



PERGAMON

International Journal of Solids and Structures 37 (2000) 3375–3398

INTERNATIONAL JOURNAL OF
**SOLIDS and
STRUCTURES**

www.elsevier.com/locate/ijsolstr

On the constitutive relations of materials with evolving microstructure due to microcracking

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Received 3 December 1998; in revised form 28 April 1999

Abstract

This paper discusses the practical implementation of a thermodynamically based procedure for the derivation of the effective nonlinear constitutive relations for composites with evolving microstructure. Examples of the procedure for the case of an elastic periodic composite with several growing cracks are presented. These examples are intended to show how the use of this procedure differs from the traditional global-local analysis approach and how well suited it is for use with general purpose structural analysis packages. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

The structural analysis of composite components characterized by evolving damage at the microscopic scale is, in general, predicated upon the availability of effective damage dependent constitutive and evolution equations. Effective constitutive equations describe the behavior of a single material point of an equivalent homogeneous medium. Ideally, these equations should be valid for any deformation history that a material point will experience. Obtaining equations of this type is the fundamental goal of any theory of effective properties of composites. Among these theories, continuum damage mechanics (CDM) and homogenization theory (HT) are perhaps the two most prominent.

CDM (Chaboche, 1981, 1988a, b; Kachanov, 1986; Krajcinovic, 1996; Lemaitre, 1996) is, in essence, a phenomenological approach where the mathematical description of a certain type of microscopic damage mechanism is postulated to be given in terms of some appropriately defined damage variables.

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Once a set of state variables (internal and external) have been selected, the constitutive equations are obtained using continuum thermodynamic theories of constitutive equations (cf Coleman and Gurtin, 1967; Coleman and Noll, 1963; Germain et al., 1983). The constitutive equations thus obtained, along with the companion evolution equation for the internal state variables, contain material constants to be determined via experiments. This approach, no matter how elegant, may be difficult to use in practice depending on the complexity of the material point internal state. In particular, in problems where the damage evolution causes the symmetry properties of material points to change and where simple evolution laws (e.g. deriving from a convex dissipation potential as is the case for J_2 materials as discussed by Maugin, 1992) cannot be postulated, extremely complex experiments are required to characterize the material constitutive equations for a wide enough range of load histories. Furthermore, small changes in microstructure (e.g. fiber volume) require a completely new set of experiments. These difficulties are greatly magnified whenever the selected damage variables are of tensorial nature. This is perhaps the reason why many of the practical applications of CDM are based on the assumption that damage preserves isotropy during its evolution (cf Kachanov, 1986).

Homogenization theories are based on the idea that given the geometric and constitutive properties of a representative volume element (RVE)² one can obtain the effective properties of an equivalent homogeneous material via averaging techniques. This process requires the definition of macroscopic variables that are spatial averages of local fields within the RVE. Also, for the effective constitutive equations to make physical sense, i.e., to conform to a thermodynamically consistent theory of constitutive equations (see e.g. Bowen, 1989; Coleman and Gurtin, 1967; Coleman and Noll, 1963; Germain et al., 1983), the macroscopic variables should be defined in such a way that one can identify what configuration of the local microscopic fields has generated such an average (Maugin, 1992; Stolz, 1986; Suquet, 1985, 1987). This type of inverse problem is often referred to as a localization procedure (or problem). Furthermore, even when the definition of an average quantity is appropriate, one must ensure that all the variables in question are independent macroscopic state variables³, i.e., that in a thought experiment it can be varied arbitrarily while keeping all other macroscopic state variables, both external and internal, fixed.

Rigorous homogenization procedures satisfying the requirements mentioned above are of general practical use in a variety of applications including linear elastic and linear viscoelastic composites with fixed microstructure (cf Bakhvalov and Panasenko, 1989; Bensoussan et al., 1978; Suquet, 1987). However, for elasto-plastic composites it has been proven that although a physically meaningful definition of macroscopic (or average) plastic strain can be defined, such an average does not allow for the construction of a successful localization procedure (Suquet, 1985, 1987). From a theoretical viewpoint, this fact leads to the conclusion that the local (or microscopic) plastic strain field, i.e., the collection of the values of the plastic strain at all points in the RVE, must be retained at the macroscopic level as the only correct descriptor of the plastic flow evolution. In other words, the formulation of effective constitutive and evolution equations for an elasto-plastic composite that are thermodynamically correct requires ‘an infinite number of internal state variables’, namely the microscopic plastic strain field at every point in the RVE (Maugin, 1992; Suquet, 1985, 1987). Clearly,

² A representative volume element is defined to be a portion of the heterogeneous material under consideration, whose average properties coincide with the average properties of the medium as a whole. In periodic media, the RVE is chosen to coincide with the periodic unit cell of the material.

³ The celebrated Vakulenko–Kachonov variable (Vakulenko and Kachanov, 1971), defined as the RVE volume average of the tensor product of the crack opening displacement function and the crack face unit normal vector field [see Eq. (11)], can be considered a typical example of a damage variable that cannot be used as a macroscopic internal damage state variable. In fact, it is not difficult to realize that such a variable, defined in terms of the displacement field within an RVE, is intrinsically dependent on the applied external loads, which, for a typical RVE, are given in terms of the average (total) strain or stress.

this result implies that practical applications of homogenization theories to elasto-plastic systems require appropriate approximation strategies such as those discussed by Aboudi (1991), Dvorak (1992), Dvorak and Benveniste (1992), Suquet (1985) and Costanzo et al. (1996).

In principle, a homogenization theory allows one to derive the effective constitutive and evolution equations if an accurate description of microscopic deformation mechanisms can be found. This makes HTs rather appealing especially for the case of media with evolving microstructure. In fact, in the case of microcracking, one can explicitly make use of fracture mechanics based concepts and crack growth criteria to derive their overall effect at the macroscopic level. However, analyses such as those given by Stolz (1986) and Costanzo et al. (1996) show that an average representation of microcracking within an RVE cannot be found if a well-posed localization procedure is to be constructed, i.e., in order to use fracture mechanics to understand how failure and crack propagation manifest themselves at the macroscopic level, one must model microcracking explicitly as it is done in a so-called global–local (GL) approach. In the GL approach, macroscopic structural components are analyzed using standard methods while every time information concerning the constitutive equations is needed, a companion micromechanics boundary value problem is explicitly solved. Consider then that if the macroscopic structural analysis is carried out using the finite element method (FEM), a companion micromechanics problem would have to be solved at every integration point in the FE grid and at every time step of the applied load history.

The main problem hindering the widespread use of a GL approach to study the nonlinear behavior of composites is the need for computational power that is usually out of the reach of most structural analysis practitioners. More importantly, GL analyses do not deliver the effective constitutive relations of a material. Rather, they provide the value of the current average stress (or strain) for the current average strain (or stress) at a material point. Therefore, a GL strategy does not provide any constitutive information that could be used in anything other than the particular problem and the particular load history at hand. Clearly, a more desirable result would be one where the effective constitutive equation for a given material could be obtained once and for all as well as separately from any particular problem. The objective of the present paper is to discuss a micromechanics based approach for the derivation of the effective constitutive equations having precisely this quality. In other words, a computational strategy is presented for the derivation of constitutive equations for composites with growing cracks that are obtained once and for all and that are valid for any load history while maintaining consistency with continuum thermodynamics. In this context, it is believed that the proposed strategy constitutes a more efficient alternative to a GL analysis approach.

The paper is structured as follows: Section 2 contains some basic equations and definitions, Section 3 describes how the proposed approach is practically implemented whereas Section 4 is devoted to the presentation and discussion of a series of examples. Finally, Section 5 contains the conclusion to the paper.

2. Background

This section is devoted to a summary of the homogenization theory presented by Costanzo et al. (1996) (see also Bui and Ehrlacher, 1980; Bui et al., 1982; Stolz, 1986). In this reference, an inelastic composite material with temperature dependence and growing cracks was considered. Since the thrust of this paper is not the establishment of general theoretical results but rather the discussion of how to practically implement a specific micromechanics-based strategy, for the sake of simplicity the system considered herein will be linear elastic and isothermal. The generalization to more complex scenarios is relatively straightforward.

