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HOMOGENIZATION TECHNIQUES FOR THERMOVISCOELASTIC SOLIDS CONTAINING CRACKS

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Abstract—In this paper mathematical techniques are developed for obtaining locally averaged (homogenized) constitutive equations for heterogeneous linear thermoviscoelastic solids. Homogenization principles will be developed for the cases wherein no internal boundaries are present, and also where internal boundaries in the form of sharp cracks are present, thus resulting in damage dependent macroscopic constitutive equations. The microthermomechanics problem will first be formulated, followed by the construction of the locally averaged equations resulting from the homogenization process. It will be shown that homogenized conservation laws and constitutive equations take the same form as do the local equations when locally linear thermoviscoelastic media are considered. However, the resulting homogenized constitutive equations will be nonlinear in the case wherein time dependent damage occurs. In addition, for materials of convolution type at the local scale, the homogenized equations will be shown to contain a term that depends on the time derivative of the strain localization tensor. Example problems will be discussed and the homogenized results will be given for these examples in order to demonstrate the technique. © 1998 Elsevier Science Ltd. All rights reserved.

INTRODUCTION

Solid media used in structural applications often are composed of multiple constituents, such as that observed in composites, alloys, and porous media. Typically, the geometric scales of these constituents are small compared to the scales of the structural components that they are deployed in. Thus, it is usually untenable to model the structural part as a fully heterogeneous medium. Often, these media can be approximated as homogeneous for design purposes even though they are actually heterogeneous. This approximation is assumed to be sufficiently accurate whenever the geometric scale of the heterogeneity is small compared to the scale of the structural part under study. These homogenization principles could, for example, be utilized to construct constitutive models (Allen and Zocher, 1997) for the thermomechanical behavior of process zones and/or cohesive zones in macroscopically monolithic media that are microscopically heterogeneous, such as metals that undergo microsuperplasticity (Shaw *et al.* 1996), and polymers that produce crazing (Kramer and Berger, 1990), as well as a variety of composite media.

The process of homogenization can be accomplished phenomenologically by simply performing material characterization experiments on specimens that are large enough to be statistically homogeneous. However, as previously discussed (Boyd *et al.* 1993), this approach may be difficult to accomplish for a variety of reasons such as material anisotropy at the macroscale. In addition, the phenomenological approach has limited usefulness since it cannot account for certain design parameters such as constituent volume fractions. A second approach for obtaining the macroscopically averaged constitutive equations is to first solve (either analytically or computationally) a microthermomechanics problem for the RVE, and then average this result. This process of averaging the microthermomechanics solution to obtain the locally averaged constitutive equations is often termed homogenization (Hill, 1963), perhaps due to the fact that a spatially heterogeneous medium is represented as a homogeneous one. The procedure appears to have grown from the early works of Hill (1963, 1965a,b, 1967), Hashin (1964) and Mandel (1964), although the idea

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was certainly contained within the earlier research by Eshelby (1957). Most of these initial efforts were devoted to elastic (Hill, 1963, 1965a; Hashin, 1964; Eshelby 1957) or elastoplastic (Hill, 1965b, 1967; Mandel, 1964) media. Several more recent works are also noteworthy on the subject (Bensoussan *et al.* 1978; Andrieux, 1981; Suquet, 1982, 1985; Mandel, 1971, 1977; Stolz, 1986). Significant progress has also been made to extend these homogenization techniques to encompass solids with stationary and/or growing microcracks (Vakulenko and Kachanov, 1971; Kachanov, 1972; Budiansky and O'Connell, 1976; Bui *et al.* 1981, 1982; Horii and Nemat-Nasser, 1983; Costanzo *et al.* 1996). However, to date few systematic efforts have been made to generalize these homogenization procedures to include thermoviscoelasticity in one or more of the phases of the RVE (Hashin, 1966; Schapery, 1967). Furthermore, these efforts have so far failed to emphasize the effects of damage (in the form of internal cracks) on the homogenized constitutive response, although a few papers have appeared wherein specific homogenized constitutive equations have been obtained for viscoelastic micromechanics problems with microcracks (Schapery, 1986; Zocher and Allen, 1997).

In the current paper the authors will briefly review the important historical results obtained in homogenization theory. Homogenization principles will then be developed for the linear thermoviscoelastic case, and example problems will be discussed in order to elucidate the technique.

SOLUTION OF THE MICROTHERMOMECHANICS PROBLEM

Our objective is to obtain macroscopically (also termed locally) averaged field and constitutive equations for the microscopically heterogeneous medium. In order to accomplish this, we must first solve a microthermomechanics problem. Thus, consider a microscopic body $V+\partial V$ that is a small subset of the global domain $V_G+\partial V_G$ and is composed of a finite number of homogeneous subphases, as shown in Fig. 1, such that the

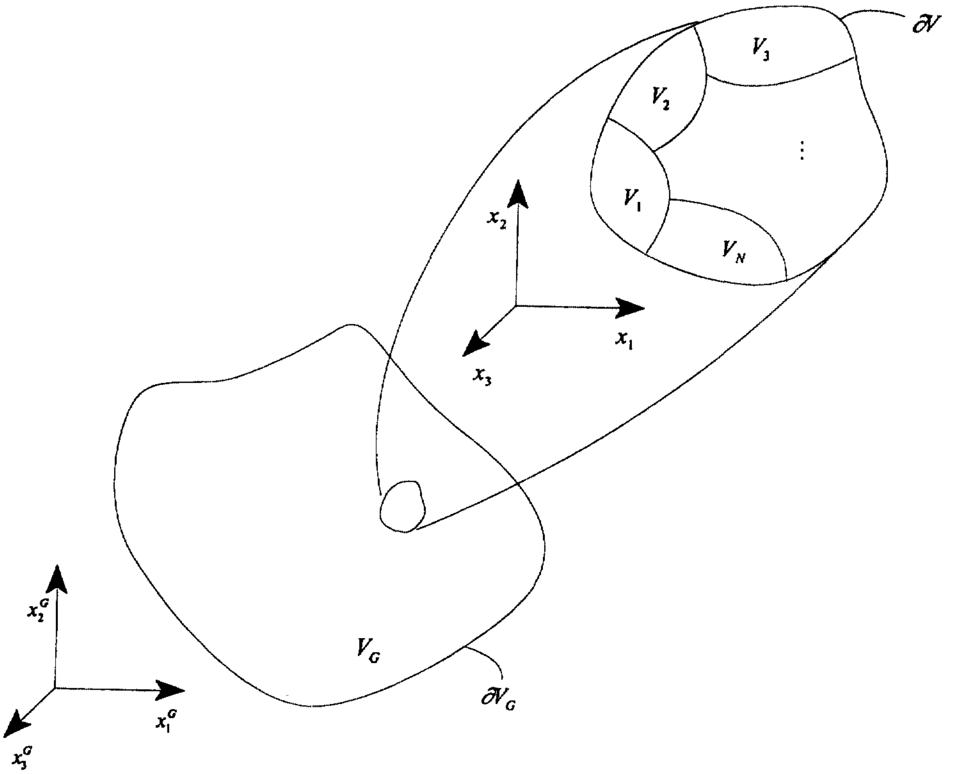

Fig. 1. Macroscopically homogeneous body of interest and microscopically heterogeneous representative volume element.

geometric scale of the body is small compared to the scale of the structural part under consideration. Note that the local (microscopic) body is endowed with coordinates $\mathbf{x}$, whereas the global body (macroscopic) body is endowed with coordinates $\mathbf{x}_G$. Also, suppose that one or more of the subphases may be cracks. Furthermore, suppose that the geometry of the subphases is such that there is either statistical homogeneity within a small subvolume, or a repetitive cell structure. In either case it is possible to consider only a small subdomain of the body, termed a representative volume element (RVE). In the latter case, this is sometimes also called a unit cell.

