

# A Macroscopic Theory of Microcrack Growth in **Brittle Materials**

J. S. Marshall, P. M. Naghdi and A. R. Srinivasa

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# A macroscopic theory of microcrack growth in brittle materials

By J. S. Marshall, P. M. Naghdi and A. R. Srinivasa Department of Mechanical Engineering, University of California, Berkeley, California 94720, U.S.A.

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This paper is concerned with the development of a macroscopic theory of crack growth in fairly brittle materials. Average characteristics of the cracks are described in terms of an additional vector-valued variable in the macroscopic theory, which is determined by an additional momentum-like balance law associated with the rate of increase of the area of the cracks and includes the effects of forces maintaining the crack growth and the inertia of microscopic particles surrounding the cracks. The basic developments represent an idealized characterization of inelastic behaviour in the presence of crack growth, which accounts for energy dissipation without explicit

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use of macroscopic plasticity effects. A physically plausible constraint on the rate of crack growth is adopted to simplify the theory. To ensure that the results of the theory are physically reasonable, the constitutive response of the dependent variables are significantly restricted by consideration both of the energetic effects and of the microscopic processes that give rise to crack growth. These constitutive developments are in conformity with many of the standard results and observations reported in the literature on fracture mechanics. The predictive nature of the theory is illustrated with reference to two simple examples concerning uniform extensive and compressive straining.

#### 1. Introduction

This paper is concerned with the construction of a (macroscopic) dynamical theory of brittle materials incorporating the growth of microcracks and their influence upon the material response, which is assumed to be perfectly elastic in the absence of cracks. Included in the class of materials addressed by the theory are geophysical materials (such as rocks), concrete and possibly also certain ceramics. Numerous experimental results reported over the past few decades by Bieniawski (1967, 1971), Peng & Johnson (1972), Sprunt & Brace (1974), Sangha et al. (1974), Dhir & Sangha (1974) and Wong (1982), among others, document the influence of microcracks on the mechanical behaviour of these materials. Also useful reviews on the state of the experiments on the subject are given by Kranz (1983) and Read & Hegemier (1986) and informative photographic evidence is contained in the paper of Sprunt & Brace (1974, figs 2–10). The continuum model constructed in this paper is largely motivated by the observations of these experimental studies.

Before providing further background material and describing in detail the scope of the paper, for clarity's sake we note that the term 'microcracking' used in the remainder of this section and elsewhere in this paper refers to a particular type of inelastic behaviour commonly found in geological materials. Such materials contain a distribution of small cracks or voids which can be seen only at a microscopic level. When a part of the material is (on the microscopic level) subjected to surface forces, 'damage' commences to accumulate at a macroscopic level and continues for the duration of the loading. This so-called 'damage' takes the form of the growth of the microcrack ranging from the cracking of a few isolated grains to the complete comminution of regions of the material.

Many of the existing developments on microcracking (see, for example, Kemeny & Cook 1986) use linear elastic solutions for the response of the material with single cracks of specific geometries for obtaining a variety of 'models'. Each of these 'models', in turn, is assumed to be applicable to a particular loading and/or crack geometry; and, in combination, are regarded to be applicable to more general situations. Although models of this type have produced interesting results in special cases, they are qualitative in nature and do not properly account for the dynamical effects of crack growth. Other developments (such as the 'damage theory' of Krajcinovic & Fonseka (1981)), attempt to correct these shortcomings by postulating direct macroscopic theories using supplementary kinematics termed 'internal variables' and identified as 'damage' variables. However, they do not adequately relate their supplementary kinematical variables explicitly to features of the deformation and crack growth. A notable exception to this trend is the study by Davison & Stevens (1973) which has some features on the microscopic level in

common with those of the present study and will be discussed in more detail at the end of the paper (see §7). The inertia effect due to microcrack growth is not included in any of the papers cited. Thus the need for a complete physical theory incorporating the effects of crack alignment, as well as the energetic and dynamical effects of crack growth, still exists. Such a theory, as discussed here, must necessarily include a procedure by which appropriate conservation laws and constitutive equations for the additional variables may be introduced in full agreement with the requirements of continuum mechanics.

It should be noted here that much of the existing literature on the subject is concerned with analysing the behaviour of a single crack of specified geometry (for a detail review, see Hutchinson (1983), who cites representative references). The present paper, on the other hand, attempts to formulate a manageable theory of microcracking for an idealized behaviour of brittle materials with a large number of microcracks.

#### 1.1. Scales of motion and modelling: macroscopic and microscopic

Before a discussion of our main objectives, we describe two distinct scales of physical modelling, namely the macroscopic and microscopic scales, which respectively represent the scale of bulk or 'smeared' response of the media and the scale on which microcracks are observed. (We need not be concerned here with a (finer) third scale of modelling, i.e. the molecular scale, at which optical, electrical and thermal phenomena occur.) Although a discrete number of cracks may exist on the microscopic scale, these cracks may not be visible on a coarser macroscopic scale. To further illustrate the nature of these levels of physical modelling, consider the motion of a material which in its initially undeformed configuration possesses a few cracks that are fairly small on the microscopic scale. Suppose further that the material is elastic in the absence of cracks. For small deformations, provided the cracks on the microscopic scale remain few and small in size, it may be possible to ignore the effect of the cracks entirely on the macroscopic scale. Next, let the material be subjected to a much larger deformation leading to the formation of new cracks and the growth of the pre-existing ones. Now, it is no longer possible to entirely neglect the effect of microcracks on the macroscopic scale. Such microscopic effects can be incorporated into the classical continuum mechanics by additional kinematical variables, together with additional conservation laws and constitutive equations. A macroscopic theory of this kind must necessarily include the classical nonlinear elasticity in the absence of microcracks. (Recall that in the absence of cracks, the macroscopic and microscopic levels become coincident.)

#### 1.2. Additional independent variables

Two additional kinematical quantities are used in the macroscopic description of the present paper. One of these is a vector-valued variable  $\bar{d}$  which is the composition of the inverse of the adjugate of the deformation gradient and a director (see equation (3.4); the adjugate  $F^*$  of an invertible second order tensor F is  $= (\det F)(F^T)^{-1}$ ; a further discussion of the adjugate of second-order tensors can be found in Chadwick's book (1976)), whose magnitude is a measure of the total area of the cracks in the microscopic description and whose direction represents the direction of the orientation of the cracks at the microscopic level. The other is a scalar-valued variable representing the crack density n defined as the limiting value of the number of cracks per unit volume in a reference configuration at the microscopic level.

Background information concerning 'directed' or 'oriented' media (also called Cosserat continua), which use a director as a kinematical variable, can be found in Green et al. (1965), Truesdell & Noll (1965), and Naghdi (1972). It should be remarked, however, that due to the differences in physical structure of the phenomena under discussion, the development of the theory with the use of a director in this paper is substantially different than that formulated in the previous works.

#### 1.3. Scope of the paper

Although the contents of the paper as listed above give an indication of the nature of its scope, some additional comments here may be helpful. Following a qualitative discussion of crack growth at the microscopic level in §2, along with some detailed development at the microscopic level in Appendix A pertaining to the identification of additional kinematical and kinetical quantities, the lagrangian form of a (macroscopic) dynamical theory of microcrack growth is constructed in §3. The development in §3 includes the consideration of balance laws for the additional independent variables  $\bar{d}$  and n described in §1.2 and an explicit development of a constrained theory after imposing an appropriate constraint on the variable  $\bar{d}$ . (This constraint (presented in §3) is not thought to be particularly suitable for laminated media because of the tendency of cracks to form along material interfaces.)

