}} + (\sigma_{0}^{\text{crit}} - \sigma_{0}^{\text{lim}})\alpha^p,$$  \hfill (20)

where $\sigma_{0}^{\text{crit}}$ represents an initial critical stress which must be met to initiate relaxation, and where $\sigma_{\text{lim}}$ is a limit (asymptotic) stress. It is clear, in an algorithmic sense, if $\sigma_{\text{rel}} - \sigma_{\text{crit}} > 0$, then we must enforce

$$\sigma_{\text{rel}} = \sigma_{\text{crit}} \Rightarrow \alpha E\varepsilon_{\text{rel}} - \sigma_{\text{lim}} - (\sigma_{0}^{\text{crit}} - \sigma_{0}^{\text{lim}})\alpha^p = 0.$$  \hfill (21)

For simplicity, consider the case when $\sigma_{\text{lim}} = 0$, and therefore $\alpha E\varepsilon - \sigma_{0}^{\text{crit}}\alpha^p = 0$, which yields

$$\alpha = \left(\frac{E\varepsilon}{\sigma_{0}^{\text{crit}}}\right)^{1/(p-1)} = \left(\frac{\sigma_{0}^{\text{crit}}}{E\varepsilon}\right)^{1/(1-p)}.$$  \hfill (22)

Clearly, a critical value is $P = 1$. For this case we have

$$\alpha(E\varepsilon - \sigma_{0}^{\text{crit}}) = 0.$$  \hfill (23)

Therefore, since for a fixed $\sigma_{0}^{\text{crit}}$, in general $(E\varepsilon - \sigma_{0}^{\text{crit}}) \neq 0$, therefore $\alpha = 0$. This violates the restriction that $\alpha > 0$, and thus the constraints cannot be satisfied, implying that the boundary value problem has no solution. For $P > 1$, for example $P = 2 \Rightarrow |\alpha| > 1$, which is physically absurd behavior. No solution exists for $P \geq 1$, that satisfies the constraint conditions and equilibrium. For these reasons, we consider ranges of $P < 1$ in this work, even though in some cases, for nonzero values of $\sigma_{\text{lim}}$, it may be possible to attain a solution for $P > 1$. To give an idea of the solution behavior, for the one-dimensional bar we plotted the stress strain curve for various values of $P < 1$, corresponding to Eq. (17) for $\sigma_{\text{lim}} \ll \sigma_{0}^{\text{crit}}$. The numerical value of $\sigma_{0}^{\text{crit}}$ corresponds to the yield strength of aluminum. Incremental loading was applied, using 1000 load increments. The condition in Eq. (21) was solved by a Newton–Raphson method at each load increment. It is clear that as $P \rightarrow 1$ the problem tends to become ill-posed, and physically absurd (Fig. 4).

Bimaterial responses were also simulated for the model shown in Fig. 5. The bimaterial one-dimensional example is analogous to three-dimensional particulate microstructures, whereby a hard particle (boron) is embedded in a softer matrix (aluminum). The material data and the response curves are shown in Figs. 4–7.

![Fig. 3. A one-dimensional representation of a constraint function.](image-url)
Fig. 4. One-dimensional bar under displacement control: a parameter study for a single material with $\sigma^{\text{lim}} \ll \sigma^\text{crit} = 40 \text{ MPa}$, $E_{\text{AL}} = 67.5 \text{ GPa}$.

Fig. 5. One-dimensional bimaterial bar model: a parameter study with $\sigma^{\text{lim}} \ll \sigma^\text{crit}_{\text{AL, B}} = 40 \text{ MPa}$, $E_{\text{AL}} = 67.5 \text{ GPa}$, $\sigma^{\text{lim}} \ll \sigma^\text{crit}_{\text{B}} = 1000 \text{ MPa}$, $E_B = 413 \text{ GPa}$.

The “double hump” nonmonotonicity occurred due to the relaxation of the inner aluminum first, and then the aluminum outer bars later (Fig. 6). The boron did not relax, but locally distorted the inner aluminum bar, i.e., causing it to relax earlier than the outer ones. The aggregate response was clearly nonmonotone due to the inhomogeneous relaxation. However, as shown in Fig. 7, if the exponents are negative there is “hardening” or growth in the constraint surface. In this one-dimensional case, there is no nonmonotonicity of the response.
Fig. 6. One-dimensional bimaterial bar model: a parameter study with $\sigma_{\text{lim}} \ll \sigma_{\text{crit}}$ = 40 MPa, $E_{\text{AL}} = 67.5$ GPa, $\sigma_{\text{lim}} \ll \sigma_{\text{crit}}^{\text{B}}$ = 1000 MPa, $E_{\text{B}} = 413$ GPa. Depicted is $\alpha$ for the aluminum in the outer bars (a) and the inner bar (b). The boron did not relax.