2.1. RVE geometry and local field equations

The first step of a homogenization procedure is the selection of an appropriate representative volume element for the material at hand. For discussion, we consider a fiber reinforced composite arranged in a square array. Then, with reference to Fig. 1, the selected RVE has volume V and external surface S_E , the latter being oriented by an outward unit normal vector n_k . The RVE contains one or more growing cracks denoted $C^i(t)$, with $i = 1, \dots, N$. The variable t denotes time. The i -th crack surface is oriented by a unit normal m_j^i and is bounded by a front denoted by $\partial C^i(t)$. The cracks are surfaces of discontinuity whereas the crack fronts are singularity lines for various mechanical fields (e.g. stress, strain and strain energy). The jump of a generic field ϕ across the crack faces is denoted by $[\phi]$ and is defined as follows:

$$[\phi] = \phi^+ - \phi^-, \tag{1}$$

where

$$\phi^\pm(z_j, t) = \lim_{\xi \rightarrow 0^+} \phi(z_j \pm \xi m_j^i, t), \tag{2}$$

and $z_j \in C^i(t) / \partial C^i(t)$ and $\xi \in \mathbb{R}$.

The system's evolution will be assumed to be quasi-static and body forces are assumed to be negligible. The local equilibrium equations are therefore given by

$$\sigma_{ij,j} = 0 \text{ in } V; \text{ and } T_i^+ = \sigma_{ij}^+ m_j^k = T_i^- = \sigma_{ij}^- m_j^k \text{ on } C^k(t), \tag{3}$$

where σ_{ij} is the Cauchy stress tensor and T_i is the traction vector. The local constitutive equations for all constituents are assumed to be those of an isothermal elastic material and are therefore expressed by the generalized Hooke's law:

$$\sigma_{ij}(x_p, t) = a_{ijkl}(x_p) \varepsilon_{kl}(x_p, t), \tag{4}$$

where x_p represents the position vector of a generic point within the RVE, $a_{ijkl}(x_p)$ represents the (position dependent) elastic moduli and ε_{ij} is the small strain tensor defined as follows:

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \tag{5}$$

where u_i is the displacement vector field.

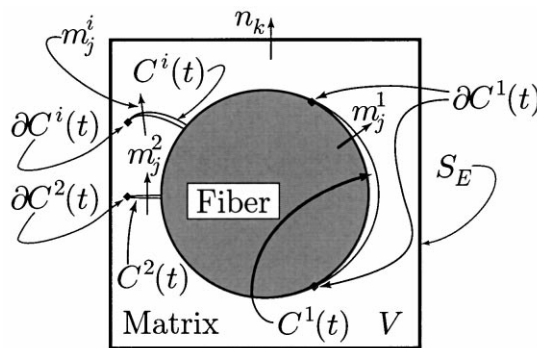


Fig. 1. RVE with linear elastic constituents and growing cracks.

2.2. Volume averages and macroscopic quantities

For an RVE without cracks, the volume average of a generic field ϕ is denoted by $\bar{\phi}$ and defined as follows:

$$\bar{\phi} := \frac{1}{V} \int_V \phi \, dV, \tag{6}$$

where V also denotes the measure of the RVE volume. This definition is made invalid by the presence of growing cracks and must therefore be modified. Hence, let $S_C^{*i}(t)$ be the envelope surface of all the spheres of radius δ having center on the i -th crack. Let c_j^i be the velocity vector characterizing the advancement of $\partial C^i(t)$ and c_j^{*i} the corresponding velocity field induced by c_j^i on S_C^{*i} . Finally, let V_C^{*i} be the volume bounded by the surface S_C^{*i} . The volume average operation is now redefined as follows (cf Bui and Ehrlacher, 1980; Bui et al., 1982; Costanzo et al., 1996; Stolz, 1986):

$$\bar{\phi} := \lim_{\delta \rightarrow 0} \left(\frac{1}{V_\delta} \int_{V_\delta} \phi \, dV \right) = \frac{1}{V} \lim_{\delta \rightarrow 0} \int_{V_\delta} \phi \, dV, \tag{7}$$

where $V_\delta := V - \sum_{i=1}^N V_C^{*i}$ (note that the $\lim_{\delta \rightarrow 0} V_C^{*i} = 0$). In the presence of growing cracks, it is important to take time derivatives of volume average variables. Hence, it is useful to have an expression for the time derivative of the quantity defined in Eq. (7). It can be shown (Bui et al., 1982; Costanzo et al., 1996) that the material time derivative of a volume averaged quantity takes on the form:

$$\dot{\bar{\phi}} = \bar{\dot{\phi}} - \frac{1}{V} \sum_{i=1}^N \lim_{\delta \rightarrow 0} \int_{\partial C^{*i}} \phi c_j^{*i} v_j^{*i} \, dA \tag{8}$$

where the dot over a quantity denotes the time derivative of that quantity, ∂C^{*i} is the envelope of all spheres with radius δ and center on ∂C^i , and v_j^* is the unit normal orienting ∂C^{*i} outward with respect to the volume enclosed by ∂C^{*i} . In order to properly use Eq. (8), one must make some assumptions concerning the strength of the singularity of the various mechanical fields in the vicinity of the crack front. Using fracture mechanics as a guide (cf Costanzo et al., 1996; Kanninen and Popelar, 1985), it is assumed that the stress and strain fields σ_{ij} and ε_{ij} are singular as $r^{-1/2}$ where r is the distance from the crack front measured on a plane perpendicular to the crack front itself.

The various mechanical fields within the RVE will be referred to as local or microscopic quantities, whereas macroscopic quantities will be those obtained by averaging local fields. Perhaps the most important macroscopic parameters are the average strain and stress. The macroscopic strain is denoted by E_{ij} and is defined as the boundary average of the tensor product between the displacement field and the unit normal orienting the RVE boundary:

$$E_{ij} := \frac{1}{2V} \int_{S_E} (u_i n_j + u_j n_i) \, dA. \tag{9}$$

In the absence of cracks this definition coincides with the volume average of the microscopic strain. When cracks are present, the relation between the average strain and the macroscopic strain is given by:

$$\bar{\varepsilon}_{ij} = E_{ij} + \sum_{p=1}^N D_{ij}^p, \tag{10}$$

where

$$D_{ij}^p := \frac{1}{2V} \int_{C^p} ([u_i]m_j^p + [u_j]m_i^p) dA \quad (11)$$

are the so-called Vakulenko–Kachanov variables (Vakulenko and Kachanov, 1971). The macroscopic stress tensor is denoted by Σ_{ij} is defined as follows:

$$\Sigma_{ij} := \frac{1}{2V} \int_{S_E} (\sigma_{ik}n_k x_j + \sigma_{jk}n_k x_i) dA. \quad (12)$$

It is not difficult to show (cf Costanzo et al., 1996) that

$$\Sigma_{ij} = \overline{\sigma_{ij}}, \quad (13)$$

where it is assumed that $\sigma_{ij}^{\pm} m_j^k = 0$ on the surface of any open crack. Also, as a consequence of Eq. (8) and of the assumption concerning the stress and strain singularities at the various crack fronts we have that

$$\dot{E}_{ij} = \frac{1}{2V} \int_{S_E} (\dot{u}_i n_j + \dot{u}_j n_i) dA \quad \text{and} \quad \dot{\Sigma}_{ij} = \overline{\dot{\sigma}_{ij}}. \quad (14)$$

2.3. Boundary conditions

Ideally, one may wish to associate to a given value of a certain macroscopic state variable the microscopic field that generates such an average while keeping the equilibrium and local constitutive equations satisfied (cf Maugin, 1992; Suquet, 1985, 1987). Clearly, this is an inverse problem which may not be always well-posed. However, this can be achieved for the macroscopic strain and stress as long as the underlying boundary conditions are chosen among the following three types.

2.3.1. Uniform stress

$$T_i(x_k, t) = \Sigma_{ij}(t)n_j, \quad (15)$$

where $x_k \in S_E$ and Σ_{ij} satisfies Eq. (13).

2.3.2. Uniform strain

$$u_i(x_k, t) = E_{ik}(t)x_k, \quad (16)$$

where $x_k \in S_E$ and E_{ij} satisfies Eq. (9).

2.3.3. Periodic boundary conditions

$$u_i(x_k, t) = E_{ik}(t)x_k + u_i^*(x_k, t), \quad (17)$$

where $x_k \in \text{RVE}$, $u_i^*(x_k, t)$ is an RVE-periodic displacement function, that is, a periodic function of space whose period is the x_q -direction in the RVE size in that direction. Eq. (17) must also be complemented with the condition that the boundary traction field be anti-periodic.