It is important to note that the theory constructed in §3 and further developed in §§4 and 5 includes the inertia effects for microcracking associated with both the rate of increase of kinetic energy of particles in a material region (in the presence of the pre-existing cracks) and the rate of increase of kinetic energy arising from fracturing processes in a non-material region (due to new cracks and the growth of the preexisting ones). Constitutive equations for the macroscopic theory, along with physically motivated constitutive restrictions resulting from appropriate conditions for the initiation of microcracking are discussed in §4. The basic constitutive restrictions in §4.1 are carried out with the use of the thermodynamical formulation of Green & Naghdi (1977) in the isothermal case (corresponding to a purely mechanical theory), and the procedure adopted in §4.2 for initiation of microcracking reduces to Griffith's (1921) criterion in an appropriate limit. Further special and explicit development of constitutive equations based on various additional physically reasonable restrictions is given in §5 with details of some of the analysis provided in Appendix B. Next in §6, after summarizing the manner in which the basic theory can be utilized, estimates for constitutive coefficients are provided in §6.2 and for purposes of illustration an analysis for uniform extensive and compressive straining of a microcracking material is carried out in §§ 6.3 and 6.4. Finally, some additional remarks are made in §7 concerning the characteristic features of the basic theory given here and its differences with the earlier literature on the subject.

# 2. Background remarks on crack growth at the microscopic level

The macroscopic theory of a medium containing microscopic cracks presented in this paper, when compared with the classical continuum mechanics, includes two additional kinematical ingredients denoted by n and d – called respectively the crack number and the director – which characterize certain features of the cracks on the microscopic level. As will become evident presently, explicit identification of these macroscopic variables with appropriate microscopic features (e.g. typical size of

cracks) is essential for motivation both of possible constraints to be imposed on the director and of restrictions to be placed on the constitutive coefficients of the macroscopic responses of the medium, as well as for physically meaningful interpretation of the macroscopic results. Preparatory to this objective and for the sake of clarity, we include here some background remarks on the nature of crack growth in terms of the microscopic description of the material.

A crack is usually defined as a void in a material which is considerably narrower in one direction, say in the direction of a unit vector  $n^*$ , than in directions on the surface normal to  $n^*$ . The area of the projection of the volume of a crack on the surface normal to  $n^*$  is taken as representing the predominant feature of the crack and is referred to in this paper simply as the 'crack area'. Crack growth is then thought to occur in two possible ways: (1) a crack may be stretched as the (microscopic) bounding surface which bounds the crack is stretched such that this surface is always material; we refer to such motions as crack deformation; and (2) a crack may grow in excess of that described in (1); we refer to such motions as crack growth. The crack growth is the consequence of the effects of actual fracture processes in which material bonds are destroyed.

The usual elasticity theory is considered to be reversible in the sense that, following any motion or deformation from a reference state, the material can always be returned to its reference state simply by reversing the motion; the reference state may, of course, be taken as the initial state. Recalling that the media under consideration is assumed to be elastic in the absence of cracks, we now define a reversible motion of the body as any motion in which every microscopic particle contained in the body may be returned to its reference state simply by reversing the deformation of the body. It is clear that during a reversible motion, the cracks in the body can undergo only crack deformation, as defined in the preceding paragraph.

Due to the possible irreversible growth of cracks, any arbitrary motion of the body is not necessarily reversible on the microscopic level. This is because the microscopic bounding surfaces (including the boundary surfaces of the microcracks) of the body are altered by the fracture processes and hence the adjoining microscopic particles do not return to their original state upon reversal of the deformation. It may be emphasized here that the concept of a reversible motion, as defined here, can be clearly defined only on the microscopic scale. However, in light of our previous discussion, the notion of a reversible motion is well defined on the microscopic scale. To elaborate, consider a typical motion which, on the macroscopic scale, takes a material point (or particle) to its corresponding place x in the current configuration  $\kappa$  of the body at time t. Such a motion is not necessarily reversible using the terminology of the preceding paragraph. It is possible, however, to associate with a given motion a different reversible motion resulting in the place x in  $\kappa$ . It follows that any motion may be decomposed into reversible and irreversible parts: the irreversible motion of the body (if present) is obtained simply by removing the corresponding reversible motion from the total motion of the body. It may be observed that the irreversible motion of the body involves only crack growth. Also, it should be noted that the concepts of reversible and irreversible motions, as defined here, are relevant not only to the body B as a whole, but also to any microscopic part of B.

It is convenient at this point to introduce some notations pertaining to the microscopic description of the body. In a fixed reference configuration  $\dagger \kappa_0^*$  the body

<sup>†</sup> The use of an asterisk attached to various symbols is for later convenience. The corresponding symbols without the asterisks are reserved for different designations to be introduced later in §3.

 $\mathscr{B}$  bounded by  $\partial \mathscr{B}$  occupies a region  $\mathscr{R}_0^*$  bounded by a closed boundary surface  $\partial \mathscr{R}_0^*$ , and in the configuration  $\kappa^*$  at time t the body occupies a region  $\mathscr{R}^*$  bounded by a closed surface  $\partial \mathscr{R}^*$ . Any arbitrary material volume  $\mathscr{S}^*$  of  $\mathscr{B}$  in the two configurations  $\kappa_0^*$  and  $\kappa^*$  occupy, respectively, the regions  $\mathscr{P}_0^* (\subseteq \mathscr{R}_0^*)$  bounded by a closed surface  $\partial \mathscr{P}^*$ . The microscopic material point (or particle)  $X^*$  within  $\mathscr{S}^*$  in the configurations  $\kappa^*$  and  $\kappa_0^*$  are identified by  $\kappa^*$  and  $\kappa^*$  in the current and reference configurations by  $\kappa^*$  and  $\kappa^*$  are identified by a closed surface  $\kappa^*$  and  $\kappa^*$  respectively. Although in anticipation of later identification of the macroscopic position vectors (in §3) with the symbols  $\kappa^*$  and  $\kappa^*$  introduced here in the context of microscopic theory, no confusion should arise between the use of the same symbols for discrete quantities defined on the microscopic level and associated continuous quantities introduced on the macroscopic scale.

We have already indicated that the most important features of any given crack (with respect to the effect of the crack on the macroscopic behaviour of the material) are the magnitude of the 'crack area' and the unit normal to the surface on which the crack area lies. Furthermore, it should be noted that energy must be supplied to the crack during crack growth to create additional surface area, and also that growth of the crack induces motion in the microscopic particles in the neighbourhood of the crack. These latter two effects, i.e. the energy supplied to the crack and the particle inertia around the crack, which are associated only with crack growth, are important for assessing the behaviour of the cracks in response to a macroscopic deformation of the material.

It was indicated previously that a typical motion of the body on a microscopic scale from a fixed reference configuration  $\kappa_0^*$  to a current configuration  $\kappa^*$  can be decomposed into an irreversible motion (from  $\kappa_0^*$  to an intermediate configuration  $\bar{\kappa}^*$ , say) and a reversible motion (from  $\bar{\kappa}^*$  to  $\kappa^*$ ). The irreversible motion of the body from  $\kappa_0^*$  to  $\bar{\kappa}^*$  is obtained by removing the reversible motion from the total motion (from  $\kappa_0^*$  to  $\kappa^*$ ). It may be noted that the location of the centre of mass of some sufficiently large region  $\mathscr{P}^*$  in the reference and intermediate configurations is the same. Additional related remarks and some analysis pertaining to crack growth on the microscopic scale are given in Appendix A.

# 3. Development of the macroscopic theory of crack growth

In the usual macroscopic description of materials, a body  $\mathcal{B}$  bounded by a closed surface  $\partial \mathcal{B}$  is regarded to consist of a set of material points (or particles) X. Here—within the context of directed media—we suppose that each material point X is endowed with an additional independent kinematical vector field, called a *director*. Remembering the background information at the microscopic level indicated in §2 (see especially the last two paragraphs of §2), in the present context the director possesses the following properties:

(i) the direction of the variable  $\bar{d}$  mentioned in §1.2 (see also equation (3.4)) represents the direction of the normal to the plane on which the projection of microscopic crack areas contained in the microscopic region  $\mathscr{P}^*$  of the intermediate configuration  $\bar{\kappa}^*$ , is a maximum (the term maximum here is unambiguous as is, in fact, an absolute maximum since it refers to the maximum of the projected (scalar) areas over all possible orientations of the projected plane);

(ii) the magnitude of  $\bar{d}$  is equal to the square root of the sum of the projections on the plane normal to  $\bar{d}$  of the microscopic crack areas (contained in the region  $\mathscr{P}^*$ ) in the intermediate configuration  $\bar{\kappa}^*$ .