3. A three-dimensional solution algorithm

In order to solve the boundary value problem, we must find a solution $u_{\text{sol}}$ and a function $\alpha$ such that the constraints and equilibrium are satisfied simultaneously. To accomplish this, we construct a global/local iteration procedure, in conjunction with incremental load stepping.
3.1. Global/local iteration process

Algorithmically, we must enforce

$$\mathcal{M} - \mathcal{K} = 0,$$

(24)

when the constraint is violated during loading. We consider

$$A(\varepsilon) \equiv \mathcal{M}(\sigma_{\text{rel}}(\varepsilon)) - \mathcal{K}(\varepsilon), \quad \mathcal{M}(\sigma_{\text{rel}}(\varepsilon)) = (g(\sigma_{\text{rel}}(\varepsilon)) : g(\sigma_{\text{rel}}(\varepsilon)))^{1/2},$$

(25)

where

$$g(\sigma_{\text{rel}}) = \eta_1 \frac{\text{tr} \sigma_{\text{rel}}}{3} I + \eta_2 \left(\sigma_{\text{rel}} - \frac{\text{tr} \sigma_{\text{rel}}}{3} I\right),$$

(26)

and where $\eta_1$ and $\eta_2$ are positive weights (different for each constituent material) which reflect the cause of failure, hydrostatic and/or deviatoric, to be expected. We define a generalization of Eq. (21) with

$$\mathcal{K}(\varepsilon) \equiv \Phi_{\text{lim}} + (\Phi_{\text{crit}} - \Phi_{\text{lim}}) \varepsilon^p,$$

(27)

where $\Phi_{\text{crit}}$ and $\Phi_{\text{lim}}$ are specified material-dependent functions, i.e., critical and limit levels of stress. When the constraint is violated, then $A(\varepsilon) = 0$ must be enforced. Following the usual procedure for problems with constraints, within a load increment $L$, requiring a global solution process, the Newton–Raphson scheme is used to satisfy the constraints locally. The displacement field, and consequently the strain field, are frozen during these local iterations.
Employing the local Newton–Raphson approach, the following are needed:

\[
\frac{\partial g(\sigma_{rel})}{\partial \sigma_{rel}} : \delta \sigma_{rel} = g(\sigma_{rel} + \delta \sigma_{rel}) - g(\sigma_{rel}) = \eta_1 \frac{\text{tr} \delta \sigma_{rel}}{3} I + \eta_2 \left( \delta \sigma_{rel} - \frac{\text{tr} \delta \sigma_{rel}}{3} I \right),
\]

\[
g(\sigma_{rel}) : g(\sigma_{rel}) = x^2 g(E : e_{rel}) : g(E : e_{rel}) = w^2 x^2 \left( \frac{\text{tr} \sigma_{rel}}{3} \right)^2 + w_x^2 \sigma_{rel} : \sigma_{rel}.
\]

\[
= x^2 \left( \eta_1^2 \left( \frac{3 \kappa}{\text{tr} e_{rel}} \right)^2 + \eta_2^2 \sigma_{rel} : \sigma_{rel} \right) \quad \text{(28)}
\]

\[
\frac{\partial g(\sigma_{rel})}{\partial \sigma_{rel}} : g(\sigma_{rel}) = \eta_1 \frac{\text{tr} g(\sigma_{rel})}{3} I + \eta_2 \left( g(\sigma_{rel}) - \frac{\text{tr} g(\sigma_{rel})}{3} I \right)
\]

\[
= \eta_1^2 \frac{\text{tr} \sigma_{rel}}{3} I + \eta_2^2 \left( \sigma_{rel} - \frac{\text{tr} \sigma_{rel}}{3} I \right).
\]

\[
\frac{\partial g(\sigma_{rel})}{\partial \sigma_{rel}} : g(\sigma_{rel}) \frac{\partial \sigma_{rel}}{\partial \alpha} = \frac{1}{2} \eta_1^2 \left( \frac{\text{tr} \sigma_{rel}}{3} \right)^2 + \eta_2^2 \left( \sigma_{rel} - \frac{\text{tr} \sigma_{rel}}{3} I \right) \cdot \left( \sigma_{rel} - \frac{\text{tr} \sigma_{rel}}{3} I \right).
\]

In the development of a solution algorithm, we employ the following somewhat standard superscript notation

- \( L \) is the load increment counter,
- \( I \) is the global solve counter (within a load increment),
- \( i \) is the local Newton–Raphson internal iteration counter (within a global solve).