Under any one of the boundary conditions listed above, one can show (cf Maugin, 1992) that the

following relation, often referred to as the Hill–Mandel macrohomogeneity condition (Hill, 1963, 1965a, b; Mandel, 1964, 1977) is satisfied:

$$E_{ij}\Sigma_{ij} = \overline{\varepsilon_{ij}\sigma_{ij}}. \quad (18)$$

Furthermore, when the damage is in the form of cracks and when the assumptions on the nature of the stress and strain singularities discussed earlier are satisfied, one can show (cf Costanzo et al., 1996) that macrohomogeneity condition can also be given the following rate form:

$$\dot{E}_{ij}\Sigma_{ij} = \overline{\dot{\varepsilon}_{ij}\sigma_{ij}}. \quad (19)$$

2.4. Crack growth laws and elastic localization

For a fixed configuration of (non-growing) cracks, Eqs. (3)–(5), (9) and (12), along with one of the boundary conditions listed in the previous section define a boundary value problem (BVP) whose solution exists and is unique (cf Suquet, 1987). The situation is slightly more complicated for problems where possible crack closure occurs but even in this case one can show existence and uniqueness of solutions (cf Andrieux, 1981; Bensoussan et al., 1978; Leguillon and Sanchez-Palencia, 1982; Suquet, 1981). The case of a problem with growing cracks changes the nature of the problem in a rather significant way. In fact, the problem becomes an initial-boundary value problem (IBVP) whose nature strongly depends on the evolution equations that govern the crack evolution.

The existence and uniqueness of solutions to an IBVP where a system of cracks grows in an elastic medium with a pointwise convex strain energy function and where the crack propagation is governed by the Griffith criterion (Griffith, 1921) has been discussed by Nguyen (1980, 1985) and Nguyen et al. (1990). These problems have been shown to have a formal structure that is essentially identical to that of IBVP characterized by the quasi-static evolution of plastic flow in an elastic perfectly–plastic medium. The consequence of this analogy is that IBVPs where a system of Griffith cracks grows quasi-statically in an elastic medium do not, in general, yield unique solutions. Furthermore, these problems may be characterized by unstable crack growth where the latter may appear while the system evolution is still unique or it may follow a stable bifurcation point (Nguyen, 1985; Nguyen et al., 1990; Triantafyllidis, 1983). The origin of this behavior is to be found in the discontinuous nature of the Griffith criterion, which does not limit the rate at which a crack can grow once the energy release rate G reaches its critical value G^{cr} . If the applied load history is such that G attempts to become larger than G^{cr} the crack will grow of an amount and at a rate that keeps $G = G^{cr}$, in the same way that plastic flow occurs so that the stress state never goes outside the yield surface in an IBVP with an elastic perfectly–plastic material. Thus, using the analogy with plasticity theory, to define a quasi-static IBVP characterized by the existence and uniqueness of stable solutions, a more regular crack growth law can be defined by including time dependence in the crack growth law. This can be accomplished in a simple way by considering a crack evolution law of the following type (cf Coussy, 1986; Schapery, 1975a, b, c):

$$\dot{l}_i = \eta_i \langle G_i - G_i^{cr} \rangle, \quad (20)$$

where $i = 1, \dots, N$, η_i will be referred to as the crack growth viscosity coefficient for the i -th crack, G_i and G_i^{cr} are the energy release rate and its corresponding critical value for the i -th crack, and where $\langle \cdot \rangle$ denote the positive part operator, that is,

$$\langle \phi \rangle = \begin{cases} 0 & \text{if } \phi \leq 0, \\ \phi & \text{if } \phi > 0, \end{cases} \quad (21)$$

ϕ being a scalar quantity. Clearly the evolution laws in Eq. (20) make sense only in a two-dimensional context and a generalization should be provided for a general three-dimensional case. Henceforth however, for convenience, we will limit ourselves to two-dimensional cases only. Before proceeding further, it should be noted that the case of crack evolution under the classical Griffith criterion can be achieved as a limit case of the laws in Eq. (20) by letting $\eta_i \rightarrow \infty$. Furthermore, the evolution law(s) in Eq. (20) can be considered time dependent since the term $G_i - G_i^{cr}$ depends on the applied strain history, which, in turn, is a function of time.

Eqs. (3)–(5), (9) and (12), along with one of the initial/boundary conditions (I/BCs) listed in the previous section, with the crack evolution laws in Eq. (20), and, finally, a crack configuration initial condition of the type

$$l_i(0) = \hat{l}_i, \quad (22)$$

define a well-posed quasi-static IBVP.

The unique solution to the IBVP defined above can be given the form

$$\varepsilon_{ij}(x_q, t) = A_{ijkl}(x_q, t)E_{kl}(t), \quad (23)$$

where the fourth-order tensor function $A_{ijkl}(x_q, t)$ is referred to as the elastic strain localization tensor (or, more concisely, localization tensor). The time dependence in the localization tensor is not a reflection of the applied load history⁴, but rather arises from the damage evolution, i.e., A_{ijkl} would be a constant function if the cracks were not present or if they did not grow.

2.5. Effective elastic moduli

Once the localization problem is solved, the effective elastic moduli, denoted by $A_{ijkl}(t)$, are obtained via a straightforward application of the macrohomogeneity condition in Eq. (19). This operation results in the following expression for the effective moduli:

$$A_{ijkl}(t) = \overline{a_{pqrs} A_{ijpq} A_{rskl}}. \quad (24)$$

Now that the effective elastic moduli have been derived a few remarks are in order.

Remark 1. (Summary of assumptions). The homogenization procedure illustrated above is built upon all of the assumptions that define the corresponding localization problem. In particular, the chosen boundary and initial conditions limit the generality of the derived effective moduli. In other words, the effective moduli in Eq. (24) are not valid for any load history and initial crack configurations but only for those assigned in the construction of the localization problem. Clearly, the dependence on initial conditions also includes the initial microcracking configuration. Furthermore, the crack growth evolution laws and the growth rates are accounted for via the localization tensor $A_{ijkl}(x_q, t)$.

Remark 2. (Practical considerations). Recalling the discussion in the introduction and in view of Remark 1, one can easily see that the effective moduli delivered by this procedure are not of immediate practical use, unless one has the capability to include in the homogenization procedure the set of all possible initial crack configurations and all possible applied load histories. This was successfully accomplished by

⁴ Here, a load history consists of a macroscopic stress history, if the I/BCs are of type 1, or of a macroscopic strain history if the I/BCs are of type 2 or 3.

Ponte-Castañeda and Zaidman (1996a, b) in the derivation of the constitutive equations of a viscoplastic (but not elastic) matrix with evolving ellipsoidal voids. In Ponte-Castañeda and Zaidman (1996a, b) the particular microstructure studied is such that the geometry of a void is completely described by six scalar parameters, i.e., the three ellipsoidal semi-axes and their direction cosines. Furthermore, the assumptions regarding the geometry of the voids and their concentration allows one to analytically construct a localization procedure in terms of Eshelby tensors (Eshelby, 1957). This is equivalent to solving the localization problem in closed form. In turn, this means that the parameters that define the I/BCs as well as the applied load history appear explicitly in the expression of the effective moduli and can therefore be varied arbitrarily. Clearly, this situation cannot be achieved for general composites with growing cracks because, in general, there are no closed form solutions of these problems unless, of course, one assumes that the cracks are flat ellipsoids surrounded by a homogeneous material.