We begin by posing microthermomechanical boundary value problem for the RVE, which has interior V and boundary ∂V. The boundary value problem for this domain is stated as follows:

(1) Conservation of linear momentum (neglecting body forces and inertial effects):

$$\sigma_{ji,j} = 0 \quad \text{in } V \tag{1}$$

where $,j$ denotes the derivative with respect to the spatial coordinate x_j, σ_{ij} is the Cauchy stress tensor, V does not contain the volume of cracks; and

$$T_i = \sigma_{ji} n_j \quad \text{on } \partial V \tag{2}$$

where T_i is the traction vector, and n_i is the unit outer normal vector on ∂V.
(2) Conservation of angular momentum (neglecting body moments):

$$\sigma_{ji} = \sigma_{ij} \quad \text{in } V + \partial V. \tag{3}$$

(3) Strain–displacement relations (assuming infinitesimal strains):

$$\varepsilon_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}) \quad \text{in } V \tag{4}$$

where u_i is the displacement vector.
(4) Conservation of energy:

$$\dot{u} = \sigma_{ij}\dot{\varepsilon}_{ij} - q_{i,i} \tag{5}$$

where the dot represents the material time derivative, u is the internal energy per unit volume, and q_i is the heat flux vector. Note that we have assumed that there is no internal source term.
(5) The entropy production inequality:

$$\dot{\eta} = \dot{\eta}^{\text{mic}} + \dot{\eta}^{\theta} = \dot{s} + \left(\frac{q_i}{\theta}\right)_{,i} \geqslant 0 \tag{6a}$$

where η is the total pointwise specific entropy production, η^{mic} is the specific entropy production due to microstructural rearrangements, η^{θ} is the specific entropy production due to heat transfer, s is the entropy per unit volume, and θ is the absolute temperature. It is assumed that the following strong form of the entropy production inequality holds (Halphen and Nguyen, 1975):

$$\theta\dot{\eta}^{\text{mic}} = \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{\theta}s - \dot{h} \geqslant 0; \quad \theta\dot{\eta}^{\theta} = -\frac{1}{\theta} q_i \theta_{,i} \geqslant 0 \tag{6b}$$

where the conservation of energy (eqn (5)) has been utilized, together with the Helmholtz free energy, defined by:

$$h \equiv u - \theta s \tag{7}$$

In this paper we will produce a strain formulation by imposing boundary displacements on the RVE. Therefore, we assume that the constitutive behavior at the local level may be determined from the Helmholtz free energy, h^{μ}, in the μth phase (with volume V_{μ}):

$$h^{\mu}(\mathbf{x}, t) = h^{\mu}{}_{\tau=0}^{\tau=t}\{\varepsilon_{ij}(\mathbf{x}, \tau), \theta(\mathbf{x}, \tau), \theta_{,i}(\mathbf{x}, \tau)\} \tag{8}$$

where the braces imply a functional mapping of the entire past history of the arguments into the current time t. Note that the choice of arguments in the above is somewhat arbitrary, and is primarily based on an artistic choice of what set of kinematic variables will constitute a minimum level of difficulty that will nevertheless be sufficient to accurately model the class of materials to be considered. Accordingly, we have selected the same set of variables that would be listed in a simple thermoelastic material, except that in thermoelastic materials the free energy depends only on the current state. Note also that we have employed a local mapping at the microscopic scale.

It can be shown by expanding h^{μ} in convolution integrals in time, taking the time derivative of this quantity (by judicious use of Leibnitz' rule), and substituting this result into the first of entropy production inequality (eqn (6b)) that (Christensen, 1982):

$$\sigma_{ij}(t) = \int_0^t D^{\mu}_{ijkl}(t, \tau) \frac{\partial \varepsilon_{kl}}{\partial \tau} \mathrm{d}\tau + \int_0^t \beta^{\mu}_{ij}(t, \tau) \frac{\partial \theta}{\partial \tau} \mathrm{d}\tau \quad \text{in } V_{\mu} \tag{9}$$

where we have dropped the spatial dependence for simplicity, and $D^{\mu}_{ijkl}(t, \tau)$ and $\beta^{\mu}_{ij}(t, \tau)$ are the relaxation modulus tensor and thermal expansion tensor, respectively. Since these are coefficients in the expansion, they are assumed to be independent of strain and temperature, thus leading to a linear constitutive theory at the microscale due to the truncation of higher order convolution integrals. Note that in the limiting case wherein D^{μ}_{ijkl} and β^{μ}_{ij} are time independent, eqn (9) reduces to linear thermoelastic behavior, so that one or more of the phases can be linear thermoelastic. Note also that in the limiting case wherein D^{μ}_{ijkl} are represented by delta functions in time, the first term in eqn (9) reduces to linear viscous behavior. Note furthermore that D^{μ}_{ijkl} and β^{μ}_{ij} are subject to the standard thermodynamic and material symmetry constraints. Thus, for example, in isotropic media

$$D^{\mu}_{ijkl}(t, \tau) = \lambda(t, \tau)\delta_{ij}\delta_{kl} + 2\mu(t, \tau)\delta_{ik}\delta_{jl} \tag{10a}$$

and

$$\beta^{\mu}_{ij}(t, \tau) = \beta^{\mu}(t, \tau)\delta_{ij}. \tag{10b}$$

Although higher order integrals could be retained in eqn (9), and many materials do indeed exhibit nonlinear behavior, multiple integral formulations are both cumbersome and inaccurate. For nonlinear extensions of the above the reader is referred to the research of Schapery (1984, 1987), wherein a practical and often accurate nonlinear single integral formulation is presented.

The first of entropy production inequality eqn (6b), together with the integral expansion of eqn (8), can also be utilized to show that

$$s = \int_0^t \beta_{ij}(t, \tau) \frac{\partial \varepsilon_{ij}}{\partial \tau} \mathrm{d}\tau + \int_0^t m(t, \tau) \frac{\partial \theta}{\partial \tau} \mathrm{d}\tau \quad \text{in } V_{\mu} \tag{11}$$

where $m(t, \tau)$ is the second order coefficient in temperature in the free energy expansion, and the second of eqn (6b) can be used to show that

$$q_i(t) \cong -k^{\mu}_{ij}(\theta_{,j}, t)\theta_{,j} \quad \text{in } V_\mu. \tag{12}$$

For the purposes of discussing the boundary conditions, it is first propititious to introduce the boundary averaged strain tensor, defined by:

$$E_{ij} \equiv \frac{1}{V}\int_{\partial V_E} \frac{1}{2}(u_i n_j + u_j n_i)\,\mathrm{d}S \tag{13}$$

where ∂V_E is the external boundary of the RVE, as well as the boundary averaged temperature, defined by:

$$\Theta(t) \equiv \frac{1}{V}\int_{\partial V_E} \theta(\mathbf{x}, t)\,\mathrm{d}S. \tag{14}$$

The above field equations are now adjoined with the following initial and boundary conditions:

(1) Initial conditions:

$$\sigma_{ij}(\mathbf{x}, t = 0) = \varepsilon_{ij}(\mathbf{x}, t = 0) = u_i(\mathbf{x}, t = 0) = 0 \tag{15a}$$

$$u(\mathbf{x}, t = 0) = 0, \quad s(\mathbf{x}, t = 0) = s_0 = \text{constant} \tag{15b}$$

$$\theta(\mathbf{x}, t = 0) = \theta_0 = \text{constant}, \quad q_i(\mathbf{x}, t = 0) = 0 \quad \text{in } V + \partial V. \tag{15c}$$

(2) Boundary conditions:

$$u_i(\mathbf{x}, t) = \hat{u}_i(\mathbf{x}, t) = E_{ij}(t)x_j \tag{16a}$$

$$\theta(\mathbf{x}, t) = \hat{\theta}(\mathbf{x}, t) = \Theta(t) \quad \text{on } \partial V_E \tag{16b}$$

where the symbol ˆ implies known quantities. Note that due to the form of boundary condition eqns (16), we consider here only Dirichlet problems. Although other boundary conditions are both possible and useful (Suquet, 1982), they will not be considered in the current paper. Note furthermore that substitution of eqn (16a) into strain–displacement eqn (4) implies that the strain field is constant in the external boundary of the RVE.