The constraint can be written as follows \((\sigma_{rel}^{L,i}) = x^{L,i} : e_{rel}^{L,i})\):

\[
A(x^{L,i} + \Delta x^{L,i}) = A(x^{L,i}) + \frac{\partial A}{\partial x} \bigg|_{x^{L,i}} \Delta x^{L,i} + \text{H.O.T.} = 0.
\]

(29)

This can be broken down into four terms

\[
A(x^{L,i}) + \frac{\partial A}{\partial x} \bigg|_{x^{L,i}} \Delta x = \gamma_1(x^{L,i}) - \gamma_2(x^{L,i}) + \gamma_3(x^{L,i}) \Delta x^{L,i} - \gamma_4(x^{L,i}) \Delta x^{L,i},
\]

(30)

where during a local iteration process, \(\sigma_{rel}^{L,i} = (x^{L,i}/x^{L,i-1})\sigma_{rel}^{L,i-1}\), and, after some algebraic manipulations

\[
\gamma_1(x^{L,i}) \overset{\text{def}}{=} (g(\sigma_{rel}^{L,i}) : g(\sigma_{rel}^{L,i}))^{1/2},
\]

\[
\gamma_2(x^{L,i}) \overset{\text{def}}{=} \phi^{\text{lim}} + (\phi^{\text{crit}} - \phi^{\text{lim}})(x^{L,i})^p,
\]

\[
\gamma_3(x^{L,i}) \overset{\text{def}}{=} \frac{\partial (g(\sigma_{rel}^{L,i}) : g(\sigma_{rel}^{L,i}))^{1/2}}{\partial x} \bigg|_{x^{L,i}} = \frac{1}{2} x^{L,i} (g(\sigma_{rel}^{L,i}) : g(\sigma_{rel}^{L,i}))^{1/2},
\]

\[
\gamma_4(x^{L,i}) \overset{\text{def}}{=} P(\phi^{\text{crit}} - \phi^{\text{lim}})(x^{L,i})^{p-1}.
\]

(31)

Thereafter, we solve for the incremental relaxation (at all points where the violations occur)

\[
\Delta x^{L,i} = -\frac{\gamma_1(x^{L,i}) - \gamma_2(x^{L,i})}{\gamma_3(x^{L,i}) - \gamma_4(x^{L,i})}, \quad x^{L,i+1} = \Delta x^{L,i} + x^{L,i}.
\]

(32)

The global problem is then resolved, with the relaxation frozen. The constraints are then locally checked, again freezing the globally updated strains.

**Remark 1.** This specific type of fixed-point choice, as opposed to a complete global Newton-type, was made because of the necessity of using small load steps to capture the small length scales inherent in the micromechanical simulations, as well as the possibility of negative (due to softening) and discontinuous (due to the heterogeneous microstructure) tangents. Furthermore, due to issues such as repeated re-forming of
(consistent) relaxed tangent stiffness matrices and the corresponding algebraic system ill-conditioning, it is unclear whether large gains in performance can be obtained from using a true Newton method. This remains a topic of investigation of the authors.

**Remark 2.** It is interesting to note that if the constraints were frozen during the load increment (updated only at the end of a load increment), then one could solve directly, with no iterations for \( i = 0 \):

\[
\gamma^{L,I} = -\left( \frac{\gamma_2(\gamma^{L-1})}{(1/\gamma^{L-1})(g(\sigma^{L-1}_{rel} : g(\sigma^{L-1}_{rel}))^{1/2})} \right).
\]

(33)

Explicitly, in the isotropic case this leads to

\[
\gamma^{L,I} = \frac{\phi^{lim} + (\phi^{crit} - \phi^{lim})(\gamma^{L-1})^p}{(\eta_1^2(3\kappa Tr(\epsilon^{L-1}_{rel})/3))^2 + \eta_2^2 4\mu^2 \epsilon^{L-1}_{rel} : \epsilon^{L-1}_{rel})^{1/2}}.
\]

(34)

Therefore, we see that the update would be the ratio between the constraint and the measure of the product of the original material values with the relaxed strains. In this case the update collapses to a scaling of a norm of a limit stress and a response produced by a material (the original unrelaxed) that is too stiff, with strains computed by employing the relaxed material.