Thus, let the material point X and the director at X, be identified by the position vector X and the value of a single director D = D(X) in a fixed reference configuration  $\kappa_0$ ; and, similarly denote the corresponding quantities in the current configuration  $\kappa$  at time t by the position vector x and the director d at x. (It is understood that the symbols such as  $\kappa$ ,  $\kappa_0$  (without an asterisk) in this section refer to configurations in the macroscopic description of the motion of  $\mathcal{B}$ .) A motion of such a body is then defined by sufficiently smooth vector functions  $\chi$  and  $\mathcal{D}$  which assign the place x and director d to each material point of  $\mathcal{B}$  at each instant of time, i.e.

$$\mathbf{x} = \mathbf{\chi}(\mathbf{X}, t), \quad \mathbf{d} = \mathcal{D}(\mathbf{D}, t).$$
 (3.1)

Clearly, in view of the dependence of D on X, the right-hand side of  $(3.1)_2$  can be expressed as a different function of X and t. The deformation gradient F and its determinant J are defined by

$$F = \partial \chi / \partial X, \quad J = \det F.$$
 (3.2)

We assume that  $(3.1)_1$ , but not  $(3.1)_2$ , is invertible for a fixed value of t so that the jacobian of transformation associated with  $(3.1)_1$  does not vanish; and, for definiteness, we stipulate further than J > 0. The ordinary particle velocity v and director velocity v are defined by

$$\mathbf{v} = \dot{\mathbf{x}}, \quad \mathbf{w} = \dot{\mathbf{d}},\tag{3.3}$$

where a superposed dot denotes material time differentiation with respect to t holding X fixed.

For reasons that will become clear presently, we introduce two additional kinematical variables. One of these, denoted by  $\bar{d}$ , is defined in terms of  $(3.1)_2$  and  $(3.2)_1$  by

$$\bar{\pmb{d}} = J^{-1} \pmb{F}^{\rm T} \pmb{d} = J^{-1} (F_{iA} \, \pmb{e}_A \otimes \pmb{e}_i) \, (d_j \, \pmb{e}_j) = J^{-1} F_{iA} \, d_i \, \pmb{e}_A = \bar{\pmb{d}}_A \, \pmb{e}_A \tag{3.4}$$

and its rate is

$$\dot{\bar{d}} = \bar{w} = \bar{w}_{4} e_{4}, \tag{3.5}$$

where  $F^{\rm T}$  denotes the transpose of F,  $e_i$  and  $e_A$  are respectively the orthonormal basis vectors in the current and reference configurations, the symbol  $\otimes$  denotes tensor product and the usual summation convention over the repeated Latin indices is understood. Also, in view of  $(3.4)_1$  and  $(3.1)_2$ , it should be clear that in terms of the function  $\mathscr D$  the variable  $\bar d = J^{-1}F^{\rm T}\bar{\mathscr D}(D,t)$  and that the values of both d and  $\bar d$  coincide with D in the reference configuration where F = I. The second kinematical variable is the crack density

$$n = n(X, t) \tag{3.6}$$

per unit volume in the reference configuration  $\kappa_0$ .

We now indicate the interpretation that may be assigned to the macroscopic variables (3.4) and (3.5) in terms of the quantities on the microscopic scale introduced in §2. In light of the microscopic description provided in Appendix A (see especially (A 4)<sub>1</sub> and (A 6)), we may identify  $\bar{d}$  as a measure of the total area and orientation of the microcracks in the intermediate configuration  $\bar{\kappa}^*$  and note that its material derivative  $\bar{d}$  can be interpreted as a measure of the rate of growth of the

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microcracks. Likewise the crack density n defined by (3.6) may be identified as the

limit of the number of cracks  $n^*$  contained in the microscopic region  $\mathscr{P}^*$  divided by the volume  $\mathscr{V}_0^*$  of  $\mathscr{S}^*$  in the configuration  $\kappa_0^*$  when  $\mathscr{V}_0^*$  tends to zero, i.e.

$$n = \lim_{\substack{\mathscr{V}_0^* \to 0}} (n^* / \mathscr{V}_0^*).$$

For later reference we recall that the lagrangian strain E is defined by

$$E = \frac{1}{2}(F^{\mathrm{T}}F - I) = E_{AB} e_A \otimes e_B, \tag{3.7}$$

where I denotes the identity tensor,  $E_{AB}=\frac{1}{2}(x_{i,A}\,x_{i,B}-\delta_{AB})$  are the rectangular cartesian components of the strain E referred to the basis  $e_A \otimes e_B$ , a comma preceding an index denotes partial differentiation, and  $x_{i,A}$  are components of the deformation gradient.

Let  $a^{K}$  (K = 1, 2, 3) designate the three principal directions of the strain measure E. Then, by standard results from linear algebra we have

$$Ea^{K} = \beta^{(K)}a^{K}$$
 or  $E_{AB}a_{B}^{K} = \beta^{(K)}a_{A}^{K}$  (no sum on  $K$ ), (3.8)

where in (3.8) K is not a tensor index and  $\beta^{(K)}$  is the associated scalar eigenvalue. Since E is a symmetric second-order tensor, the three directions  $a^{K}$  are mutually orthogonal and must satisfy the conditions

$$a^{I} \cdot a^{J} = a_{A}^{I} A_{A}^{J} = \begin{cases} 1 & \text{if } I = J, \\ 0 & \text{if } I \neq J, \end{cases} \quad (I, J = 1, 2, 3).$$
 (3.9)

We recall that as a consequence of the motion specified by the vector function  $\mathbf{z}$ the material point X in  $\mathcal{B}$  occupies the place x in the configuration  $\kappa$  given by  $(3.1)_1$ . Under another motion, which differs from the given one only by a superposed rigid body motion, the material point X moves to  $x^+$  in the configuration  $\kappa^+$  at time  $t^+$ t+a, where a is a constant. It is well known that under such superposed rigid body motions  $x^+$ ,  $d^+$  and  $F^+$  transform as

$$x^{+} = a + Qx, \quad F^{+} = QF, \quad d^{+} = Qd,$$
 (3.10)

where a is a vector function of t and Q is a proper orthogonal tensor function of t and satisfy the conditions

$$Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = I, \quad \det Q = +1.$$
 (3.11)

Under superposed rigid body motion (3.10)<sub>1</sub>, the variable  $\bar{d}$  and the number of cracks n transform as

$$\bar{d}^+ = \bar{d}, \quad n^+ = n. \tag{3.12}$$

The first of (3.12) readily follows from the definition  $(3.4)_1$  and  $(3.10)_{2.3}$ , while  $(3.12)_2$ represents a physically reasonable stipulation that the number of cracks will remain unaltered by a superposed rigid body motion.

It is convenient at this point to define certain additional quantities which occur in the balance laws to be introduced presently. The mass density  $\rho_0 = \rho_0(X)$  and  $\rho =$  $\rho(X,t)$  of  $\mathcal{B}$  in the configurations  $\kappa_0$  and  $\kappa$ , respectively; the rate of production h=h(X,t) of the number of cracks per unit volume in the reference configuration; the stress vector  $\mathbf{R} t = \mathbf{R} t(X, t; N)$  and the director stress vector (or the stress couple)  $_{\rm R}m = _{\rm R}m(X,t;N)$ , each measured per unit area with an outward unit normal N in the reference configuration  $\kappa_0$ ; the external body force b = b(X, t) and the external directory body force l = l(X, t), each per unit mass in the reference configuration; and the intrinsic director force  $_{R}\mathbf{k} = _{R}\mathbf{k}(\mathbf{X},t)$  per unit volume in the reference configuration. We also assume in the present paper that the quantities  $_{R}\mathbf{m}$ ,  $\mathbf{l}$  and  $_{R}\mathbf{k}$  make no contributions to the moment of momentum.