For fixed surface area of cracks eqns (1)–(9), (11), and (12), together with initial and boundary condition eqns (15) and (16) form a well-posed linear initial boundary value problem which will in the linear cases possess a unique solution. However, the above equations must be adjoined with an appropriate crack advancement criterion when crack growth is to be predicted in the analysis. One way to obtain this criterion is to perform a global thermodynamic analysis of the micromechanics problem. Since this is also necessary in order to obtain homogenized field equations, the subject of the crack growth criterion will be discussed in a later section.

The solution for the kinematic variables in the microthermomechanics problem can be written in the following convenient way (Hill, 1967):

$$\varepsilon_{ij}(\mathbf{x}, t) = \Lambda_{ijkl}(\mathbf{x}, t)E_{kl}(t) \tag{17a}$$

$$\theta(\mathbf{x}, t) = \Pi(\mathbf{x}, t)\Theta(t) \tag{17b}$$

where Λ_{ijkl} is called the strain localization tensor, and we denote Π as the temperature localization field. Both localization variables will clearly depend on the damage state in the RVE.

Note that in the case of linear thermoelastic behavior the strain localization tensor will be time independent; that is, the solution given by eqn (17a) will be separable in time and space. Unfortunately, the same cannot be said to be true in all cases for thermoviscoelastic media. This is due to the fact that while there exists a correspondence principle (Christensen, 1982; Alfrey and Doty, 1945) which states that if all of the boundary conditions are proportional to one another in time, the solution will be separable, this correspondence principle does not hold for heterogeneous media. This point will become important in the next section.

The solution to the microthermomechanics problem may be obtained either analytically or computationally. In the following section it will be assumed that this solution has been obtained, so that the strain localization tensor is known *a priori* for the homogenization problem of interest.

HOMOGENIZATION OF THE MICROTHERMOMECHANICS FORMULATION

It is desirable to produce locally averaged (macroscopic) equations for the global domain $V_G + \partial V_G$ that are similar in form to the pointwise equations described in the previous section. If this objective can be achieved, then significant simplification of the global problem is possible. The process of homogenizing the microthermomechanics formulation is accomplished by the conceptually simple task of volume averaging the pointwise equations posed in the previous section. While conceptually straightforward, this process is nevertheless mathematically complicated due to several factors. First, although the material is homogenized by this process, it is nevertheless spatially variable due to both the time dependent nature of thermoviscoelastic media, as well as the possibility of spatial heterogeneity of the damage on the macroscopic scale. Furthermore, the evolution of the damage requires the use of a transport theorem in order to evaluate time derivatives of the macroscopic state variables (Costanzo *et al.*, 1996; Costanzo and Allen, 1993).

For the purpose of obtaining macroscopically averaged quantities in the RVE, it is convenient to introduce the following notational device for a generic function, f:

$$\bar{f}(\mathbf{x}_G, t) \equiv \frac{1}{V}\int_{V(\mathbf{x}_G)} f(\mathbf{x}, t)\,\mathrm{d}V. \tag{18}$$

Note that since local spatial coordinates $\mathbf{x}$ are integrated out of $\bar{f}$, any quantities obtained in this way cannot contain a length scale, thus obviating macroscopically nonlocal constitutive theories. In the case wherein the nature of the heterogeneity in the RVE is not statistically homogeneous, it may be necessary to integrate the pointwise state variables against spatial functions such as Legendre polynomials. This possibility will not be considered in the current paper. It should be pointed out, however, that there will nevertheless be spatial dependence in the homogenized or locally averaged variables, since in the global problem $V = V(\mathbf{x}_G)$, thus explicitly indicating that the RVE is continuously transportable in the global domain V_G.

From the standpoint of a viewer who cannot see the interior of the RVE, it is apparent that the locally averaged state variables of interest to the homogenization procedure should be boundary averaged quantities. Therefore, similar to eqns (13) and (14), we introduce the boundary averaged stress tensor:

$$\Sigma_{ij}(\mathbf{x}_G) \equiv \frac{1}{V}\int_{\partial V_E(\mathbf{x}_G)} \sigma_{ik} n_k x_j\,\mathrm{d}S \tag{19}$$

and the boundary averaged heat flux vector:

$$Q_i(\mathbf{x}_G) \equiv \frac{1}{V}\int_{\partial V_E(\mathbf{x}_G)} q_i\,\mathrm{d}S. \tag{20}$$

As a point of interest, note that the following identity can be easily established when the internal boundaries are traction free by volume integrating conservation of linear momentum eqn (1) and employing the divergence theorem:

$$\Sigma_{ij} = \overline{\sigma_{ij}}. \tag{21}$$

Also, it can be shown by similar use of eqns (4) and (16a) that:

$$E_{ij} = \overline{\varepsilon_{ij}} - \alpha_{ij} \tag{22}$$

where

$$\alpha_{ij} \equiv \frac{1}{V} \int_{S_C} \frac{1}{2}(u_i n_j + u_j n_i)\,\mathrm{d}S \tag{23}$$

where $S_C \equiv \partial V - \partial V_E$. α_{ij}, sometimes called the Vakulenko–Kachanov tensor (Vakulenko and Kachanov, 1971), was apparently first mentioned in a footnote by Hill (1963).

In the case wherein there are no internal boundaries, the boundary averaged strain tensor is equivalent to the volume averaged strain tensor since in this case α_{ij} is identically zero. However, we emphasize here that the natural interpretation of the homogenized strain tensor is given by the boundary averaged strain, E_{ij}, since it is observable on the boundary of the RVE.

In order to accomplish this formidable task, it is then necessary to volume average the pointwise field equations postulated in the previous section. For example, by assuming that the volume V of the RVE is a continuously varying function of global coordinates, it can be easily shown by volume averaging the pointwise conservation of linear momentum (eqn (1)) and substituting eqns (19) and (21) that

$$\Sigma_{ji,j} = 0 \quad \text{in } V_G \tag{24}$$

similar to the pointwise conservation of linear momentum eqn (1), except that the spatial derivatives are now taken with respect to global coordinates $\mathbf{x}_G$. Similarly, due to eqns (2) and (19):

$$T_i = \Sigma_{ji} n_j \quad \text{on } \partial V_G \tag{25}$$

where by definition there are no internal boundaries in V_G, and

$$\Sigma_{ji} = \Sigma_{ij} \quad \text{in } V_G + \partial V_G. \tag{26}$$

Similarly, volume averaging the pointwise strain–displacement equations and utilizing eqn (22) results in:

$$E_{ij} = \tfrac{1}{2}(\bar{u}_{i,j} + \bar{u}_{j,i}). \tag{27}$$

Construction of macroscopically averaged thermodynamic energy balance and entropy production statements similar to eqns (5) and (6) are much more involved than eqns (24)–(27). This is at least in part due to the fact that these last two are in rate form, and the presence of time dependent crack growth in the RVE necessitates the careful use of a transport theorem. The first author and coworkers have carried out this procedure in previous research (Costanzo *et al.* 1996; Costanzo and Allen, 1993), so that we need only review these results briefly. Thus, volume averaging the pointwise conservation of energy (eqn (5)), employing the divergence theorem and a transport theorem for the growing crack surfaces results in:

$$\dot{U} = \Sigma_{ij}\dot{E}_{ij} - Q_{i,i} \tag{28}$$

where the macroscopic specific internal energy U is defined by:

$$U \equiv \bar{u} + \frac{1}{V}\int_{S_C} 2\gamma \, \mathrm{d}S \tag{29}$$

where $\gamma = \gamma(\mathbf{x}, t)$ is the specific reversible fracture energy per unit area of crack extension, and as described in Costanzo and Allen (1993), S_C is the surface area of cracks produced during the time period $0 \leqslant \tau \leqslant t$. In addition, the first term on the right hand side of eqn (28) is obtained by constructing a rate form of the Hill–Mandel macrohomogeneity condition (Hill, 1965a; Suquet, 1982; Mandel, 1971; Costanzo *et al.* 1996):

$$\Sigma_{ij}\dot{E}_{ij} = \overline{\sigma_{ij}\dot{\varepsilon}_{ij}}. \tag{30}$$