### 3.2. An overall computational algorithm

In the algorithm to follow, within each load increment, the equilibrium/constraint system is resolved until the constraints and equilibrium are satisfied. The chosen measure to determine the global violation of the constraints is

\[
||\mathcal{M} - \mathcal{K}||_C \overset{\text{def}}{=} \frac{1}{\Omega} \int_{\Omega} \max_{\mathcal{K}} (\mathcal{M}, \mathcal{K}) - \mathcal{K} \frac{d\Omega}{\mathcal{K}}.
\]

(35)

Algorithmically the system can be solved, for example under displacement control, by:

\[
\begin{align*}
L &= 1, \quad \gamma^{L} = 1 \quad \forall x \in \Omega \\
(1) \text{INCREMENT LOAD : } &u^{L-1}_{rel}|_{r_0} = u^{L-1}_{rel}|_{r_0} + \delta u^{L}_{rel}|_{r_0}, \quad I = 1 \\
(2) \text{GLOBALLY COMPUTE } &u^{L,I}_{rel} \text{ AND } \gamma^{L,I} \overset{\text{def}}{=} ||\mathcal{M}^{L,I} - \mathcal{K}^{L,I}||_C \\
\text{FLAG} &= 0 \\
\text{IF (} &\gamma^{L,I} > \text{TOL)} \text{ THEN} \\
\text{FLAG} &= 1 \\
\text{ENDIF} \\
\text{FOR EACH } &x \in \Omega: \\
\text{IF (} &\mathcal{M}^{L,I} > \mathcal{K}^{L,I} \text{ THEN} \\
&\text{UPDATE } \gamma^{L,I} \text{ UNTIL } A(\gamma^{L,I}) = 0 \\
\text{ENDIF} \\
\forall x \in \Omega \text{ UPDATE } &\gamma^{L,I} \text{ AND } \mathcal{E}^{L,I}; \quad I = I + 1 \\
\text{IF (FLAG = 1)} \text{ THEN} \\
\text{GOTO (2)} \\
\text{ENDIF} \\
L &= L + 1 \text{ AND GOTO (1)}
\end{align*}
\]

(36)

Essentially, the presented algorithm is a global fixed-point or Picard iteration process with local internal Newton corrections for the constraints. Typically, the convergence of such algorithms is inversely dependent on the load step size. Therefore, if the internal iterations at a load step converge too slowly, or do not converge at all, then the load step should be reduced to decrease the spectral radius. We have found that simple load bisection algorithms, i.e., those bisecting the load step size when, within a load step, the number
of global/local iterations exceeds a limit, to be quite successful in reducing computational cost while maintaining accuracy and convergence. However, in the simulations presented in the next section, for the sake of comparison between different levels relaxation (P), we used relatively small step sizes where convergence was never in question, and thus no load step adaptation was necessary. The analysis of fixed point schemes for partial differential equations dates back at least to 1929 to Perron [8] with subsequent studies by Ostrowski [9,10], Ortega and Rockoff [11], Kitchen [12] and numerous others. For overviews, see [7].

4. Numerical relaxation simulations

To study the 3-D model, standard loadings used in micromechanical simulations, applied uniform strains (via linear displacements) were incrementally increased in a multiaxial tension test on a cubical sample:

$$
\begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33}
\end{bmatrix}
\begin{bmatrix}
 u_1 \\
u_2 \\
u_3
\end{bmatrix}
= 
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix},
$$

(37)

We note that by the use of Gauss’s Divergence theorem one can show that $\langle \varepsilon_{ij} \rangle_\Omega = \varepsilon_{ij}$, which makes this a convenient load control parameter for the incremental relaxation tests to come later. The quantities of interest were the six response curves, $\langle \sigma_{ij} \rangle_\Omega$ vs. $\langle \varepsilon_{ij} \rangle_\Omega = \varepsilon_{ij}$. However, before undertaking the incremental relaxation tests, we performed a set of preliminary numerical experiments, with the load fixed ($\varepsilon_{ij} = 0.001$), with a purely linear elastic material model, in order to determine a reasonable sample size for a statistically representative response. In other words, we determined the minimum size of a cube containing a group of particulate suspensions which when loaded would give approximately invariant overall responses ($\langle \sigma_{ij} \rangle_\Omega$ vs. $\langle \varepsilon_{ij} \rangle_\Omega$) with sample size enlargement.