Motivated by considerations at the microscopic level and the identification of the material point of the continuum on the macroscopic scale with the centre of mass of the microscopic region (discussed in detail in Appendix A), we assume that the kinetic energy  $\kappa$  per unit mass in the reference configuration associated with the particle X has the form

$$\kappa = \frac{1}{2}(\mathbf{v} \cdot \mathbf{v} + y \,\overline{\mathbf{w}} \cdot \overline{\mathbf{w}}),\tag{3.13}$$

where  $\overline{w}$  is defined by (3.5). The inertia coefficient y in (3.13) in general requires a constitutive equation, which apart from its dependence on X could also depend on the kinematical variables  $(E, \overline{d}, n)$  inasmuch as the region containing the microcracks is not necessarily material. In this connection, it should be noted that a constitutive equation for the inertia coefficient in the form y = y(E, d, n; X) can still satisfy the invariance requirement  $y^+ = y$ , in view of the invariance properties of (E, d, n) under superposed rigid body motions. Moreover, it is worth observing that consistent with the identifications made previously for x and  $\overline{d}$  in regard to features on the microscopic level, it is assumed that no coupling term involving  $v \cdot \overline{w}$  contributes to the macroscopic kinetic energy in (3.13).

In view of (3.13), we define the momentum per unit mass corresponding to the velocity v and the director momentum per unit mass corresponding to the director velocity w by

$$\partial \kappa / \partial v = v, \quad \partial \kappa / \partial \overline{w} = y \overline{w}.$$
 (3.14)

Consistent with the identification of x and d with corresponding quantities in §2, we may regard the magnitude of the ordinary inertia coefficients in (3.14) to be simply the magnitude of the inertia coefficients which this microscopic region would have had if no crack growth had occurred. The magnitude of the director inertia in (3.14) may then be interpreted as the magnitude of the additional inertia of the microscopic particles in this region due to the growth of cracks. Thus the magnitude of the inertia of any microscopic particle in the neighbourhood of a crack may be divided into two parts, namely the part which would have been present regardless of the motion of the cracks and the part due to the irreversible growth of the cracks. Appropriate averages of each of these two parts over all microscopic particles in the microscopic region may be identified with the magnitudes of the ordinary and director inertias, respectively, of the macroscopic particle X. Also, the physical dimensions of  $\rho_0$ , R, D are:

$$\begin{array}{c} \text{phys. dim. } \rho_0 = [ML^{-3}], \quad \text{phys. dim. } _{\mathbf{R}} \boldsymbol{t} = [ML^{-1}T^{-2}], \\ \text{phys. dim. } \boldsymbol{b} = [LT^{-2}], \end{array}$$

where the symbols [L], [M] and [T] stand for the physical dimensions of length, mass and time. The physical dimensions of the vector fields  $_{R}m$ , l,  $_{R}k$  depend upon the physical dimension of d. Here we assume that d and hence  $\overline{d}$  have the dimension of length and then  $_{R}m$ , l will have the same physical dimensions as  $_{R}t$  and b in (3.15) while  $_{R}k$  will have the physical dimension of  $[ML^{-2}T^{-2}]$ . (It should be noted that if d is specified to be dimensionless, then the physical dimension of  $_{R}m$  will be  $[MT^{-2}]$  corresponding to a physical dimension of a stress couple.)

The balance laws utilized in the present paper, aside from being in lagrangian form, consist of those ordinarily adopted in the classical continuum mechanics and

and

two others, which are associated with the kinematical variables n and  $\bar{d}$  and which will be discussed presently. We note here that the basic ingredients that enter the balance law associated with  $\bar{d}$  are assumed to make no contributions to the balance of moment of momentum. (Further comments on this point will be made below in the paragraph following (3.20).) Thus we first record the local forms of the ordinary conservation laws for mass and momentum which can be stated for every material point in the reference configuration  $\kappa_0$  as

$$\rho_0 = \rho J, \quad \rho_0 \, \dot{\boldsymbol{v}} = \rho_0 \, \boldsymbol{b} + \text{Div} \, \boldsymbol{P}, \quad \boldsymbol{P} \boldsymbol{F}^{\text{T}} = \boldsymbol{F} \boldsymbol{P}^{\text{T}}, \quad {}_{\text{R}} \boldsymbol{t} = \boldsymbol{P} \boldsymbol{N}, \tag{3.16}$$

where P is the first non-symmetric Piola–Kirchhoff stress tensor. The equations  $(3.16)_{1,2,3}$  represent, respectively, the referential form of conservation of mass, the consequences of momentum and that of moment of momentum. Also in (3.16), the notation 'Div' stands for the divergence operator with respect to X, N denotes the outward unit normal to any surface in the reference configuration  $\kappa_0$  and the remaining quantities were defined in the preceding paragraph.

The nature of the additional balance laws for any part of the body  $\mathcal{B}$ , which is motivated in Appendix A, may be stated in words as:

rate of change of crack number = rate of production of new cracks (3.17)

$${\text{rate of change of momentum} \atop \text{associated with crack growth}} = {\text{all forces arising from (and maintaining)} \atop \text{the effect of crack growth}}.$$
(3.18)

Then, in terms of the definitions introduced previously, statements for balance of crack number and the rate of change of momentum associated with crack growth embodied in (3.17) and (3.18) for any part  $\mathscr{P}_0$  bounded by a closed surface  $\partial \mathscr{P}_0$  in  $\kappa_0$  are:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathscr{P}_0} n \, \mathrm{d}V = \int_{\mathscr{P}_0} h \, \mathrm{d}V, \tag{3.19}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathscr{P}_0} \rho_0 \, y \, \overline{\boldsymbol{w}} \, \mathrm{d}V = \int_{\mathscr{P}_0} \rho_0 \, \boldsymbol{l} \, \mathrm{d}V - \int_{\mathscr{P}_0} {}_{\mathbf{R}} \boldsymbol{k} \, \mathrm{d}V + \int_{\partial \mathscr{P}_0} {}_{\mathbf{R}} \boldsymbol{m} \, \mathrm{d}A, \tag{3.20}$$

where dV is an element of volume and dA is an element of area in the fixed reference configuration.

Two features of the above balance laws should be noted: (a) there is no coupling of inertia terms between the balances of ordinary momentum and director momentum (3.20), as is evident from the left-hand sides of (3.16)<sub>2</sub> and the right-hand side of (3.13), and (b) the balance of angular momentum (3.16)<sub>3</sub> does not involve any contributions from the director and the kinematical and kinetical quantities associated with the director which occur in (3.20). Support for these features of the balance laws for the present purpose can be readily provided through a derivation from a balance of energy, together with the invariance requirements under superposed rigid body motions, which demonstrates that the classical conservation laws together with the local form of (3.20) are consistent with the invariance properties of the kinetical quantities  $_{\bf R} m$ ,  $_{\bf R} k$  (see (3.24)<sub>1,2</sub> below), and (iii) the invariance properties of

the balance of energy under superposed rigid body motions. The details of such a derivation are not included here.

By usual procedures and under suitable continuity assumptions, it follows from (3.19) and (3.20) that

$$\dot{n} = h$$
,  $\rho_0 \dot{y} \dot{w} = \rho_0 l - {}_{\mathbf{R}} k + \text{Div}_{\mathbf{R}} M$ ,  ${}_{\mathbf{R}} m = {}_{\mathbf{R}} M N$ , (3.21)

where  $_{\mathbf{R}}\mathbf{M}$  is the director stress tensor measured per unit area of the surfaces in the reference configuration.

Within the scope of the macroscopic theory under discussion, the expression for the mechanical power P can be reduced to

$$P = \mathbf{S} \cdot \dot{\mathbf{E}} + {}_{\mathbf{R}} \mathbf{k} \cdot \overline{\mathbf{w}} + {}_{\mathbf{R}} \mathbf{M} \cdot \operatorname{Grad} \overline{\mathbf{w}}, \tag{3.22}$$

where the notation 'Grad' stands for the gradient operator with respect to X and S is the second (symmetric) Piola–Kirchhoff stress tensor defined through

$$S = F^{-1}P$$
,  $S = S^{\mathrm{T}}$ .