The veracity of the above identity can be proven by integrating the conservation of linear momentum against the rate of change of the displacement field over the volume of the RVE, and once again employing the divergence theorem. Finally, the last term in eqn (28) is obtained by utilizing eqn (20) and the divergence theorem to define:

$$Q_{i,i} \equiv \frac{1}{V}\int_{\partial V_E} q_i n_i \, \mathrm{d}S \tag{31}$$

where the flux of heat across the internal boundaries is accounted for in the last term in eqn (29) (Costanzo *et al.* 1996).

A similar procedure may be utilized to construct the following locally averaged form of the entropy production inequality:

$$\Sigma_{ij}\dot{E}_{ij} - \dot{\Theta}S - \dot{H} \geqslant 0; \quad \overline{-\frac{1}{\theta}q_i\theta_{,i}} \geqslant 0 \tag{32}$$

where the specific macroscopic entropy S is defined by:

$$S \equiv \frac{\overline{\dot{\theta}s}}{\dot{\Theta}} \tag{33}$$

and the specific macroscopic Helmholtz free energy is defined to be:

$$H \equiv U - \overline{\theta s} = \bar{h} + \frac{1}{V}\int_{S_C} 2\gamma \, \mathrm{d}S. \tag{34}$$

Thus, it is possible to construct a macroscopic formulation that is similar in form to the microscopic formulation presented in the previous section. The important issue that remains is what effect the introduction of cracks, as encompassed within the last terms in eqns (29) and (34), will have on the locally averaged constitutive equations. This issue will be taken up in the next section.

HOMOGENIZED CONSTITUTIVE EQUATIONS

It is desirable for the homogenization procedure to result in a relationship between the locally boundary averaged quantities that is similar in form to pointwise thermomechanical constitutive eqns (9). Furthermore, this relationship should be simply derivable with the aid of the microthermomechanics solution (eqn (17)). The advantages to this similarity are numerous. For example, there may be times when the micromechanics solution is untenable.

In these circumstances, if the homogenized form of the constitutive equations is known, it will help in the determination of what experiments will need to be carried out in order to construct the locally averaged constitutive equations by the phenomenological approach. Alternatively, suppose that the micromechanics solution is obtained computationally such as with the finite element method. If the general character of the equations is retained at the global scale, then it may be possible to utilize the same algorithm (with a minimum of modification) to also solve the global problem.

One way that the macroscopically averaged constitutive equations can be obtained from the micromechanics solution is to solve the Hill–Mandel theorem for the macroscopic stress and substitute the microthermomechanics solution (eqn (17)) into this result (an essentially equivalent procedure is to use the principle of virtual work). While this procedure is often convenient for elastic media, there is a second approach that yields identical results that is often easier to evaluate, especially for viscoelastic media. This involves simply substituting pointwise thermomechanical constitutive eqn (9) directly into eqn (21) to obtain:

$$\Sigma_{ij} = \frac{1}{V}\int_V \left[\int_0^t D_{ijkl}(t,\tau)\frac{\partial \varepsilon_{kl}}{\partial \tau}\mathrm{d}\tau + \int_0^t \beta_{ij}(t,\tau)\frac{\partial \theta}{\partial \tau}\mathrm{d}\tau\right]\mathrm{d}V. \tag{35}$$

Substitution of micromechanics solution (eqn (17)) into the above will result in

$$\begin{aligned}\Sigma_{ij} = {} & \frac{1}{V}\int_V \left[\int_0^t D_{ijkl}(t,\tau)\Lambda_{klmn}(\mathbf{x},\tau)\frac{\partial E_{mn}}{\partial \tau}\mathrm{d}\tau + \int_0^t D_{ijkl}(t,\tau)E_{mn}\frac{\partial \Lambda_{klmn}(\mathbf{x},\tau)}{\partial \tau}\mathrm{d}\tau\right]\mathrm{d}V \\ & + \frac{1}{V}\int_V \left[\int_0^t \beta_{ij}(\mathbf{x},t,\tau)\Pi(\mathbf{x},\tau)\frac{\partial \Theta(\tau)}{\partial \tau}\mathrm{d}\tau + \int_0^t \beta_{ij}(\mathbf{x},t,\tau)\Theta(\tau)\frac{\partial \Pi(\mathbf{x},\tau)}{\partial \tau}\mathrm{d}\tau\right]\mathrm{d}V\end{aligned} \tag{36}$$

where we have retained the partial derivatives in E_{mn} and Θ due to the fact that in the global problem these state variables depend on global coordinates.

Due to the second and fourth terms involving the localization tensors on the right hand side of the above equation, it is evident that the macroscopic constitutive equations may not be equivalent in form to the microscopic form in the RVE. For elastic media, the localization tensor is independent of time, so that global and local distinctions disappear. However, in the current scenario of linear viscoelastic behavior, this is not necessarily the case, as demonstrated by eqn (36). Furthermore, although a correspondence principle exists (Christensen, 1982; Alfrey and Doty, 1945) that will show that the strain localization tensor is time independent for certain Dirichlet problems, as previously mentioned, this correspondence does not generally hold true in heterogeneous media.

Fortunately, there is an alternative way of writing eqn (36) that will retain the single integral form of the micromechanical viscoelastic behavior. This may be constructed by using integration by parts to obtain

$$\Sigma_{ij}(t) = \int_0^t D^G_{ijkl}(t,\tau)\frac{\partial E_{kl}}{\partial \tau}\mathrm{d}\tau + \int_0^t \beta^G_{ij}(t,\tau)\frac{\partial \Theta}{\partial \tau}\mathrm{d}\tau \tag{37}$$

where

$$D^G_{ijkl}(t) = \frac{1}{V}\int_V \left[D_{ijmn}(t)\Lambda_{mnkl}(0) + \int_0^t D_{ijmn}(t,\tau)\frac{\partial \Lambda_{mnkl}(\tau)}{\partial \tau}\mathrm{d}\tau\right]\mathrm{d}V \tag{38a}$$

and

$$\beta^G_{ij}(t) = \frac{1}{V}\int_V \left[\beta_{ij}(t)\Pi(0) + \int_0^t \beta_{ij}(t,\tau)\frac{\partial\Pi(\tau)}{\partial\tau}\,\mathrm{d}\tau\right]\mathrm{d}V. \tag{38b}$$

It can be seen that the first terms in each of eqns (38) correspond to the first and third terms on the right hand side of eqn (36), and the second terms in each of eqns (38) correspond to the second and fourth terms in eqn (36). Thus, it is clear from eqn (38a) that the volume of the micromechanical relaxation modulus tensor integrated against the initial value of the strain localization tensor does not necessarily equate to the macroscopic relaxation modulus tensor, $D^G_{ijkl}(t)$, as is the case in linear elastic media. One may well ask the question as to how much error will be introduced by neglecting the last term in eqn (38). The answer to this question is that it will depend on the geometry and material properties contained in the micromechanics problem. Neglecting this term is sometimes called the quasi-elastic assumption since it is customary in this case to utilize the strain localization tensor that would be obtained from the corresponding elastic microthermomechanics problem (Schapery, 1984).