4.1. Preliminary tests

The matrix material was aluminum containing $N$ spherical nonintersecting boron particles randomly distributed throughout a unit cube. The material data are shown in Table 1. This material combination is representative of the typical mismatches in industrially used metal matrix dispersed particulate materials. We controlled the amount of embedded boron via particle/sample size ratio. This was done by defining a subvolume size $V_{\text{def}} = L \times L \times L / N$, where $N$ was the number of particles in the entire cubical ($L \times L \times L$) sample. A generalized diameter, $d$, was defined as the diameter of the smallest sphere that can enclose a single particle of possibly nonspherical shape, although in this work we restricted ourselves to spherical shapes. The ratio between the generalized diameter and the subvolume was the fixed control parameter defined by $\zeta_{\text{def}} = d / V^{1/3}$. The number of particles contained in a sample was increased holding the volume fraction constant. We used $\zeta = 0.75$, which resulted in a (fixed) volume fraction of approximately 22%. During the tests, we repeatedly refined the mesh to obtain invariant macroscopic responses. For a variety of numerical tests (discussed momentarily), the typical mesh density to deliver invariant volumetrically averaged responses was approximately $9 \times 9 \times 9$ trilinear finite element hexahedra (approximately 2200–3000 DOF) per particle.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\kappa$ (Gpa)</th>
<th>$\mu$ (Gpa)</th>
<th>$\phi_{\text{dev}}^{\text{crit}}$ (Mpa)</th>
<th>$\phi_{\text{all}}^{\text{crit}}$ (Mpa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum (matrix)</td>
<td>77.9</td>
<td>24.9</td>
<td>40</td>
<td>80</td>
</tr>
<tr>
<td>Boron (particle)</td>
<td>230.0</td>
<td>172.0</td>
<td>1000</td>
<td>1000</td>
</tr>
</tbody>
</table>

Table 1

Material property values of the constituents used in experiments
Table 2
Results of successive sample/particle enlargements ($W \equiv 1/|\Omega| \int_\Omega \epsilon : E : \epsilon \, d\Omega$)

<table>
<thead>
<tr>
<th>Part</th>
<th>$d/L$</th>
<th>DOF</th>
<th>$W$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.595</td>
<td>5184</td>
<td>0.001444</td>
</tr>
<tr>
<td>4</td>
<td>0.472</td>
<td>10.125</td>
<td>0.001408</td>
</tr>
<tr>
<td>8</td>
<td>0.375</td>
<td>20.577</td>
<td>0.001386</td>
</tr>
<tr>
<td>16</td>
<td>0.298</td>
<td>41.720</td>
<td>0.001375</td>
</tr>
<tr>
<td>32</td>
<td>0.236</td>
<td>81.000</td>
<td>0.001365</td>
</tr>
<tr>
<td>64</td>
<td>0.188</td>
<td>151.959</td>
<td>0.001358</td>
</tr>
</tbody>
</table>

The following particle per sample sequence was used to study the dependence of the effective responses on the sample size: 2 (5184 DOF), 4 (10,125 DOF), 8 (20,577 DOF), 16 (41,720 DOF), 32 (81,000 DOF) and 64 (151,959 DOF) particles. In order to obtain more reliable response data for each particle number set, the tests were performed five times and the responses averaged. We tracked the normalized strain energy density (Table 2) for the dependency with growth in sample size. As Table 2 indicates, the difference between successive stored strain energy densities was less than 1% for samples containing approximately above 20 particles. With this somewhat ad hoc justification, we used 20 particle microstructures in the incremental relaxation simulations to follow. We remark that during the computations, to increase the resolution of the internal geometry, we applied a “2/$S$” Gauss rule, i.e., a $2 \times 2 \times 2$ integration rule if there was no material discontinuity in the element, and a $5 \times 5 \times 5$ integration rule if there was a discontinuity. This process, which was not the subject of this work, has been studied more in detail in [13,14]. Also, throughout the tests a conjugate gradient (CG) solver was used. This was important in the incremental relaxation simulations to follow, since this allowed the re-use of the previous increment’s solution as a starting vector for the next one, in order to speed up the solution process.