We have previously indicated that under superposed rigid body motions (SRBM) the place  $\mathbf{x}^+$ , the director  $\mathbf{d}^+$  and the crack number  $n^+$  are specified by (3.10) and (3.12)<sub>1,2</sub>. Now, all the local conservation equations in (3.16) and (3.21) and the various fields occurring in these equations should be properly invariant under superposed rigid body motions (3.10) and (3.12): For example, as is well known, the stresses  $\mathbf{P}$  and  $\mathbf{S}$  transform according to the formulae

$$P^+ = QP, \quad S^+ = S. \tag{3.23}$$

Supplementary to  $(3.23)_{1,2}$ , we stipulate the invariance properties

$$_{\mathbf{R}}\mathbf{M}^{+} = _{\mathbf{R}}\mathbf{M}, \quad _{\mathbf{R}}\mathbf{k}^{+} = _{\mathbf{R}}\mathbf{k}.$$
 (3.24)

There seems to be reasonable support in the literature for the assumption that

the growth of cracks tends to occur along a surface which is normal to the particular principal direction of the strain E in the macroscopic theory for which the associated eigenvalue is maximum. (3.25)

The assumption (3.25) is supported by experimental studies for nearly isotropic materials and in the presence of small deformation (for which the principal directions of stress and strain are the same) such as those of Sangha et al. (1974) for sandstone, Bieniawski (1974) for coal and Williams & Ewing (1972) for two-dimensional cracks in thin plates. For anisotropic materials, the principal direction of E, although not usually recorded in studies of crack growth, can be roughly estimated and our assumption (3.25) seems to be at least qualitatively in agreement with available studies, for instance that of Peng & Johnson (1972) for anisotropic granite. Of course for certain laminated composites the assumption (3.25) may at times be expected to break down due to the tendency of the cracks to propagate along material interfaces. We do not assert here that the growth of every crack necessarily conforms to the assumption (3.25), but merely assert that a fair majority of cracks grow in this way. Although the support for this assumption in the literature may not be entirely conclusive for anisotropic media, we adopt it in what follows because it seems to be in reasonable agreement with observations in the literature and because it provides an idealized model which leads to a substantial simplification of the theory.

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Let  $\mathbf{a}^3$  refer to the principal direction of E which possesses a maximum eigenvalue  $\beta^{(3)}$ . Recalling that the  $\overline{\mathbf{w}}$  defined by  $(3.4)_1$  may be identified with the rate of the crack growth and in line with the observations mentioned in the last paragraph, we now require that  $\mathbf{w}$  be constrained to be parallel to  $\mathbf{a}^3$ , so that by (3.9) we may write

$$\begin{array}{ccc} \overline{w} = \alpha \boldsymbol{a}^3 & \text{or} & w_A = \alpha a_A^3, \\ \overline{w} \cdot \boldsymbol{a}^1 = \overline{w} \cdot \boldsymbol{a}^2 = 0 & \text{or} & \overline{w}_A a_A^1 = \overline{w}_A a_A^2 = 0 \end{array}$$
 (3.26)

for all X and t. Since  $\mathbf{a}^3$  can be determined from (3.8) once  $\mathbf{E}$  is known and since  $\mathbf{d}$  can be calculated from the time history of  $\mathbf{w}$ , the constraint (3.26) reduces the number of additional independent variables incorporated into the theory to account for the presence of cracks from four (i.e. n and  $\mathbf{d}$  or  $\mathbf{w}$ ) to only two (i.e. n and  $\alpha$ ). (A discussion of constraints for a directed medium with a single director is included in a paper of Green  $et\ al.\ (1970, \S 6)$ . The nature of the constraint (3.26) and subsequent derivation of constraint responses given below by (3.29) are similar to a previous development carried out in a different context by Naghdi (1982, §6.2), where additional references on the subject can be found.)

In the special case in which the body is subjected to all around uniform tension or compression, the deviatoric part of the strain E (at least for small strain) may vanish, in which case the direction  $a^3$  will become indeterminate. To resolve this indeterminacy, a choice for the direction  $a^3$  in (3.26) must be made by some other criteria. In such cases the cracks are usually observed to continue growing in whatever material plane in which they were growing just prior to the vanishing of the deviatoric part of E. If the deviatoric part of E was initially zero, the direction normal to the plane along which the cracks are most pronounced is a good choice for  $a^3$  (in this case  $a^3$  is parallel to  $\overline{d}$ ).

Returning the constraint imposed on  $\bar{d}$  by (3.26), we now proceed to determine its affect on the kinetical quantities which enter the equations of motion (3.16)<sub>2</sub> and (3.21)<sub>2</sub>. Thus, we assume that each of the response functions S,  $_Rk$ ,  $_RM$  are determined to within an additive constraint response  $\bar{S}$ ,  $_R\bar{k}$ ,  $_R\bar{M}$  so that

$$S = \bar{S} + \hat{S}, \quad _{\mathbf{R}}\mathbf{k} = _{\mathbf{R}}\bar{\mathbf{k}} + _{\mathbf{R}}\hat{\mathbf{k}}, \quad _{\mathbf{R}}\mathbf{M} = _{\mathbf{R}}\bar{\mathbf{M}} + _{\mathbf{R}}\hat{\mathbf{M}}, \tag{3.27}$$

where  $\hat{S}$ ,  $_{R}\hat{k}$ ,  $_{R}\hat{M}$  are to be specified by constitutive equations and the constraint responses which are workless are independent of the kinematical variables  $(\dot{E}, \bar{w}, \text{Grad } \bar{w})$  and are only arbitrary functions of position and time. Thus, recalling the expression (3.22) for mechanical power, we have

$$\bar{\mathbf{S}} \cdot \dot{\mathbf{E}} + {}_{\mathbf{R}}\bar{\mathbf{k}} \cdot \bar{\mathbf{w}} + {}_{\mathbf{R}}\bar{\mathbf{M}} \cdot \operatorname{Grad} \bar{\mathbf{w}} = 0. \tag{3.28}$$

Multiplying the constraint  $(3.26)_{2,3}$  by the Lagrange multipliers  $\gamma^{\alpha}$  ( $\alpha = 1, 2$ ), subtracting from (3.28) and noting that the resulting equation must remain valid for all values of  $\dot{E}$ ,  $\bar{w}$ , Grad  $\bar{w}$ , we deduce that

$$\bar{S} = {}_{R}\overline{M} = 0, \quad {}_{R}\bar{k} = \sum_{\alpha=1,2} \gamma^{\alpha} a^{\alpha}.$$
(3.29)

Substituting the result  $(3.29)_3$  into the director momentum equation  $(3.21)_2$ , after using (3.28), results in

$$\rho_0 \dot{\vec{y}w} = \rho_0 \mathbf{l} - {}_{\mathbf{R}} \hat{\mathbf{k}} + \text{Div}_{\mathbf{R}} \hat{\mathbf{M}} - {}_{\mathbf{R}} \bar{\mathbf{k}}, \tag{3.30}$$

where  $_{\mathbf{R}}\mathbf{k}$  is given by  $(3.29)_3$ .

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The relevant equations adopted and developed in the section are the mass conservation equation  $(3.16)_1$ , the crack number balance  $(3.21)_1$ , the ordinary momentum equation  $(3.16)_2$ , the constraint  $(3.26)_1$  and the reduced form of the director momentum equation resulting from the inner product of (3.30) and  $a^3$  with vanishing of  $_{\rm R}\bar{k}\cdot a^3$  provide a sufficient number of equations to determine the unknown variables  $\rho$ , n, v and  $\bar{d}$ .

#### 4. Constitutive equations for the macroscopic theory

It is common in the continuum mechanics literature to use the various balance laws and inequalities of thermomechnical theory to place restrictions on constitutive equations for both thermal and mechanical response functions. Since the primary objectives of this paper have to do only with mechanical aspects of crack growth, the present theory is constructed only in a purely mechanical context. However, to motivate certain restrictions on the constitutive equations of the theory, limited use is made here of more general thermodynamical results in the special case of isothermal conditions. The present theory may, of course, be extended to encompass more general thermomechanical effects; however, it is felt that such an extension may obscure the basic features of the purely mechanical theory which we wish to emphasize.