Alternatively, one could expand the macroscopic Helmholtz free energy, H, in terms of kinematic variables in order to obtain the macroscopic thermomechanical constitutive equations. Although this is not actually necessary, as demonstrated by the above results obtained from the homogenization process, some interesting results can be obtained. Therefore, consider the macroscopic free energy, given by eqn (34). It is clear that in the absence of internal boundaries in the RVE, H is equivalent to the volume average of the microscopic free energy, h. Thus, it can be shown that, in the absence of damage:

$$H = H^{\tau=t}_{\tau=0}\{E_{kl},\Theta\} \tag{39}$$

where the dependence on macroscopic temperature gradient is disallowed due to the macroscopic form of the second law (eqn (32)). Although it has already been shown by volume averaging the stress above, it can further be shown by expanding H in convolution integrals (for the undamaged case), employing the second law, and neglecting higher order terms, that the thermomechanical constitutive relation given by eqn (37) is recovered. Of course, the microthermomechanical approach discussed above is more concise, since it results in the thermomechanically based descriptions of the macroscopic modulus $D^G_{ijkl}(t,\tau)$ and thermal expansion $\beta^G_{ij}(t,\tau)$ given by eqns (38a) and (38b). Thus, the expansion of H is redundant in the undamaged case, although it does at least confirm symmetry and positive semidefiniteness constraints on the macroscopic properties.

In the case of growing internal boundaries due to crack extension, the results are more complicated. This can be readily seen by observing macroscopic thermomechanical constitutive eqns (37). Clearly, when the internal boundaries are changing with time, the strain localization tensor and temperature localization field Π will reflect this dependence. Verification of this fact is evidence by the last term in eqn (34), which represents the energy stored during crack extension. This term is explicitly dependent on the crack surface area, S_C. However, note that the volume average of the local free energy also depends implicitly on the energy released due to crack extension (as well as energy dissipated due to thermoviscoelasticity).

We have previously shown that the macroscopic form of the entropy production inequality (eqn (32)) may be written in the following form:

$$\overline{\theta\dot{\eta}^{\mathrm{mic}}} + D_F + D_C \geqslant 0 \tag{40}$$

where we take the following strong form of the second law:

$$D_F = \frac{1}{V}\int_{S_C} [q_i]n_i\,\mathrm{d}A \geqslant 0 \tag{41}$$

where $[q_i]$ is the heat flux jump across the crack faces. Also, when γ is spatially constant in the rth crack:

$$D_C = \frac{1}{V}\sum_{r=1}^{N}(G^r - 2\gamma^r)\dot{S}_C^r \geqslant 0 \tag{42}$$

where (Costanzo and Allen, 1993; Nguyen, 1980; Costanzo and Allen, 1966)

$$G^r \equiv \lim_{\delta\to 0}\frac{1}{\dot{S}_C^r}\int_{S_\Gamma^r}(hc_i^{*r}v_i^r + \sigma_{ij}\dot{u}_i v_j^r)\,\mathrm{d}A \tag{43}$$

is the energy release rate of the rth crack, where c_i^{*r} is the crack tip velocity of the rth crack, and v_i^r is the unit outer normal vector of the manifold S_Γ^r with radius δ surrounding the rth crack (Costanzo and Allen, 1993, 1996).

In the current scenario of thermoviscoelastic material behavior, G^r is clearly not path independent, so that the limit must be taken in eqn (43) in order to recover the energy released by the crack itself. This can pose difficulties both when attempting to evaluate γ experimentally, and also when attempting to evaluate G^r in order to predict crack extension in the micromechanics problem. Fortunately, this issue has been addressed both for linear viscoelastic (Knauss, 1974; Schapery, 1975a,b,c) and a class of nonlinear viscoelastic media (Schapery, 1984, 1987). Using a correspondence principle it is possible to construct a path independent integral in a corresponding elastic space, so that the two difficulties mentioned above can be surmounted. Thus, eqn (42) can be utilized as a criterion for predicting crack advance in the microthermomechanics problem. This criterion then completes the description of the microthermomechanics problem, as discussed in that section.

In the case wherein the specific reversible fracture energy γ is independent of spatial coordinates, the damage dependent macroscopic free energy is postulated to take the following from:

$$H = H_{\tau=0}^{\tau=t}\{E_{kl}, \Theta, \Theta_{,k}, S_C\} \tag{44}$$

where a significant difficulty arises due to the fact that the first three variables are locally averaged quantities, whereas S_C represents the entire surface area of cracks in the RVE. A second difficulty is due to the fact that crack extension can cause severe thermal gradients, especially when there is crack face friction. In order to deal with this problem, we will make the assumption that there is no crack face friction, and that the temperature is spatially homogeneous in the RVE. This will also serve to mitigate issues associated with non-equilibrium thermodynamics (DeGroot and Mazur, 1962; Glansdorff and Prigogine, 1971). Thus, the term $\Theta_{,k}$ is neglected in eqn (44).

In order to deal with the field associated with S_C, there are several possible courses of action. One is to simply evaluate the thermomechanical constitutive equations by the microthermomechanical approach, as given in eqns (37) and (38). In this approach, the moduli will naturally take on a form that depends on the structure of the microcracks in the RVE. Kachanov (1994) has utilized this approach for a variety of geometries in elastic media. For the limits of completely ordered cracks and completely disordered cracks, this approach may be useful, especially wherein analytic microthermomechanical results are available. However, there will undoubtedly be cases wherein the crack structure in the RVE precludes analytic microthermomechanical solutions. In these cases it may be preferable to expand the macroscopic free energy H in convolution integrals, similar to the procedure taken in the section on microthermomechanics. Two pragmatic approaches to this expansion come to mind. One would involve expanding the free energy explicitly in terms of the arguments in eqn (44). A second approach would be to expand H only in terms of E_{ij} and Θ, thus producing expansion coefficients in the convolution integrals that are functions of S_C. Based on experience, the latter approach will be taken here. As with the micromechanics approach, the result is that given by eqn (37), except that the moduli in eqn (38) are now functions of S_C, thus resulting in a form that is essentially equivalent to the microthermomechanics solution. This approach is thus clearly redundant when the strain localization tensor can be evaluated, especially analytically. Since this is not always the case, consider the case wherein the only microthermomechanical solution is computational in nature. In this case, it appears to be useful to expand the coefficients D^G_{ijkl} and β^G_{ij} in some phenomenologically based damage parameter. Clearly, since the quantity S_C represents the entire surface area of cracking in the RVE, it is untenable. If the damage in the RVE is statistically homogeneous in spatial coordinates, then one possible way to account for crack orientation would be to utilize a tensor valued representation of the damage similar to that given by eqn (23). Suppose we use

$$d_{ijkl} \equiv \frac{1}{E_{kl}V}\int_{S_C}\frac{1}{2}(u_i n_j + u_j n_i)\,\mathrm{d}S. \tag{45}$$

Expanding the relaxation modulus tensor and thermal expansion tensor in two first order Taylor series in d_{ijkl} results in

$$D_{ijkl} = D_{ijmn}(\delta_{km}\delta_{ln} - d_{mnkl}) \tag{46a}$$

and

$$\beta_{ij} = \beta_{mn}(\delta_{im}\delta_{jl} - d_{mnij}). \tag{46b}$$

In certain limiting cases these results may turn out to be exact. However, they will in the general case entail some approximation. Nevertheless, when only computational results are available they can be utilized to evaluate an evolution law for d_{ijkl}, so that the need for a global–local scheme is obviated. We have now completed the description of the macroscopic initial boundary value problem. In the next section several example problems will be solved in order to demonstrate the homogenization procedure.