3. Damage space definition and discretization

In view of Remark 1, the localization problem discussed in Section 2.4 is given the following reformulation (cf Germain, 1982; Maugin, 1992; Nguyen, 1985; Nguyen et al., 1990):

$$\dot{l}_i(t) = \eta_i \langle G_i(t) - G_i^{cr} \rangle, \tag{25}$$

$$G_i(t) = - \frac{\partial \mathcal{H}(E_{ij}(t); l_1(t), \dots, l_N(t))}{\partial l_i}, \tag{26}$$

$$\mathcal{H}(E_{ij}(t); l_1(t), \dots, l_N(t)) = \min_{u_k^* \in K(E_{ij}(t); l_1(t), \dots, l_N(t))} \mathcal{E}(u_k^*(x_q, t), l_1(t), \dots, l_N(t)), \tag{27}$$

$$\mathcal{E}(u_p(x_q, t), l_1(t), \dots, l_N(t)) = \int_V \frac{1}{2} a_{ijkl} \varepsilon_{ij}(x_q, t) \varepsilon_{kl}(x_q, t) dV, \tag{28}$$

$$K(E_{ij}(t); l_1(t), \dots, l_N(t)) = \begin{cases} u_i(x_j, t) = E_{ij}(t)x_j & \text{for } x_j \text{ on } S_E, \\ \varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) & \text{for } x_q \in V, \\ [u_m] \geq 0 & \text{on } C^i, \quad i = 1, \dots, N, \end{cases} \tag{29}$$

$$l_i(0) = \hat{l}_i, \tag{30}$$

where K represents the set of all RVE kinematically admissible displacement fields, $\mathcal{E}(u_p(x_q, t), l_1(t), \dots, l_N(t))$ is the RVE total potential energy corresponding to a given displacement field u_p and a given crack configuration $l_1(t), \dots, l_N(t)$, $\mathcal{H}(E_{ij}(t); l_1(t), \dots, l_N(t))$ is the RVE total (Helmholtz) free energy of the equilibrium solution corresponding to a given microscopic strain E_{ij} and a given crack configuration $l_1(t), \dots, l_N(t)$. Clearly, the set K and the form of the total potential energy of the RVE must be changed when using BCs other than those of uniform strain type, although the overall procedure would not change.

The above reformulation is useful because it shows that the evolution of the RVE can be reduced to the study of the IVP consisting of the ordinary differential equations in (25) together with the ICs in (30) as long as the function \mathcal{H} is available. Furthermore, this reformulation shows that the function \mathcal{H}

can be constructed without any reference to a specific load history because time appears in \mathcal{H} only implicitly. Finally, it should be noticed that the function

$$H(E_{ij}(t); l_1(t), \dots, l_N(t)) = \frac{\mathcal{H}}{V}, \quad (31)$$

is the macroscopic Helmholtz free energy of the homogenized equivalent homogeneous material, i.e., it can be easily shown that

$$\Sigma_{ij}(t) = \frac{\partial H(E_{kl}(t); l_1(t), \dots, l_N(t))}{\partial E_{ij}}. \quad (32)$$

Eq. (32) indicates that the N variables $l_1(t), \dots, l_N(t)$ appear in the homogenized constitutive equations of the material as Internal State Variables (ISVs), thus recovering, at least formally, a formulation similar to that sought by continuum damage mechanics.

The above discussion implies that the effective constitutive and evolution equations can be simply obtained once and for all and without reference to a particular load history as long as one properly constructs the function \mathcal{H} . Clearly, it would be impractical to determine the value of \mathcal{H} for all possible values of length of the N cracks present in the problem. However, what can be practically achieved is the computation of the function \mathcal{H} at some specific set of crack length values, while the determination of the value of \mathcal{H} for other crack length configurations can be obtained via interpolation. This strategy will be described next.

With reference to Fig. 2, let the various crack paths of interests be selected and let λ_i represent the non-dimensional length of the i -th crack, that is,

$$\lambda_i = \frac{l_i}{l_{i0}}, \quad 0 \leq \lambda_i \leq 1, \quad i = 1, \dots, N, \quad (33)$$

where l_{i0} represents the maximum crack length achievable by the i -th crack. An N -tuple of values $(\lambda_1, \dots, \lambda_N)$ identifies the coordinates of a point in an N -dimensional space which will be referred to as the damage space. In this context, the set of values $(\lambda_1, \dots, \lambda_N)$ defines a point in the damage space unit cube UC defined as follows:

$$UC = \{(\lambda_1, \dots, \lambda_N) \mid \lambda_i \in [0, 1], \quad i = 1, \dots, N\} \quad (34)$$

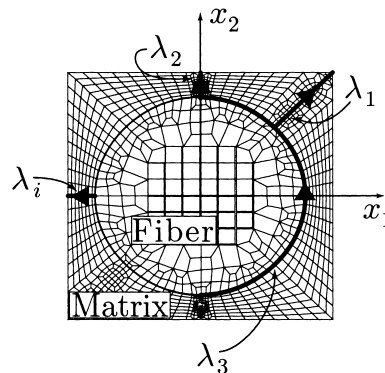


Fig. 2. Schematic RVE with selected crack paths.

Now, for each λ_i consider a finite and discrete set of values $\{\lambda_i^k\}$, with $k = 1, \dots, M_i$, obtained by partitioning the interval $[0, 1]$ in M_i parts:

$$0 = \lambda_i^1 < \lambda_i^2 < \dots < \lambda_i^M = 1. \tag{35}$$

The set $\{\lambda_i^k\}$ will be referred to as a discretization of the i -th crack path. This discretization generates a corresponding discretization of UC given by the Cartesian products of all the sets $\{\lambda_i^k\}$. An example of damage space discretization is depicted in Fig. 3, where, with reference to Fig. 2, it has been assumed that λ_1 and λ_2 are the only cracks present in the RVE. The set of points appearing in Fig. 2 is one of the many sets that one could use to discretize the UC . Going back to the discussion concerning the RVE free energy, one can see that by explicitly calculating H (or \mathcal{H}) at the discrete points $(\lambda_1^k, \lambda_2^k, \dots, \lambda_N^k)$, for a discrete set of macroscopic strain values, all possible values of H for any damage configuration and strain levels can be obtained via an interpolation scheme. The latter would then allow one to obtain all the information necessary to use the constitutive and evolution equations of the composite material. To exemplify this last point consider a case where the system behaves linearly elastically for a fixed configuration of the cracks. Hence, the overall scheme reduces to calculating a finite number of elastic moduli corresponding to the values that these moduli take on at the various points of the discretized UC . In fact, in this case we have

$$H(\lambda_1, \dots, \lambda_N) = \begin{cases} \frac{1}{2} A_{ijkl}(\lambda_1, \dots, \lambda_N) E_{ij} E_{kl} & \text{for } E_{ii} \geq 0, \\ \frac{1}{2} A_{ijkl}(0, \dots, 0) E_{ij} E_{kl} & \text{for } E_{ii} < 0, \end{cases} \tag{36}$$

where, in an approximate sense, the case with $E_{ii} < 0$ is taken to identify crack closure. Specifically, for a damage space discretization such as that depicted in Fig. 3, one only needs to compute the elastic moduli at the 48 points defining the UC discretization using standard homogenization schemes. A possible and simple interpolation scheme to determine the value of the elastic moduli at all other points in the UC can be constructed as follows. Again, with reference to Fig. 3, consider the rectangle of vertices $P_1 = (\lambda_1^m, \lambda_2^n)$, $P_2 = (\lambda_1^{m+1}, \lambda_2^n)$, $P_3 = (\lambda_1^{m+1}, \lambda_2^{n+1})$ and $P_4 = (\lambda_1^m, \lambda_2^{n+1})$, with $1 \leq m \leq M_1$ and $1 \leq n \leq M_2$. Now let A^q_{ijkl} , with $q = 1, 2, 3, 4$, be the values of the elastic moduli at the points P_1, \dots, P_4 . The value of the elastic moduli at points within said rectangle can therefore be determined via the use of the appropriate Lagrange polynomials (cf Hughes, 1987): $\phi_1(\lambda_1, \lambda_2), \dots, \phi_4(\lambda_1, \lambda_2)$, and expressed as follows:

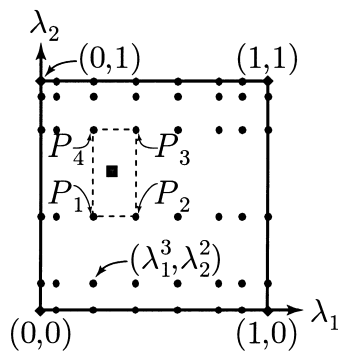


Fig. 3. Discretization scheme for a 2-D damage space.

$$A_{ijkl}(\lambda_1, \lambda_2) = \sum_{q=1}^4 A_{ijkl}^q \phi_q(\lambda_1, \lambda_2), \quad (37)$$

where $\lambda_1 \in [\lambda_1^m, \lambda_1^{m+1}]$ and $\lambda_2 \in [\lambda_2^n, \lambda_2^{n+1}]$. An interpolation scheme of this type is represented in Fig. 4 depicting the value of the coefficient A_{1111} over the entire damage space for a case where the active cracks in the RVE are λ_1 and λ_3 . Clearly, other and more sophisticated interpolation schemes can be constructed in a similar way.