To motivate these constitutive restrictions we appeal to the thermodynamical formulation of Green & Naghdi (1977). In this formulation, the energy equation, after combination with a balance law for entropy and elimination of the heat supply and body force terms, takes a reduced form which is then regarded as an identity for all processes. The lagrangian form of this reduced energy equation, before specialization to the isothermal case, reads as

$$-\rho_{0}(\dot{\psi}+\eta\dot{\theta})+P+\frac{1}{2}\rho_{0}\dot{y}\bar{w}\cdot\bar{w}-\rho_{0}\theta\xi-\theta^{-1}\boldsymbol{q}_{\mathrm{R}}\cdot\boldsymbol{g}_{\mathrm{R}}=0,$$

where  $\theta$  is the absolute temperature,  $\psi$  the specific Helmholtz free energy,  $\eta$  the specific entropy,  $\mathbf{g}_{\mathrm{R}}$  the temperature gradient,  $\mathbf{q}_{\mathrm{R}}$  the heat flow vector measured per unit area in the reference configuration  $\mathbf{\kappa}_{\mathrm{0}}$  and the term  $\rho_{\mathrm{0}}\,\theta\xi$  is a measure of internal rate of production of heat (or energy dissipation) arising from an internal generation of entropy  $\boldsymbol{\xi}$ . For the special case of isothermal deformation ( $\theta = \mathrm{const.}, \ \dot{\theta} = 0, \ \mathbf{g}_{\mathrm{R}} = 0$ ), this reduced energy identity has the form

$$P = \rho_0 \dot{\psi} + \rho_0 \xi - \frac{1}{2} \rho_0 \dot{y} \overline{w} \cdot \overline{w}, \tag{4.1}$$

where  $\psi$  and  $\xi$  must be specified by constitutive equations as functions of the independent variables of the theory. (The notation  $\xi$  here corresponds to  $\theta \xi$  (with  $\theta$  standing for temperature) of Green & Naghdi (1977) and the first (un-numbered) equation of this section.) The functions  $\psi$  and  $\xi$  are referred to here as the 'stress potential' and the 'rate of energy dissipation', respectively, both per unit mass. It may be noted that the independent variables on which  $\psi$  may depend are not limited to only the strain E; and, hence,  $\psi$  is not the same as the 'strain energy' of usual elasticity theory. The rate  $\dot{\psi}$  in (4.1) may be interpreted as the rate of energy storage due to the macroscopic deformation of the material minus the rate of crack surface energy increase associated with crack growth. Additionally, a certain portion of the mechanical work may be dissipated in the material during the creation of new crack surfaces, both through breaking of molecular bonds in the creation of a crack bounding surface and during plastic flow in the microscopic region surrounding a

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crack. Of course, in a perfectly brittle material the latter contribution is negligible. It is common in theories of crack growth in brittle media to neglect dissipation altogether and lump all the energy spent in the creation of a new crack surface into the surface potential energy. However, strictly speaking, the surface potential energy should only be identified with energy that can be recovered upon elimination of the crack surface. The difference between energy required to create a crack surface and that gained by its elimination should properly be called dissipation.

#### 4.1. Basic constitutive development

We now proceed with the development of the constitutive responses in the constrained theory discussed at the end of  $\S 3$ . Because of the presence of the last term on the right-hand side of the reduced energy equation (4.1), we introduce a new vector-valued variable K defined by

$$K = {}_{\mathrm{R}}\hat{k} + \frac{1}{2}\rho_0 \dot{y}\bar{w} \tag{4.2}$$

and assume that

$$\{\hat{\boldsymbol{S}}, \boldsymbol{K}, {}_{\mathrm{R}}\hat{\boldsymbol{M}}\} \tag{4.3}$$

and the scalar  $\psi$  depend on the variables

$$\mathscr{U} = (E, \bar{d}, n). \tag{4.4}$$

We also stipulate similar constitutive assumptions for  $\xi$  and h which, in addition to the variables (4.4), are assumed to depend on  $\overline{w}$  defined by (3.5). For later reference, it is convenient to specifically indicate the constitutive forms of  $\psi$ ,  $\xi$  and h as:

$$\psi = \hat{\psi}(\mathscr{U}) \tag{4.5}$$

and

$$\xi = \hat{\xi}(\mathcal{U}, \overline{w}), \quad h = (\mathcal{U}, \overline{w}). \tag{4.6}$$

With the above constitutive assumptions, the reduced energy equation (4.1) becomes

$$\hat{\mathbf{S}} \cdot \dot{\mathbf{E}} + \mathbf{K} \cdot \overline{\mathbf{w}} + {}_{\mathbf{R}} \hat{\mathbf{M}} \cdot \operatorname{Grad} \overline{\mathbf{w}} = \rho_0 \left( \frac{\partial \hat{\psi}}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}} + \frac{\partial \hat{\psi}}{\partial \overline{\mathbf{d}}} \cdot \overline{\mathbf{w}} + \frac{\partial \hat{\psi}}{\partial n} h + \hat{\xi} \right), \tag{4.7}$$

where in obtaining (4.7) use has been made of the conservation equation (3.21)<sub>1</sub> and the fact that the mechanical power P in (3.22) will now involve only the determinate parts of the stresses in (4.3). In view of the assumed dependence of (4.3) on the variables  $\mathscr{U}$  in (4.4), the coefficient K in (4.7) is necessarily independent of rate variables such as  $\bar{w}$ ; this, however, does not place any restriction on the coefficient  $y = y(\mathscr{U}; X)$  but implies that only the sum of the determinate part  ${}_{\mathbf{R}}\hat{\mathbf{k}}$  and  ${}_{\mathbf{I}}^{\dagger}\rho_{0}\,\dot{y}\bar{w}$  is independent of rates. It is important to note also that the term  ${}_{\mathbf{I}}^{\dagger}\rho_{0}\,\dot{y}\bar{w}\cdot\bar{w}$  (a part of  $K\cdot\bar{w}$  in (4.7)) represents the inertia effect of microcracking associated with the rate of increase of kinetic energy due to fracturing processes in a non-material region; the latter arises from formation of new cracks and the growth of the pre-existing ones.

To avoid unnecessary complications, in the rest of this paper we specialize the constitutive assumptions  $(4.6)_{1,2}$  and suppose that both the rate of energy dissipation and the rate of production of new cracks depend linearly on  $\overline{w}$  so that we may write

$$\xi = \xi \cdot \overline{w}, \quad h = h \cdot \overline{w} \tag{4.8}$$

with vector fields  $\boldsymbol{\xi}$  and  $\boldsymbol{h}$  being dependent only on (4.3), i.e.

$$\boldsymbol{\xi} = \hat{\boldsymbol{\xi}}(\mathcal{U}), \quad \boldsymbol{h} = \hat{\boldsymbol{h}}(\mathcal{U}). \tag{4.9}$$

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Introduction of (4.8) and (4.9) into (4.7) results in an equation which is linear in the variables

$$(\dot{E}, \overline{w}, \operatorname{Grad} \overline{w})$$
 (4.10)

with coefficient functions which are independent of (4.10). Since this equation must hold for every choice of the variables (4.10), we conclude that

$$\hat{\mathbf{S}} = \rho_0 \, \partial \hat{\psi} / \partial E, \quad {}_{\mathbf{R}} \hat{\mathbf{M}} = \mathbf{0}, \quad \mathbf{K} = \rho_0 (\partial \hat{\psi} / \partial \bar{\mathbf{d}} + (\partial \hat{\psi} / \partial n) \, \hat{\mathbf{h}} + \hat{\boldsymbol{\xi}}). \tag{4.11}$$

The restriction (4.11) enables us to calculate the determinate parts of the internal stresses in terms of the response functions for  $\hat{\psi}$ ,  $\hat{\xi}$  and  $\hat{h}$ . Further restrictions may be imposed on the constitutive result (4.11) by consideration of special processes and are discussed in the remainder of this section.