Fig. 8. A sample of aluminum embedded with 20 boron particles occupying approximately 22% of the volume fraction. The brute force meshing scheme is used. Actual orthogonal cross-sections of the geometry as “seen” by the mesh density used (46,875 DOF). The lighter grey shade represents boron, while the darker represents aluminum.
4.2. Incremental relaxation tests

In the incremental relaxation simulations, the load step size was set to 40 displacement controlled increments to guide the following load history:

\[
\begin{bmatrix}
\delta_{11} & \delta_{12} & \delta_{13} \\
\delta_{21} & \delta_{22} & \delta_{23} \\
\delta_{31} & \delta_{32} & \delta_{33}
\end{bmatrix} = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} \rightarrow \begin{bmatrix}
0.005 & 0.005 & 0.005 \\
0.005 & 0.005 & 0.005 \\
0.005 & 0.005 & 0.005
\end{bmatrix}.
\]

(38)

Fig. 9. Twenty spheres (24 x 24 x 24 mesh/46,875 numerical DOF): Relaxation of an aluminum/boron composite with \( v_2 \approx 0.22, \) \( (\eta_1, \eta_2) = (1, 1) \) and \( P_x = -0.95. \)
For the relaxation tests, the constraint function was selected as follows:

\[
\mathcal{K}(x) \equiv \phi^{\text{lim}} + (\phi^{\text{crit}} - \phi^{\text{lim}})x^p,
\]

\[
\phi^{\text{crit}} = \sqrt{\eta_1^2 (\phi^{\text{crit}}_{\text{del}})^2 + \eta_2^2 (\phi^{\text{crit}}_{\text{dev}})^2},
\]

\[
\phi^{\text{lim}} = \beta \% \times \phi^{\text{crit}}.
\]

Fig. 10. Twenty spheres (24 × 24 × 24 mesh/46,875 numerical DOF): Relaxation of an aluminum/boron composite with \(v_2 \approx 0.22\), \((\eta_1, \eta_2) = (1, 1)\) and \(P_\sigma = -0.5\) (a), \(-0.1\) (b).
where $\phi_{\text{crit}}^{\text{dil}}$ and $\phi_{\text{crit}}^{\text{dev}}$ are specified material parameters, i.e., critical levels of stress (shown in Table 1). We chose $\beta_p = 50\%$ and $\eta_1 = \eta_2 = 1$. The normalized tolerance on the overall constraint violation in Box (36) was set to $\gamma \leq 0.0001 = \text{TOL}$.

Seven different levels of progressively stronger constraint surface contractions (more positive $P$ more contraction) were used: $P = -0.95$, $-0.5$, $-0.1$, $0.0$, $0.1$, $0.5$ and $0.95$. The same fixed random 20 particle microstructural distribution was used for all tests.

The meshes employed were uniform, and repeatedly refined until no significant changes in the responses occurred, for the entire load path. A mesh density of $24 \times 24 \times 24$ trilinear finite element hexahedra, 46875

![Graph](image)

Fig. 11. Twenty spheres ($24 \times 24 \times 24$ mesh/46,875 numerical DOF): Relaxation of an aluminum/boron composite with $v_2 \approx 0.22$, $(\eta_1, \eta_2) = (1,1)$ and $P_\alpha = 0.0$ (a), 0.1 (b).
numerical total unknowns ($\approx 9 \times 9 \times 9$ trilinear finite element hexahedra or 2344 numerical DOF per particle), was found to deliver stable results throughout the tests. As in the previous tests, to increase the resolution of the internal geometry, we applied the “2/5” Gauss rule. Cross-sections of the actual geometry, as resolved by this mesh density, are shown in Fig. 8. As one would intuitively expect, the macroscopic responses are clearly more strongly relaxing with increasing $P$. The relaxation began almost immediately, due to the fact that the inter-particle stresses in the matrix were high. The ability of the model to capture nonmonotonic responses, due to inhomogeneous relaxation, is noteworthy. This is an effect that is impossible to capture with macroscopic damage models without embedded (phenomenologically constructed)