Before illustrating some examples of application of this procedure a number of remarks are in order.

Remark 3. (Damage space discretization and FEM). Fig. 2 shows an RVE along with a number of crack paths and an underlying Finite Element grid. As discussed in Section 4, the latter was used in the solution of the micromechanics problems necessary to determine the elastic moduli at the various points defining the *UC* discretization. What should be noted here is that the FEM grid used to solve the micromechanics problems and the *UC* discretization need not coincide. In fact, in principle the micromechanics necessary to evaluate the function H (or \mathcal{H}) does not need to be carried out using the FEM at all.

Remark 4. (Interpolation within the damage space). The method selected to interpolate the values of the function H (or \mathcal{H}) within the *UC* must be chosen so as to accommodate the smoothness requirements dictated by the selected crack evolution law. In fact, with reference to Eqs. (25) and (26), one sees that the evaluation of the energy release rates requires that the interpolation functions be at least once differentiable. However, if one were to choose linear interpolation functions for the elastic moduli, there may be instances where the energy release is a constant function of the parameters $\lambda_1, \dots, \lambda_N$ for a certain range of these parameters. Hence, depending on the desired accuracy, one may need to use interpolation functions that are smoother than the minimum required by the particular evolution law at hand.

Remark 5. (*UC* discretization and thermodynamics). From the viewpoint of continuum thermodynamics, the choice of a crack path is equivalent to the definition of an ISV. Hence, the example depicted in Fig. 3 along with Eqs. (36), defines a nonlinear material with two internal state variables. The corresponding

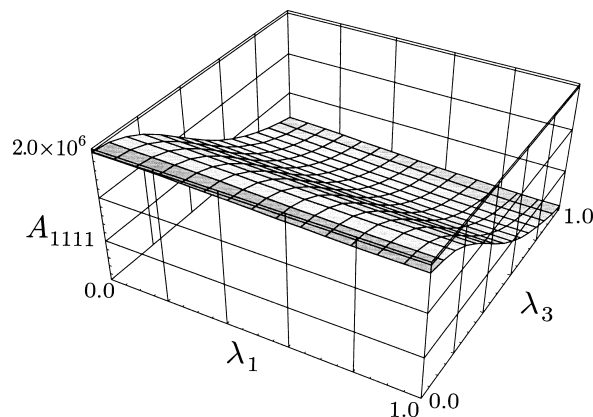


Fig. 4. Surface representing the elastic coefficient A_{1111} as a function of the two damage variables λ_1 and λ_3 , obtained using a bilinear interpolation scheme.

crack growth laws in Eqs. (25) provide the necessary internal state evolution laws. Thus, the procedure outlined above delivers equations of the same type as those usually proposed within a phenomenological theory such as CDM. To stress the fact that the present approach is actually homogenization-based and that the final form of the effective constitutive equations are obtained using the concept of damage space discretization, it will be referred to as a Discretized Damage Space Homogenization Method (DDSHM). The DDSHM differs from a global–local approach in that the DDSHM delivers the constitutive equations of the composite material at hand without reference to a particular applied load history. This quality originates from the selection of a finite number of crack paths. Hence, it could be argued that, depending on the complexity of the system's microstructure, the DDSHM is just as numerically involved as a full scale GL analysis. However, for some problems there may be conditions that may make this approximation scheme preferable and significantly more flexible than a GL analysis. In fact, experience tells us that not all theoretically possible crack paths are relevant to the understanding of a given composite material system. Furthermore, even if one were to perform a GL analysis choices must be made as to the selection of these paths and for this reason a GL analysis would yield essentially as much accuracy as the proposed approach, without the added benefit of having a 'stand-alone' set of constitutive equations. Hence, despite the fact that the approach proposed above may not prove to be always more efficient than a corresponding GL analysis, there may be a rather wide spectrum of problems for which it may indeed be more efficient.

4. Examples

In this section we present results of numerical calculations to illustrate the implementation of the theory presented in Sections 2 and 3. In the examples reported herein, we have limited the maximum dimension of the damage space to 2, i.e., there are at most two possible crack paths active at any one time. This will simplify the graphical presentation of the results. For each of the examples, the crack evolution laws used are those in Eq. (25). For the one-dimensional case, the damage space discretization consisted of 29 points, whereas a total of 464 points were used in the two-dimensional case. To calculate the homogenized elastic coefficients at these points an FEM based homogenization scheme was used where the FEM grid employed is that in Fig. 2 and the boundary conditions were chosen to be of the 'uniform strain' type. As far as the interpolation strategy adopted in the following examples is concerned, second-order Lagrange polynomials (cf Hughes, 1987) were used in both the one- and two-dimensional cases.

One of the goals of this work is to develop and demonstrate a theory for modeling constitutive relations for nonlinear composite materials with growing cracks which is suitable for use with general purpose structural analysis packages. In this regard, it is important to note that all results that follow have been obtained by assigning a strain history to a material point whose constitutive relations had been derived with no prior knowledge of the applied load history, i.e., not by solving a micromechanics problem for each point in time as one would do if using a GL approach. The strain histories assigned to said material point are precisely the type of load history definition used in the ABAQUS (HKS, 1998) finite element program. Simple monotonic and more complex cyclic strain histories were studied. In all cases, the coupled set of nonlinear ordinary differential equations in (25) was solved numerically using a Runge–Kutta algorithm with adaptive time step size control (Press et al., 1986).

4.1. Single crack problem

With reference to Fig. 2, a square RVE with a single crack is now considered. The single crack path selected in this example is that denoted by λ_3 , that is, a disbond crack. The RVE constituents are assumed to behave linearly elastically, so that the resulting effective constitutive equations of the composite are of those in Eq. (36), with $N = 1$.

The composite material response to three different applied strain histories of the type $E_{11} = E_{12} = E(t)$, $E_{22} = 0$, is depicted in Fig. 5 where the initial disbond condition has been chosen to be $\lambda_3(0) = 0.2$. The nominal value of E_0 used in this case was 0.005. This simple one-dimensional example yields the expected evolution of the microstructural state: due to the evolutions laws in Eq. (25), the rate at which the crack propagates is higher for the higher applied strain rate.

Figs. 6 and 7 illustrate the sensitivity of the effective material response to various values of the regularization parameter η in Eq. (25). In particular, Figs. 6 and 7 represent the response to a ‘relaxation’ test-type load $E_{22}(t) = E_{22}^0 = \text{const.}$, where the value given to E_{22}^0 was chosen to be just large enough to cause crack growth. As the value of η increases the damage evolution seems to take on an unstable character, that is, λ_3 jumps almost instantaneously from its initial length to an equilibrium value which depends on the magnitude of the applied strain. This behavior can be explained by recalling that as the value of η is increased, the crack evolution law in Eq. (25) tends to approximate the crack growth behavior that is governed by the Griffith criterion. The latter allows one to predict stable crack growth only when the second derivative of the elastic strain energy with respect to crack length is positive (Nguyen et al., 1990). Since the material discussed herein contains λ_3 as the only ISV, using Eq. (36), and recalling that the example at hand is characterized by $E_{11} = E_{12} = 0$ while $E_{22} = E_{22}^0 = \text{const.}$, this positivity condition takes on the form

$$\frac{d^2H}{d\lambda_3^2} = \frac{1}{2} \frac{d^2A_{2222}}{d\lambda_3^2} (E_{22}^0)^2 > 0. \tag{38}$$

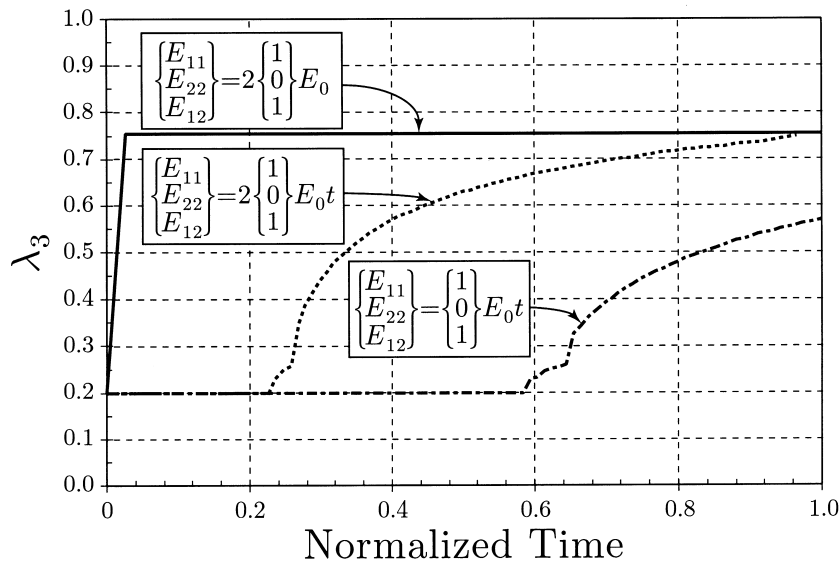


Fig. 5. Evolution of the ISV λ_3 due to three different applied strain histories.