#### 4.2. Conditions for initiation of microcracking

The constitutive results (4.11) have been deduced from (4.1) by consideration of processes in which the variables (4.10) may assume arbitrary non-zero values. However, we now examine an important class of motions for which  $\bar{w}$  (or at least one of its components) vanish and derive appropriate conditions for the initiation of microcracking. For this purpose, we stipulate the notion of impossibility of crack healing, i.e. the notion that once a crack is formed in a material it cannot recover (with the faces rejoined); and this, in turn, implies that the total area of cracks in a material can only increase. Since the area of cracks on the macroscopic scale is represented by the magnitude of  $\bar{d}$  in (3.4), we restrict attention to processes in which the magnitude of  $\bar{d}$ , i.e.  $\|\bar{d}\| = (\bar{d} \cdot \bar{d})^{\frac{1}{2}}$ , is increasing. This statement is equivalent to requiring that the rate of change of  $\|\bar{d}\|$  be non-negative so that

$$\|\dot{\overline{d}}\| \geqslant 0 \quad \text{or} \quad \overline{d} \cdot \overline{w} \geqslant 0.$$
 (4.12)

Moreover, in view of the constraint condition  $(3.26)_1$ , the second of (4.12) can be rewritten as

$$\alpha \bar{\mathbf{d}} \cdot \mathbf{a}^3 \geqslant 0. \tag{4.13}$$

Since only the directions of  $\bar{d}$  and  $a^3$  and not their senses are defined, for definiteness we choose  $\bar{d}$  and  $a^3$  such that

$$\bar{\mathbf{d}} \cdot \mathbf{a}^3 \geqslant 0. \tag{4.14}$$

With the choice (4.14) the condition (4.13) is satisfied provided that

$$\alpha \geqslant 0. \tag{4.15}$$

As noted in the last paragraph of §3, a relevant differential equation of motion in the constrained theory arises from the inner product of (3.30) with  $a^3$ ; and, after also using (4.11)<sub>2</sub>, is given by

 $\rho_0 \dot{\overline{y}} = -_{R} \hat{k} \mathbf{1} \cdot \mathbf{a}^3 + \rho_0 \mathbf{l} \cdot \mathbf{a}^3. \tag{4.16}$ 

Given the fact that  $\overline{w}$  and hence  $\alpha$  are assumed to be continuous functions of time t (and position), we need to consider the behaviour of  $\dot{\alpha}$  on the left-hand side of (4.16) in light of the condition (4.15). To this end, we examine the behaviour of  $\dot{\alpha}$  during a small closed time interval  $[t_0,t_{\rm f}]$  such that at time  $t^*\in(t_0,t_{\rm f})$  and at some material point  $X^*$  in the reference configuration of the body

$$\alpha(X^*, t^*) = 0. \tag{4.17}$$

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It can then be argued that since the only admissible motions are those for which (4.15) holds and since at time  $t^*$  (and position  $X^*$ ) the coefficient  $\alpha$  must be zero by (4.17), we must have

$$\dot{\alpha}(X^*, t^{*+}) \geqslant 0. \tag{4.18}$$

With  $\rho_0$  and the inertia coefficient y both positive at  $t=t^*$  and  $X=X^*$ , the right-hand side of (4.16) at  $t=t^*$  and  $X=X^*$  is non-negative whenever  $\alpha$  (but not  $\dot{\alpha}$ ) vanishes.

In view of the conclusions reached in the preceding paragraph and with l = 0 (actually we only need to specify  $l \cdot a^3 = 0$ ), the equation of motion (4.16) and the constitutive result (4.11), yield the following condition for erack initiation:

$$-\rho_0 \left(\partial \hat{\psi}/\partial \overline{d} + (\partial \hat{\psi}/\partial n) \, \hat{h} + \hat{\xi}\right) \cdot a^3 \geqslant 0. \tag{4.19}$$

Thus, depending on whether or not conditions (4.17) and (4.18) hold (with  $t^*$  being any time), the constitutive expressions for K can be summarized as

$$K = \begin{cases} \mathbf{0}, & \text{if } \alpha = 0 \text{ and } (4.19) \text{ is not satisfied,} \\ & \text{right-hand side of } (4.11)_3, & \text{if } \alpha \neq 0 \text{ or if } (4.19) \text{ is satisfied.} \end{cases}$$
(4.20)

(Alternatively, we could stipulate a criterion for  $_{\rm R}\hat{k}$  (instead of K) in which case the right-hand side of  $(4.20)_1$  remains unchanged whereas that of  $(4.20)_2$  reads as 'right-hand side of  $(4.11)_3 - \frac{1}{2}\dot{y}\bar{w}$ '.) The specification  $(4.20)_1$  holds during reversible processes in which the material is elastic, while  $(4.20)_2$  holds during irreversible processes and represents a constitutive equation for the determinate part of the 'crack stress' K.

It should be noted that (4.19) is only a necessary condition for crack growth in the sense that satisfaction of (4.19) does not necessarily ensure the initiation of crack growth. However, it should be possible to impose supplementary conditions for initiation of the crack growth so long as they are compatible with (4.19).

Before closing this section, an interpretation can be provided in regard to the crack initiation condition (4.19). Let the left-hand side of (4.19) be designated by g and note that this quantity is a function of the variables  $\mathcal{U}$ . For fixed values of  $(\bar{d}, n)$ , the equation

$$g(\mathcal{U}) = \text{left-hand side of } (4.19) = 0 \tag{4.21}$$

represents a closed hypersurface  $\partial \mathscr{E}$  of dimension five, enclosing an open region  $\mathscr{E}$  in a six-dimensional strain space. Then, the function g is such that  $g(\mathscr{U}) < 0$  for all points in  $\mathscr{E}$  and corresponds to a region in which arrested cracks do not grow. The surface represented by (4.21) can then be interpreted as the surface of initiation of crack growth and  $g(\mathscr{U}) > 0$  may be interpreted as the region of accelerating crack growth in strain space. It should be noted that such interpretations, although interesting, are by no means essential for the theory presented here and will not be referred to in the remainder of the paper.

# 5. Special constitutive equations

We specialize here the general constitutive development of §4; and, in particular, impose further restrictions on the form of the response functions for  $\psi$ ,  $\xi$  and h. Thus we assume that  $\psi$  is a quadratic function of the strain E with coefficients which are arbitrary functions of the variables

$$\mathscr{V} = (\overline{d}, n), \tag{5.1}$$

and that the vector fields  $\boldsymbol{\xi}$  and  $\boldsymbol{h}$  are only linear in  $\boldsymbol{E}$  with coefficients which are arbitrary functions of the variables (5.1). Moreover, in the interest of simplicity, we restrict attention to materials which are isotropic in the absence of cracks. We note, however, that the analysis for the more general anisotropic material is not substantially different from that for the isotropic case.