EXAMPLE PROBLEMS

In this section several micromechanics problems will be solved to demonstrate the homogenization principle described above. As also mentioned in the previous section, micromechanics problems that involve viscoelastic materials are notoriously difficult to solve, especially by analytic means. Although there exist two broad classes of problems for which correspondence principles exist that relate the elastic to the viscoelastic solutions for linear media (Schapery, 1984), these correspondence principles often break down when heterogeneous media are considered. In general, this problem arises from the fact that the material interfaces in the interior of the micromechanical problem do not have the same time dependent behavior as the external boundaries, thereby often leading to viscoelastic solutions that are not separable in space and time. To illustrate this point, we consider herein three very simple micromechanical problems for which closed form solutions exist.

Example I

In the first example, consider an assemblage of two bars in parallel, as shown in Fig. 2. The horizontal bar at the base of the assemblage is assumed to deform vertically (as a rigid body) without rotation under vertical loading, so that the solution to this problem is statically determinant, and the deformations in the two bars are equivalent. For simplicity, we consider here the case where bar a is linear elastic with modulus E_a and bar b is linear viscoelastic with relaxation modulus described by a Maxwell model, i.e.,

$$D_b(t) = E_M\,\mathrm{e}^{-\frac{E_M t}{\eta_M}}. \tag{47}$$

Assuming that each bar has unit cross-sectional area and length, it is easily shown that eqn (38a) results in

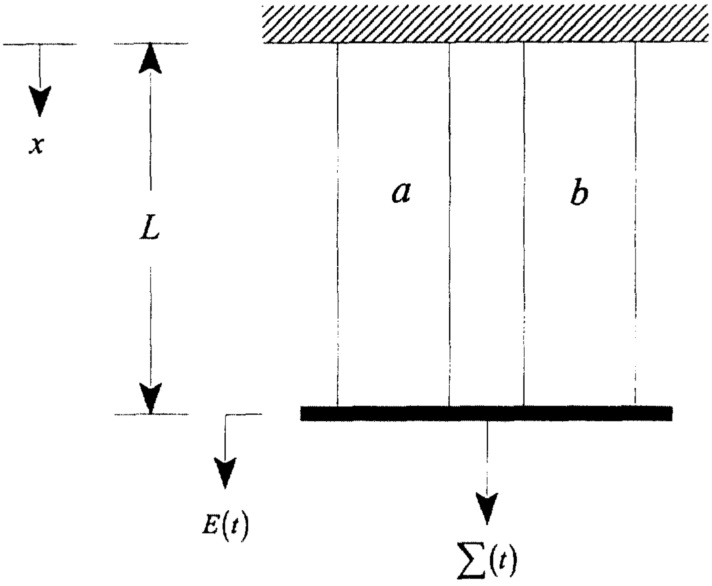

Fig. 2. Two uniaxial bars in parallel.

$$D^G(t) = E_a + E_M e^{-\frac{E_M t}{\eta_M}} \tag{48}$$

which can be seen to be equivalent to a standard linear solid analog. In this case the second term in eqn (38a) is identically zero because the solution is separable in time and the localization tensor Λ_{ijkl} is time independent. Therefore, no error is introduced by considering only the first term in eqn (38a).

Example II

In the second example, consider an assemblage of two bars in series, as shown in Fig. 3. Note that this problem represents the one-dimensional analog to the three-dimensional ellipsoidal inclusion problem (Eshelby, 1957). Once again, the assemblage is subjected to

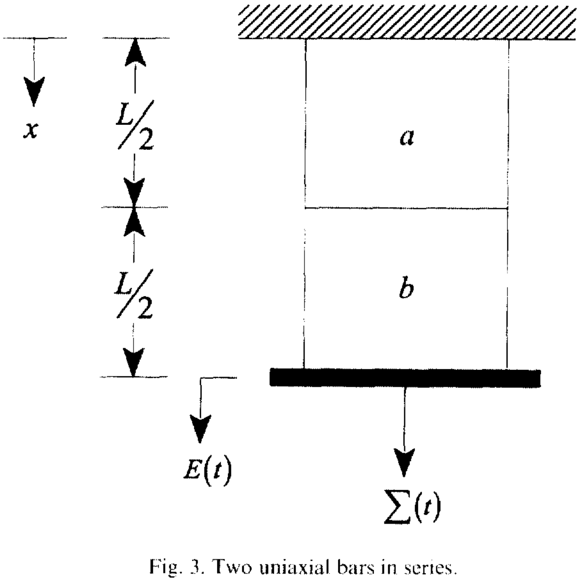

Fig. 3. Two uniaxial bars in series.

loading in the vertical direction. Also, the upper section is assumed to be linear elastic with modulus E_a, and the lower section is assumed to be linear viscoelastic with the Maxwell model relaxation modulus given by eqn (47). Each section is assumed to be of unit length and cross-sectional area. In this example the solution is somewhat more complicated than in Example I because the strains in the two sections are unequal and time dependent, thus leading to a spatially heterogeneous strain localization tensor. It is easily shown that the strain localization tensor in each section is given by

$$\Lambda^a = \frac{2E_M}{E_a + E_M} e^{-\frac{E_a E_M}{\eta_M (E_a + E_M)} t} \tag{49}$$

and

$$\Lambda^b = 2\left\{1 - \frac{E_M}{E_a + E_M} e^{-\frac{E_a E_M}{\eta_M (E_a + E_M)} t}\right\}. \tag{50}$$

Substituting the above results into the first term in eqn (38a) results in

$$D^H(t) = \frac{E_a E_M}{E_a + E_M}\left\{1 + e^{-\frac{E_M}{\eta_M} t}\right\}. \tag{51}$$

The correct result, obtained by evaluating both terms in eqn (38a), is

$$D^G(t) = \frac{2E_a E_M}{(E_a + E_M)} e^{-\frac{E_a E_M}{\eta_M (E_a + E_M)} t}. \tag{52}$$

The above two results are plotted in Fig. 4 for a set of material properties that are representative of a typical continuous carbon fiber polymer composite. It is observed that significant error can be introduced if the second term is not included in the evaluation of eqn (38a). Although this example is statically determinate, it illustrates that care must be taken due to the fact that the displacements in the body are not separable.

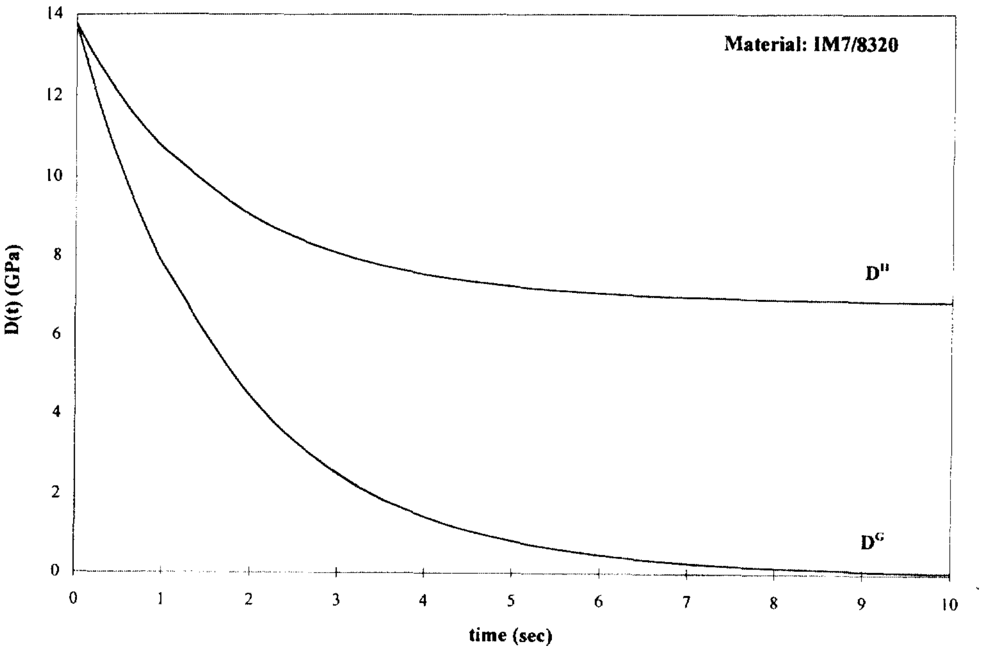

Fig. 4. Results for Example II.