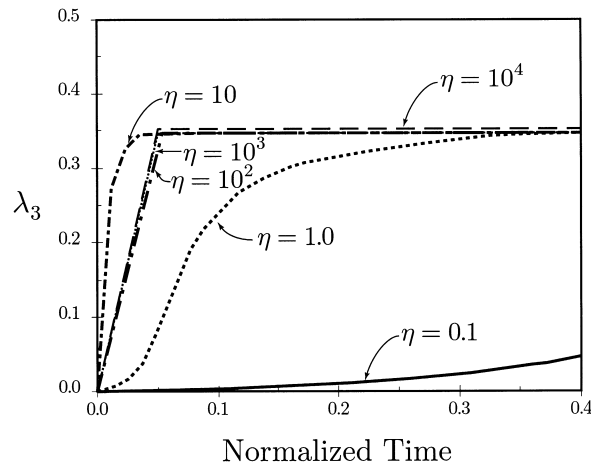


Fig. 6. Evolution of the ISV λ_3 due to a constant applied strain as a function of the parameter η .

In other words, said positivity condition can be translated into a positivity condition for the second derivative of the elastic modulus A_{2222} with respect to the damage variable λ_3 . As displayed in Fig. 8, the elastic moduli of the effective medium at hand are characterized by a downward concavity for $\lambda_3 = 0$, i.e., at the initial condition used to generate Figs. 6 and 7, thus confirming that an initial unstable behavior under the constraints imposed by the Griffith criterion is to be expected. It should be noted that the equilibrium value reached by the ISV λ_3 of roughly 0.35 corresponds to a region of shallow but positive concavity of the A_{2222} elastic modulus, the latter being the only relevant elastic modulus in this discussion.

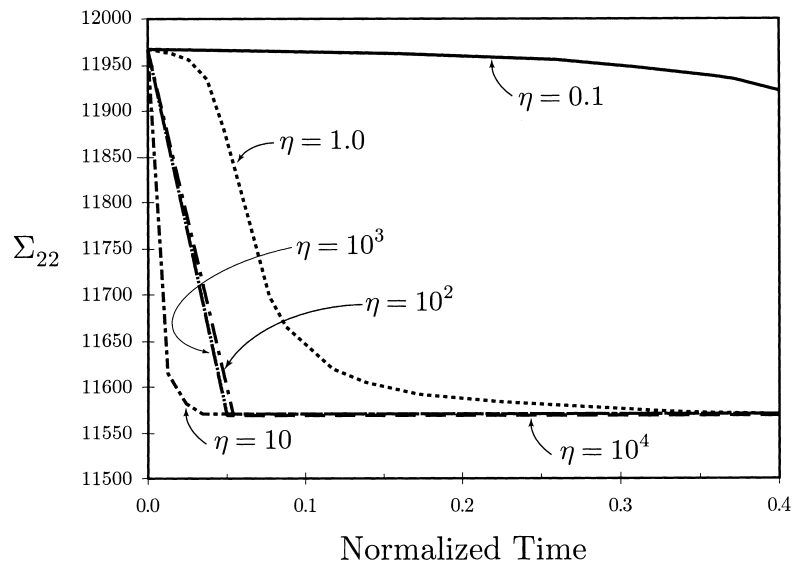


Fig. 7. Evolution of the macroscopic stress component Σ_{22} corresponding to the damage evolution displayed in Fig. 6, due to a constant applied strain and as a function of the parameter η .

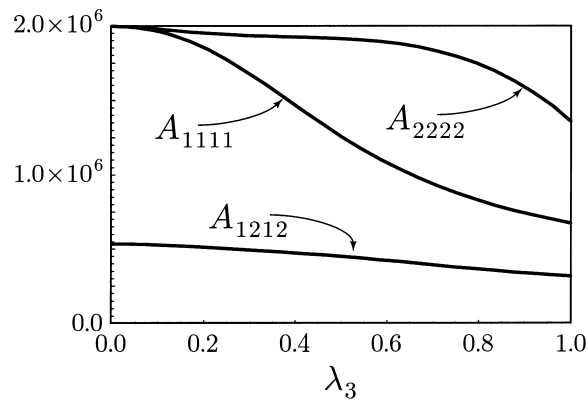


Fig. 8. Effective elastic moduli for the two-dimensional RVE in Fig. 2, as a function of the damage variable λ_3 (while $\lambda_1 = \lambda_2 = 0$).

We now consider a case with cyclic loading. The applied load history, ISV evolution, and macroscopic stress versus macroscopic strain results for this case are shown in Figs. 9–11. It should be noted that the strain history depicted in Fig. 9 regards only the E_{11} component of the strain tensor since the other two components are null throughout the loading sequence. Careful examination of Fig. 11 reveals slight nonlinearity at the end of the first load increment due to the small growth of the fiber–matrix disbond (cf Fig. 10). The return path (during the first unloading) is linear since there is no further damage growth during unloading, but differs slightly from the initial load path due to the reduced effective stiffness. The disbond reaches its full extent near the end of the third time step (as E_{11} approaches 0.008). Finally note the unload–reload stiffness, as E_{11} goes from 0.008, back to 0 and up again to 0.010, is very different from its initial value.

4.2. A case with a two-dimensional damage space: monotonic, cyclic and general loadings

In this section we present results regarding the evolution of a linear elastic material with two damage internal state variables. Despite the fact that the number of ISVs is limited to two, these examples illustrate features typical of constitutive equations with several ISVs. In fact, they show that

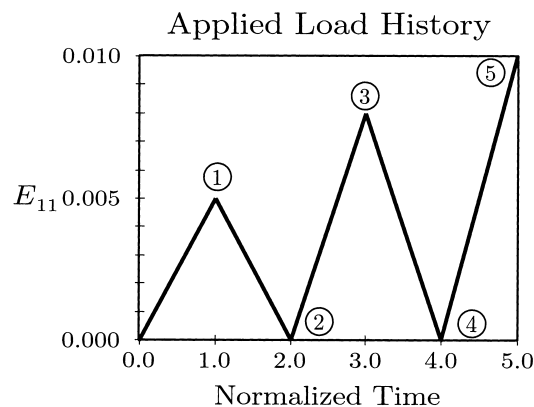


Fig. 9. Cyclic loading case: applied macroscopic strain as a function of time.

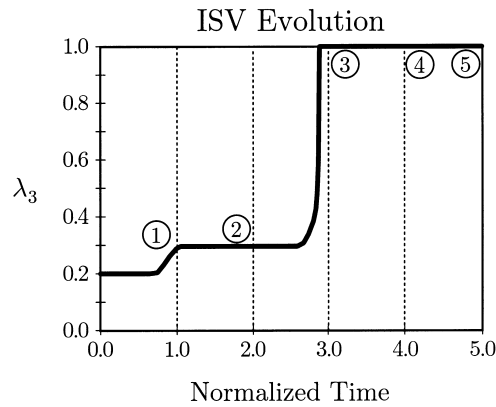


Fig. 10. Cyclic loading case: response of the effective medium in terms of the internal state variable λ_3 .

microstructural evolution in an RVE with multiple possible damage paths depends on many factors such as the applied strain history, the initial damage state, and the value of the critical energy release rates G_i^{cr} for each damage path.