Fig. 12. Twenty spheres ($24 \times 24 \times 24$ mesh/46,875 numerical DOF): Relaxation of an aluminum/boron composite with $v_2 \approx 0.22$, $(\eta_1, \eta_2) = (1, 1)$ and $P_e = 0.5$ (a), 0.95 (b).
“trigger” mechanisms. The nonmonotonicity of the responses is a direct consequence of inhomogeneous relaxation, as exemplified by the one-dimensional examples discussed earlier in the work. This nonmonotonicity was expected since

$$\sigma_{rel} = \alpha \varepsilon : \varepsilon_{rel} \Rightarrow d\sigma_{rel} = \frac{d\varepsilon}{d\varepsilon_{rel}} E : \varepsilon_{rel} = \varepsilon^{\text{TAN}} : d\varepsilon_{rel}.$$ (40)

Clearly, when the change in $\alpha$ is large, a nonpositive definite tangent modulus can occur. The tangent can be explicitly written out by observing that when relaxation occurs we have

$$dA = \frac{\partial A}{\partial \sigma_{rel}} : d\sigma_{rel} + \frac{\partial A}{\partial \alpha} d\alpha = 0,$$ (41)

Fig. 13. Left to right, and top to bottom: the relaxation (distributions of $\alpha$) in the microstructure after five, ten, twenty and forty load increments ($P_x = -0.5$). The depicted values of $\alpha$ were averaged over each finite element.
which leads to

$$d\mathbf{\varepsilon} = -\left( \frac{\partial A}{\partial \mathbf{\sigma}_{\text{rel}}} : \mathbf{\sigma}_{\text{rel}} \right) \left( \frac{\partial A}{\partial d} \right)^{-1} = A : d\mathbf{\sigma}_{\text{rel}}. \quad (42)$$

Substituting Eq. (42) into Eq. (41) we obtain

$$d\mathbf{\sigma}_{\text{rel}} = \left( I + \mathbf{\varepsilon}_{\text{rel}} \otimes A \right)^{-1} : A \mathbf{\varepsilon}_{\text{rel}} : d\mathbf{\varepsilon}_{\text{rel}}. \quad (43)$$

A typical example of the progressive relaxation is seen in Fig. 9, where one observes that in an overall volumetrically averaged sense, the relaxation $\langle \mathbf{x} \rangle_A$ is strong early in the loading history. Therefore, the overall relaxed tangent response will lose positive-definiteness. We observe that the responses develop "texture" with increasing loads. In other words, responses like $\langle \sigma_{11} \rangle_A$ vs. $\langle \varepsilon_{11} \rangle_A$ and $\langle \sigma_{22} \rangle_A$ vs. $\langle \varepsilon_{22} \rangle_A$, which would be identical if the macroscopic response were perfectly isotropic, began to deviate (Figs. 9–12). This is attributed to the inhomogeneous relaxation spreading nonuniformly through the structure. This can be seen by studying the (framed) load sequence in Fig. 13.

5. Concluding remarks

In this work we have formulated a model to describe the microscopic deterioration of materials containing heterogeneities. The effects of local microscopic failure were modeled by a variational boundary value problem with constraints on the microfields. In the model, in order to satisfy equilibrium and the constraints simultaneously, the original material had to relax on the microstructural level. Mathematically, this was achieved by reducing the eigenvalues of the elasticity tensor at points throughout the heterogeneous body. As with most micromechanical approaches, the computations are somewhat intensive. In this regard, domain decomposition methods, such as those found in [15–17], are possibly helpful to achieve efficient simulations. Such techniques are also useful in extracting statistical information by performing such simulations on multiple samples. The benefits of computational micromechanical approaches, such as the one presented here, are relatively simple descriptions on the microscale, containing parameters that are physically meaningful. In other words, the phenomenological aspects of the modeling are reduced. In closing, within the last few years, there have been processing methods developed to control the orientation of particulate matter by coating them in a conducting liquid material and introducing them into the molten matrix material. Thereafter, an electrical current is applied, forcing the particles to align themselves along the field lines. This can produce particulate microstructures which deliver anisotropic macroscopic responses. The approaches developed here are directly applicable to such microstructures, as well as to the more common fiber-reinforced cases.

References