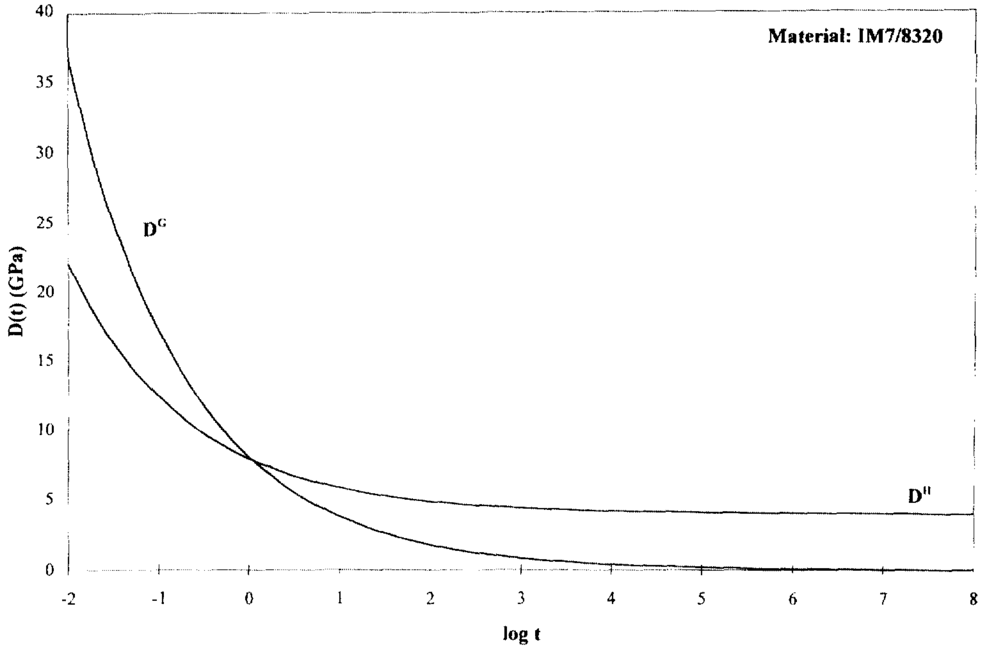

Fig. 5. Results for Example III.

Example III

This example is identical to the second example, except that the lower member is assumed to be modelled by a power law material with viscoelastic relaxation modulus given by

$$D_b(t) = E_\infty + E_1 t^n, \quad -1 < n \leqslant 0. \tag{53}$$

Values of the constants have been chosen to be representative of the relaxation modulus in the fiber direction of IM7/8320 at 195°C, a typical continuous fiber polymer composite. In this case the first term in eqn (38a) results in

$$D^H(t) = \frac{2E_a}{E_a+E_\infty+E_1}\left[E_\infty + \frac{E_1}{2}(1+t^n)\right], \quad t \geqslant 1 \tag{54}$$

whereas the correct answer is

$$D^G(t) = \frac{2E_aE_\infty}{E_a+E_\infty}\mathscr{L}^{-1}\left\{\frac{1}{S}\left[\frac{S^n + \dfrac{E_1\Gamma(1+n)}{E_\infty}}{S^n + \dfrac{E_1\Gamma(1+n)}{E_a+E_\infty}}\right]\right\} \simeq \frac{2E_a}{E_a+E_\infty}(E_\infty + E_1 t^n) \tag{55}$$

where $\mathscr{L}^{-1}$ { } is the inverse Laplace transform. The above two results are plotted in Fig. 5. It is apparent that the error introduced by neglecting the second term in eqn (38a) is mitigated by reducing the rate of change of the relaxation modulus in time. Thus, for many real materials, the error introduced by neglecting the time dependence in the strain localization tensor may in fact be negligible (Schapery, 1996).

Example IV

We consider now the case of a viscoelastic composite containing cracks. We have recently studied just such a problem (Zocher and Allen, 1997), and the macroscopically averaged axial modulus will be discussed here for demonstrative purposes. The problem consists of a single ply of orthotropic viscoelastic material subjected to homogeneous displacements on the boundary except for the two vertical faces at the ends, which are subjected to a unit horizontal displacement that is constant in time. Matrix cracks are assumed to have previously developed normal to the loading direction, as shown in Fig. 6. We have obtained the micromechanics solution to this problem both analytically and computationally (by the finite element method) (Zocher and Allen, 1997), and the analytic solution is utilized therein to obtain the macroscopically averaged axial modulus as a function of the damage. This result will be discussed further below.

Now suppose that an alternative approximate result is obtained by the method discussed above using the damage parameter, d_{ijkl}. An evaluation of this parameter gives

$$d_{1111} = \frac{h}{a}\sum_{n=1}^{\infty} \frac{2^4 \tanh\left[\sqrt{\frac{G_T}{C_T}}\left(\frac{2n-1}{2}\right)\frac{\pi a}{h}\right]}{\pi^3(2n-1)^3\sqrt{\frac{G_T}{C_T}}}. \tag{56}$$

Thus, eqn (46a) can be utilized to obtain the axial relaxation modulus D^{G}_{1111}. The initial value of the axial relaxation modulus obtained from the above equation, along with the exact modulus given in Zocher and Allen (1997), as well as a result obtained from the finite

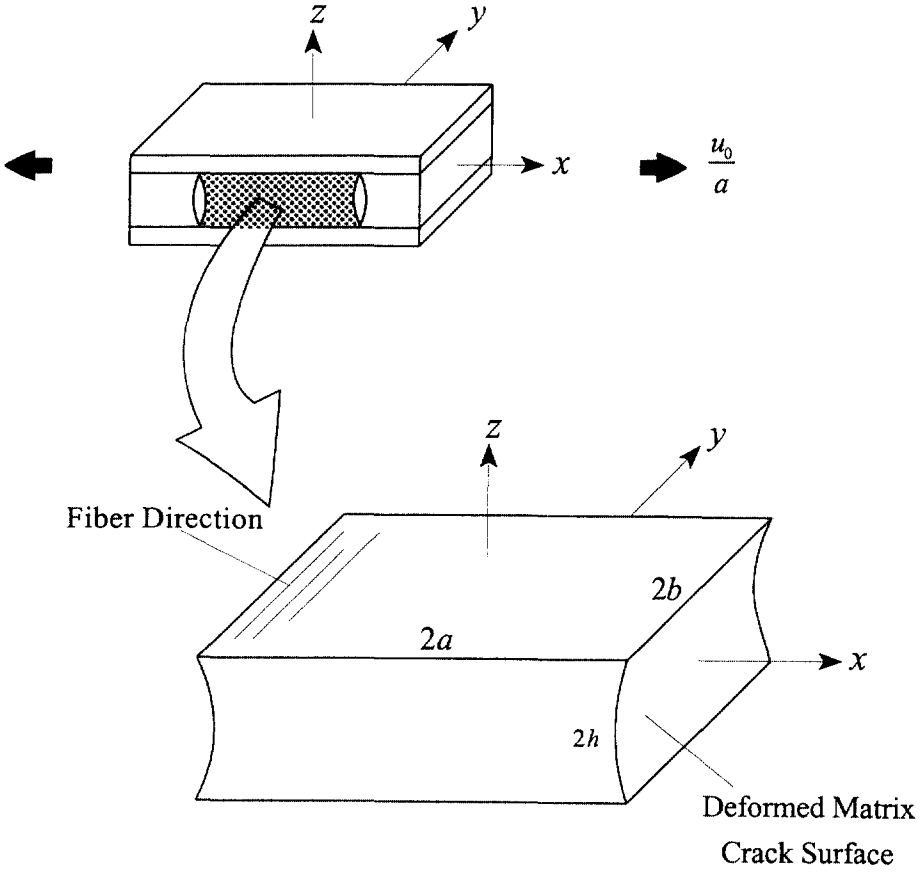

Fig. 6. An orthotropic viscoelastic ply with matrix cracks.