Results, both in terms of the ISV evolution and stress–strain response, for a monotonic uniaxial tension strain in the ‘11’ direction and a monotonic shear strain in the ‘12’ direction are shown in Figs. 12 and 13, respectively. The ISVs λ_1 and λ_3 are those defined in Fig. 2. In both Fig. 12 and Fig. 13 the stress–strain behavior is characterized by a pronounced drop coinciding with the beginning of damage growth. In particular, Fig. 12 shows a rather sharp drop in the stress due to the fact that both λ_1 and λ_3 start growing almost simultaneously, whereas the gradual softening or rounding of the shear stress–strain curve in Fig. 13 is a direct result of the fact that there is a noticeable delay in the λ_1 growth with respect to that of λ_3 . Also, although it is difficult to detect it from the figures, the branches of the stress–strain curves corresponding to a growth of the ISVs are non-linear. Linearity in the stress–strain behavior is recovered only when the ISVs reach their maximum value. In both cases, the fact that said nonlinear behavior is barely noticeable is caused by the dominating behavior of λ_3 which (in both cases) reaches its maximum value rather quickly after it starts growing.

Fig. 14 shows the ISVs propagation trajectories in the two-dimensional damage space unit cube (cf Fig. 3). The applied strain history used to obtain the various curves appearing in Fig. 14 consists of a

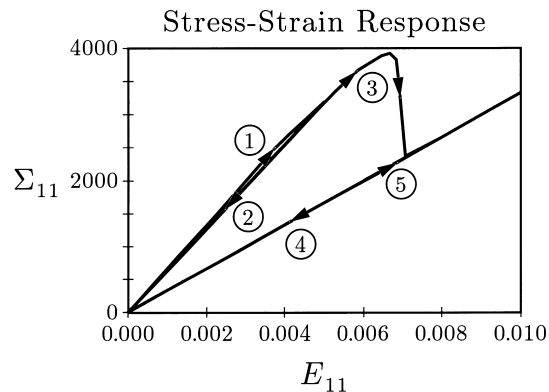


Fig. 11. Cyclic loading case: effective medium response in terms of the Σ_{11} – E_{11} stress–strain curve.

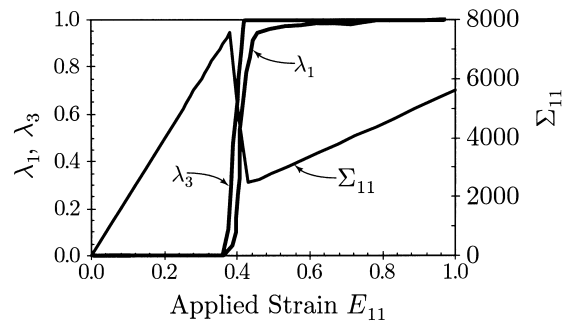


Fig. 12. Constitutive response with two ISVs: monotonic tensile loading consisting of an applied strain in the ‘11’ direction while the other components of strain are kept equal to zero.

linear function of time:

$$\begin{Bmatrix} E_{11}(t) \\ E_{22}(t) \\ E_{12}(t) \end{Bmatrix} = \begin{Bmatrix} 0.005 \\ 0.000 \\ 0.005 \end{Bmatrix} t. \quad (39)$$

Said curves differ from one another by the value given to initial conditions, i.e., the initial value of the damage state. That the initial conditions affect the damage evolution paths is a result to be expected since the ISV trajectories are governed by the gradient of the Helmholtz free energy with respect to the damage state vector. In this case, such a gradient is directly associated to the slope of the surfaces of the elastic moduli (cf Fig. 4). Another factor that strongly influences the trajectory followed by the system in damage space is the relative value of the critical energy release rates for a given ISV with respect to that of all other ISVs. This effect is illustrated in Fig. 15 depicting various trajectories obtained using the strain history in Eq. (39), with a fixed initial condition, a fixed value of G_1^{cr} and various values of G_3^{cr} . For $G_3^{cr} = G_1^{cr}$, λ_3 grows faster than λ_1 , and, as the value of G_3^{cr} is increased relative to G_1^{cr} , the trajectory in damage space will tend to become dominated by the λ_1 growth, as expected.

Results for a cyclic load history are summarized in Figs. 16–18. Several different instantaneous stiffnesses are present during the load–reload cycles due to the staggered growth of the ISVs. The lagging of λ_1 behind λ_3 , and the ultimate very quick propagation of this crack near the end of the third time step, produces the interesting ratcheting stress–strain curve shown in Fig. 18. A final lower bound

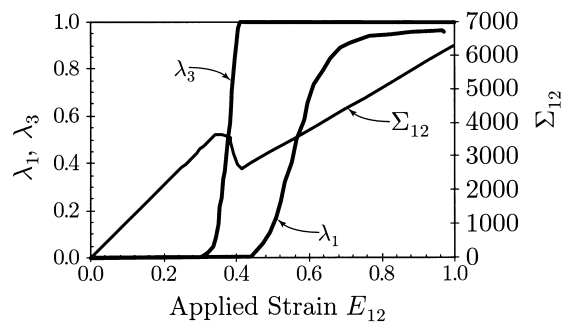


Fig. 13. Constitutive response with two ISVs: monotonic shear loading consisting of an applied strain in the ‘12’ direction while the other components of strain are kept equal to zero.

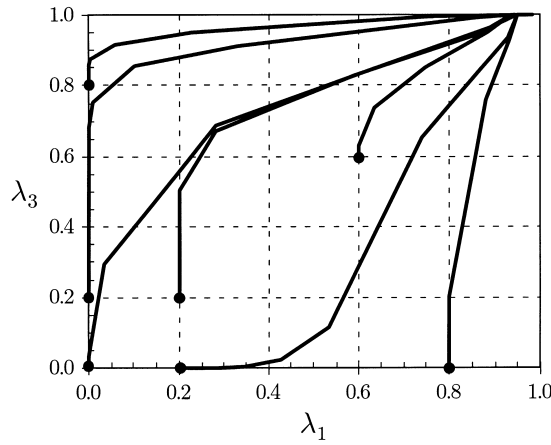


Fig. 14. Monotonic loading case: evolution of the ISVs as a function of initial conditions.

for the effective macroscopic stiffness is obtained during the final load cycle since both ISVs have reached their maximum values.

We now investigate the effect that the applied strain history sequence can have on damage evolution. In particular, with reference to the top two graphs in Fig. 19, we subject the homogenized material point to a load function having both an E_{12} and an E_{22} strain history component. The applied strain history two differs from the applied strain history one only in that the application of the E_{12} history precedes the E_{22} history, contrary to what was done in the applied strain history one. However, the final loading stage for both sequences is the same, and, overall, the maximum strain at any given time is the same for both applied strain sequences. These loading sequences were chosen so as to address the following questions:

1. do both load histories eventually produce the same damage state; and
2. are the final apparent effective moduli or macroscopic stresses equal?

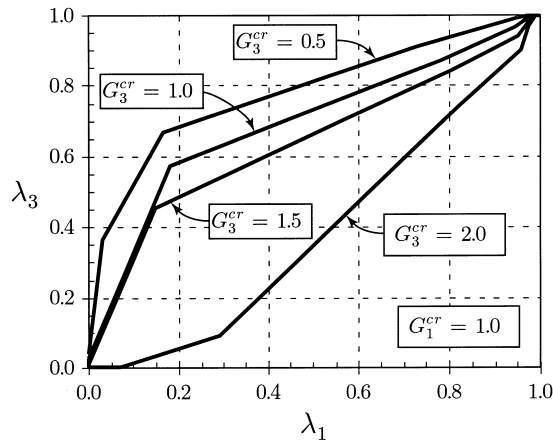


Fig. 15. Monotonic loading case: evolution of the ISVs as a function of the ratio G_3^{cr}/G_1^{cr} , that is, the ratio between the critical values of the energy release rates of the two ISVs characterizing the effective constitutive response of the material.

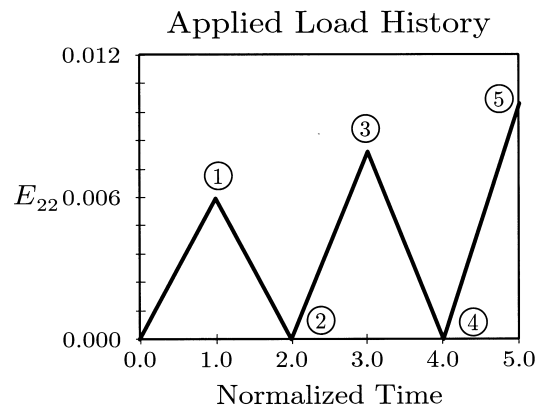


Fig. 16. Cyclic loading case: applied strain history.