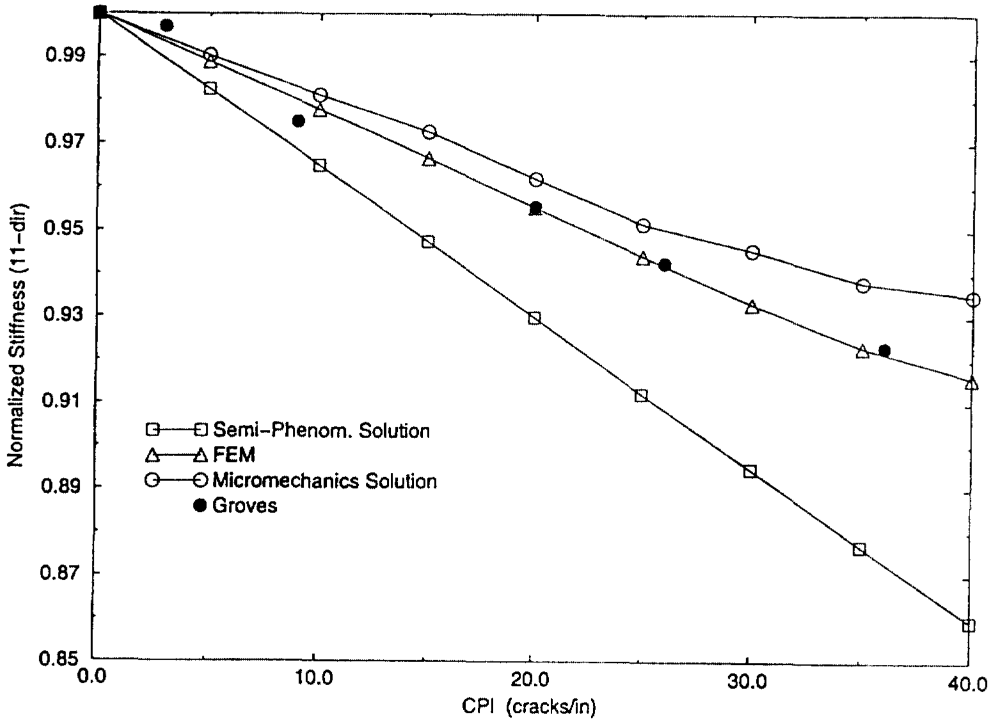

Fig. 7. Comparison of initial axial modulus vs crack density for Example IV.

element method (Groves *et al.* 1987), are plotted against crack density in Fig. 7. Also shown in the figure are experimental data from Groves *et al.* (1987). The exact and approximate results shown above are also plotted vs time in Fig. 8. It can be seen that while the approximate damage dependent relaxation modulus given by eqn (56) is somewhat different from that given in Zocher and Allen (1997), it may be sufficiently accurate for modelling purposes under some circumstances. Furthermore, it is a vastly simpler mathematical statement.

CONCLUSION

The authors have described herein a thermomechanically consistent homogenization principle for heterogeneous linear thermoviscoelastic media with stress–strain behavior of convolution type. It has been shown that the nonseparable nature of the microthermomechanics solution can lead to macroscopically averaged relaxation moduli that are erroneous unless care is taken into account for the time dependent nature of the strain localization tensor obtained from the microthermomechanics solution. However, this error may be negligible in many real materials.

We have also discussed the microthermomechanical problem at length, and its relation to the homogenized macrothermomechanical boundary value problem. An interesting byproduct of the homogenization process is that the second law serendipitously produces an energy based fracture criterion for crack growth in the microthermomechanical problem.

The approach taken herein will perhaps be a convenient way to obtain homogenized macroscopic properties in linear viscoelastic composites. However, we should point out some shortcomings of the homogenization approach. First, while the microthermomechanical solution will normally lead to homogenized equations that are more descriptive than their counterpart phenomenologically (experimentally) obtained macroscopic equations, they may require a great deal of effort to produce due to the complexity of the microthermomechanical boundary value problem. Second, although the homogenized

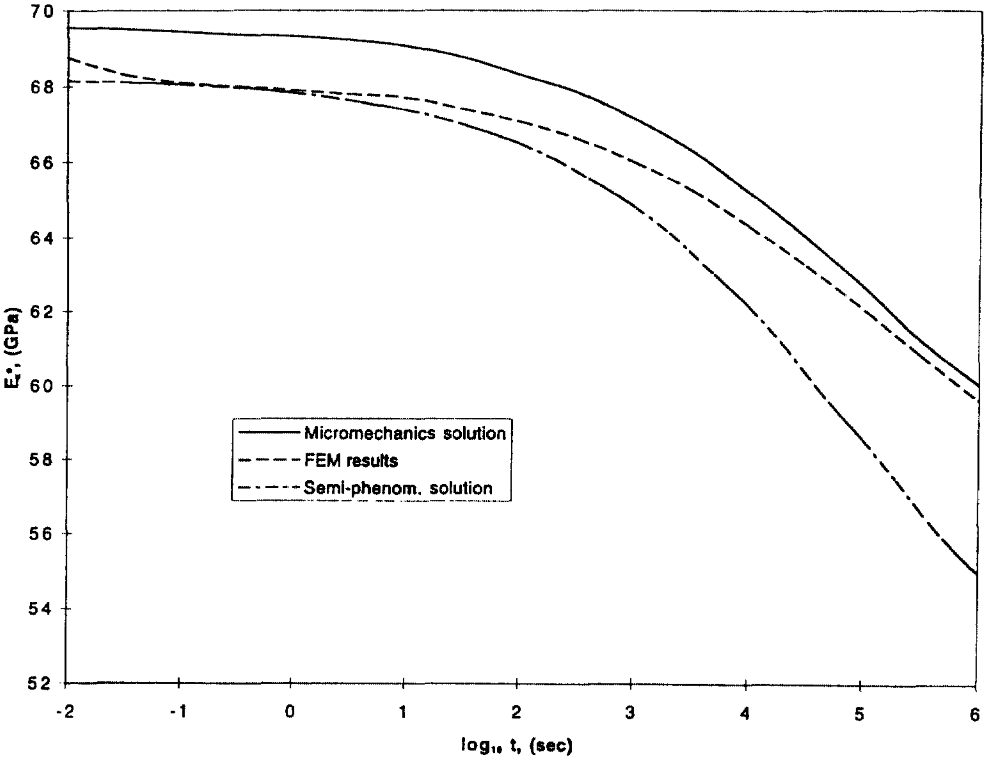

Fig. 8. Comparison of approximate and exact relaxation modulus vs time for Example IV.

relaxation modulus will be spatially homogeneous for media without cracks, it will necessarily be a function of coordinate location for media with cracks that are distributed nonhomogeneously. This will render the approach discussed herein somewhat less tractable when the microthermomechanical solution is obtained computationally. In this case, it may be advisable to utilize the damage parameter proposed in eqn (45) together with an evolution law in order to avoid the necessity to invoke a potentially cumbersome global–local scheme. Finally, the microthermomechanical approach makes the implicit assumption that the properties of the constituents do not change when they are processed together. There will doubtless be cases wherein this assumption will be invalid, and in these cases, more thought will need to be given to the problem.

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