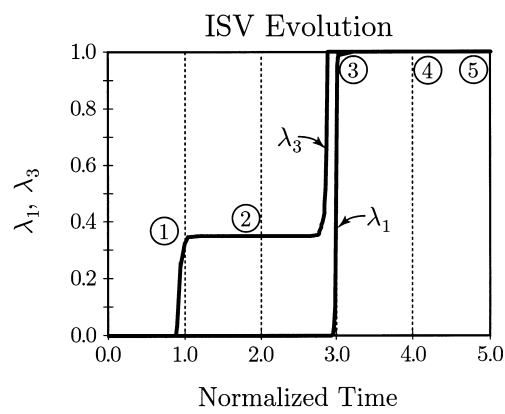


Fig. 17. Cyclic loading case: evolution of the ISVs as a function of time.

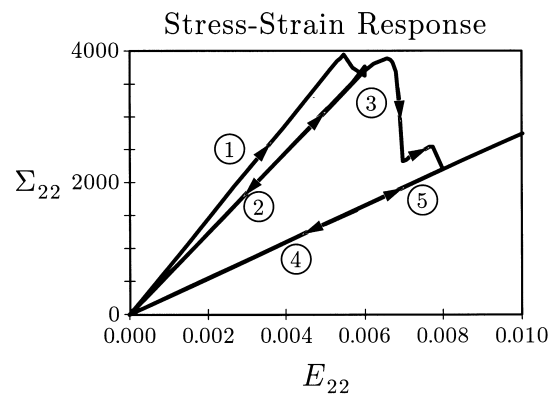


Fig. 18. Cyclic loading case: stress-strain curve.

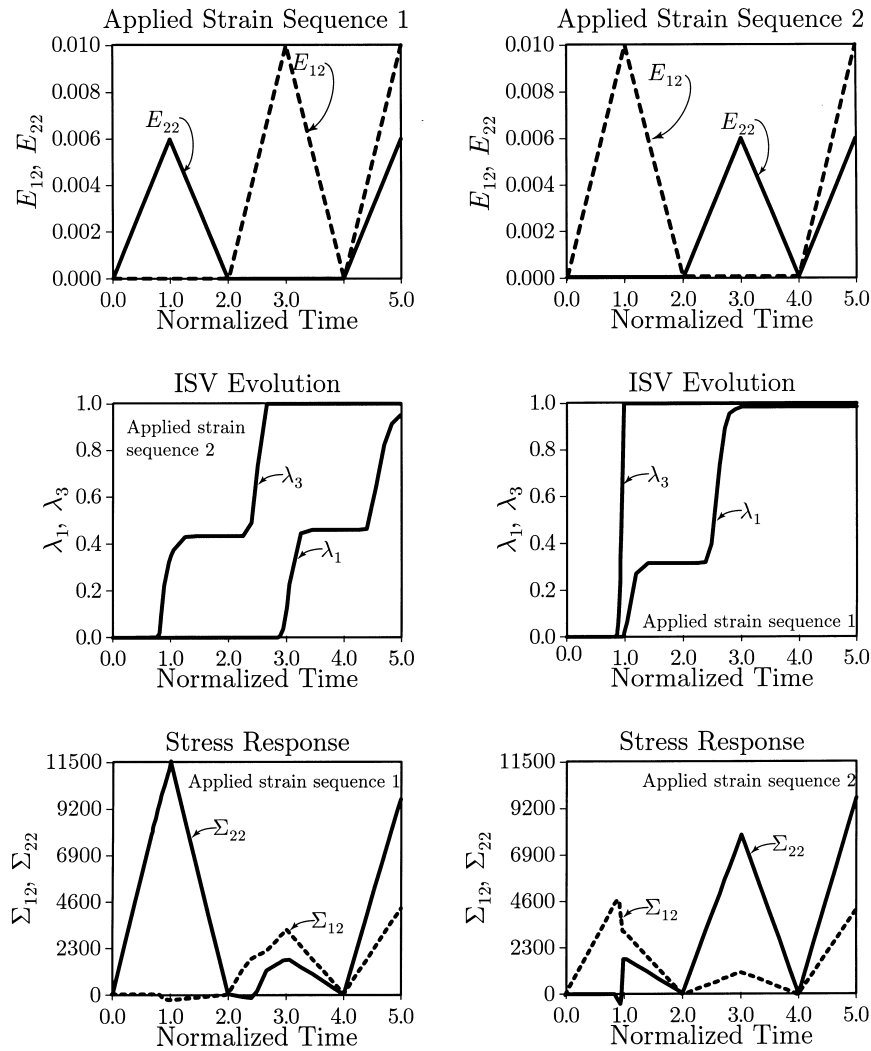


Fig. 19. Effects of the applied strain history sequence on the material response.

To address these issues, consider load sequence 2, where a shear E_{12} strain is applied first. Near the end of the first step, i.e., for $t = 1$, the disbond crack reaches its full extent (i.e., $\lambda_3 = 1$). This is reflected in a small but sudden drop in the stresses, as shown in the bottom right graph in Fig. 19. The microstructural change associated to λ_3 taking on its maximum value, is also reflected in an increase in the available energy release rate driving the evolution of λ_1 ⁵. This explains why, despite the unloading taking place for $1 \leq t \leq 2$ in the first load sequence, λ_1 starts growing. This behavior should be contrasted to that caused by the first load sequence, where λ_3 reaches its full extent only after $t = 2.5$ and where λ_1 never quite reaches its maximum. The latter is achieved during sequence two soon after $t = 2.5$. Also, if one compares the behavior in terms of stresses due to the two applied strain histories, it

⁵ For fixed values of E_{22} and λ_1 , $G_1(\lambda_1, \lambda_3)$ is a monotonic increasing function of λ_3 .

is clear that the maximum stresses reached during the load sequences differ, except, perhaps, at $t = 5.0$ when both λ_1 and λ_3 have fully extended and a linear stress–strain behavior is recovered. This indicates that, while the maximum applied strain, whether in the ‘12’ or ‘22’ direction, is the same for the two load sequences, the overall evolution responses produced are very different in the two cases. The fact that, once the damage parameters reach their full extent, the subsequent material response is linear although with reduced macroscopic moduli is consistent with the so-called characteristic damage state proposed by other authors such as Reifsnider and Masters (1982).

From a practical viewpoint, these analyses reinforce the physically intuitive idea that the overall stress response depends not only on the damage growth caused by the current load step, but also on the current value of all of the ISVs caused by the entire preceding load history. In turn, this means that in an experimental setting one cannot rely on the idea that a given load history for an individual strain component (while keeping fixed all other components of strain) induces a characteristic damage accumulation which is applicable to all load histories.

5. Conclusions

The computational procedure described in this paper, delivers a set of constitutive and evolution equations for composite materials with growing cracks without knowledge of the load history to be later imposed on a given (homogenized) material point. The effective elastic moduli are determined by solving a sequence of BVPs for a finite set of crack paths and values of the selected ISVs, where the latter are chosen to represent a direct measure of crack configuration rather than some average measure. Microstructural evolution under applied load histories are obtained by numerically integrating the set of ODEs that result from energy based crack growth laws. The results presented in this paper were all generated by applying different load strain histories to a single set of constitutive equations. For each case the behavior resulting from the application of said histories was shown to be physically sound, thus showing that the proposed approach does yield constitutive equations applicable to the study of a wide range of diverse loading conditions. Also, because the damage state is known at all points in the time history, sufficient information is available to calculate and report instantaneous stiffness and average RVE stress, as well as to precisely determine the occurrence of local (i.e., pointwise) material instability. This is precisely the information needed when implementing a so-called user defined constitutive relation in a global structural analysis package (e.g. ABAQUS, HKS, 1998). Finally, given its sensitivity to load history, this method can be used as a guide in the design of experiments for the characterization of complex material behavior which is history dependent.

The issues that remain to be addressed to make this approach fully operational, include establishing reliable criteria for the choice of the damage space, that is, what is the type and number of damage paths to select for a given RVE in order to predict damage accumulation to a satisfactory approximation level. A quantitative comparison of the computational efficiency/accuracy that this approach offers when used in an FEM analysis with respect to a full scale GL approach should also be made. These issues will be the object of forthcoming publications.

Acknowledgements

Partial support for this research was provided by the National Science Foundation through the NSF Grant No. CMS-9733653.

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