Let c be the unit vector in the direction of  $\bar{d}$  and write

$$\bar{\boldsymbol{d}} = \bar{\boldsymbol{d}}\boldsymbol{c}, \quad \boldsymbol{c} = c_B \boldsymbol{e}_B, \tag{5.2}$$

where  $\bar{d}$  is the magnitude of  $\bar{d}$  and  $c_B$  are the rectangular cartesian components of c referred to the basis  $e_B$ . Keeping  $(5.2)_1$  in mind, the constitutive equation for  $\psi$  given by (4.5) can be rewritten as

$$\psi = \bar{\psi}(E, c, \mathscr{V}), \tag{5.3}$$

along with similar expressions for  $\xi$  and h. Recalling the assumptions introduced in the opening paragraph of this section, especially that  $\xi$  and h are linear in E, and the functional form indicated in (5.3), by standard results in the theory of invariants we may write (see Spencer 1971, p. 328, or Green & Adkins 1970, §1.13, eqs (1.13.12)):

$$\psi = \frac{1}{2} [\mathscr{C}E] \cdot E + \mu_0,$$

$$\xi = [\phi_0 + \phi_1 \operatorname{tr} E + \phi_3 (c \cdot Ec)] c + \phi_2 Ec,$$

$$h = [\epsilon_0 + \epsilon_1 \operatorname{tr} E + \epsilon_3 (c \cdot Ec) c + \epsilon_2 Ec.$$
(5.4)

In  $(5.4)_{1-3}$ , the coefficients  $\mu_0$ ,  $\phi_0$ ,  $\epsilon_0$ ,  $\phi_1$ , ...,  $\phi_3$ ,  $\epsilon_1$ , ...,  $\epsilon_3$  are functions of the variables (5.1), the fourth-order tensor  $\mathscr{C}$  in  $(5.4)_1$  is given by

$$\mathscr{C} = \mathscr{C}_{ABCD} \, \mathbf{e}_A \otimes \mathbf{e}_B \otimes \mathbf{e}_C \otimes \mathbf{e}_D \tag{5.5}$$

and its components  $\mathscr{C}_{ABCD}$  are defined by

$$\mathscr{C}_{ABCD} = \mu_1 \, \delta_{AB} \, \delta_{CD} + \frac{1}{2} \mu_2 (\delta_{AC} \, \delta_{BD} + \delta_{AD} \, \delta_{BC}) 
+ \frac{1}{2} \mu_3 (\delta_{AC} \, c_C \, c_D + \delta_{CD} \, c_A \, c_B) 
+ \frac{1}{2} \mu_4 (\delta_{AC} \, c_B \, c_D + \delta_{AD} \, c_B \, c_C) + \mu_5 \, c_A \, c_B \, c_C \, c_D,$$
(5.6)

where the coefficients  $\mu_1, ..., \mu_5$  are functions of (5.1).

Introducing  $(5.4)_{1-3}$  into  $(4.11)_{1,3}$ , we obtain the following expressions for  $\hat{S}$  and K:

$$\hat{\mathbf{S}} = \rho_0 \mathscr{C} \mathbf{E},\tag{5.7}$$

$$\textbf{\textit{K}} = \rho_0 \left\{ \left[ \frac{\partial \psi}{\partial \overline{d}} + \phi_0 + \epsilon_0 \frac{\partial \psi}{\partial n} + \left( \phi_1 + \epsilon_1 \frac{\partial \psi}{\partial n} \right) \operatorname{tr} \textbf{\textit{E}} + \left( \phi_3 + \epsilon_3 \frac{\partial \psi}{\partial n} \right) (\textbf{\textit{c}} \cdot \textbf{\textit{Ec}}) \right] \textbf{\textit{c}} \right\}$$

$$+ \left[ \frac{2}{\overline{d}} \mu_3 \operatorname{tr} \mathbf{E} + \phi_2 + \epsilon_2 \frac{\partial \psi}{\partial n} + 4\mu_5 \mathbf{c} \cdot \mathbf{E} \mathbf{c} \right] \mathbf{E} \mathbf{c} + \frac{2}{\overline{d}} \mu_4 \mathbf{E} (\mathbf{E} \mathbf{c}) \bigg\}, \tag{5.8}$$

where in obtaining (5.7)–(5.8) we have also used the relationship

$$\frac{\partial \hat{\psi}}{\partial \bar{d}} = \frac{\partial \psi}{\partial d} c + \frac{1}{\bar{d}} \frac{\partial \psi}{\partial c} \tag{5.9}$$

between  $\hat{\psi}$  in (4.5) and  $\psi$  in (5.4).

Several restrictions must be placed on the coefficients appearing in  $(5.4)_{1-3}$  so that the resulting equations governing the macroscopic material behaviour do not admit 'physically unrealistic' results. One such restriction is that the stress  $\hat{S}$  should vanish

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and the 'crack stress'  $K \cdot a^3$  should be non-negative as the strain E vanishes. On the basis of the constitutive results (5.5) and (5.6), such a restriction implies that

$$\frac{\partial \mu_0}{\partial n} e_4 = 0, \quad \frac{\partial \mu_0}{\partial \bar{d}} + \phi_0 + e_0 \frac{\partial \mu_0}{\partial n} \geqslant 0. \tag{5.10}$$

Since the material is regarded to be isotropic in the absence of cracks, we must recover the usual elasticity coefficients in the limit as  $\bar{d} \to 0$ . Thus, in this limit

$$\begin{array}{l} 2\rho_0\,\mu_1 \rightarrow \lambda, \quad \rho_0\,\mu_2 \rightarrow \mu, \\ (\mu_3,\,\mu_4,\,\mu_5,\,\hat{\boldsymbol{\xi}}) \rightarrow 0, \end{array} \quad \text{as} \quad (n,\,\overline{d}\,) \rightarrow 0,$$

where  $\lambda$  and  $\mu$  are the Lamé constants.

It has been observed that for materials subjected to all around uniform (hydrostatic) compressions, failure occurs under very high load (or pressure) mainly by crushing of the material rather than by microcracking. Since the present theory is not intended to include such crushing processes, we require the value of  $K \cdot a^3$  be non-negative (corresponding to a decrease in the rate of microcracking) as the deviatoric part  $E^{d}$  of the strain tensor approaches zero with the mean normal strain  $\bar{E}I$  being negative. Such a requirement when applied to  $K \cdot a^3$  with the use of (4.14) results in

$$\begin{aligned} & \epsilon_0 \, \partial \mu_0 / \partial n + \partial \mu_0 / \partial \overline{d} + \phi_0 \geqslant 0, \\ & (\phi_1 + \frac{1}{3}\phi_2 + \frac{1}{3}\phi_3) + (\partial \mu_0 / \partial n) \, (\epsilon_1 + \frac{1}{3}\epsilon_2 + \frac{1}{3}\epsilon_3) \leqslant 0, \\ & \frac{\partial}{\partial \overline{d}} \left( \mu_1 + \frac{1}{3}\mu_2 + \frac{1}{3}\mu_3 + \frac{1}{9}\mu_4 + \frac{1}{9}\mu_5 \right) + \epsilon_0 \frac{\partial}{\partial n} \left( \mu_1 + \frac{1}{3}\mu_2 + \frac{1}{3}\mu_3 + \frac{1}{9}\mu_4 + \frac{1}{9}\mu_5 \right) + \epsilon_0 \frac{\partial}{\partial n} \left( \mu_1 + \frac{1}{3}\mu_2 + \frac{1}{3}\mu_3 + \frac{1}{9}\mu_4 + \frac{1}{9}\mu_5 \right) \geqslant 0, \\ & (\epsilon_1 + \frac{1}{3}\epsilon_2 + \frac{1}{3}\epsilon_3) \frac{\partial}{\partial n} \left( \mu_1 + \frac{1}{3}\mu_2 + \frac{1}{3}\mu_3 + \frac{1}{9}\mu_4 + \frac{1}{9}\mu_5 \right) \leqslant 0. \end{aligned}$$

For microcracking materials of the type under consideration, it is usual to assume that as the total crack area  $\bar{d}^2$  increases, the surface potential energy  $\mu_0$  will increase while the 'difference' energy  $\psi - \mu_0$  decreases. This assumption is consistent to that first introduced by Griffith (1921, p. 166), who asserted that '... the total decrease in potential energy due to the formation of a crack is equal to the increase in strain energy less the increase in surface energy'. We, therefore, impose the restrictions

$$\frac{\partial \mu_0}{\partial \overline{d}} \geqslant 0, \quad \frac{\partial}{\partial \overline{d}} (\psi - \mu_0) \leqslant 0$$
 (5.12)

for all admissible processes. Next, with the use of the decomposition (5.6), we note that the condition  $(5.12)_2$  implies that the fourth order tensor  $\mathscr{C}$  must be negative semi-definite for all vectors  $\boldsymbol{c}$ , i.e.

$$\frac{\partial}{\partial \bar{d}} \mathscr{C} \leqslant 0, \tag{5.13}$$

and this, in turn, implies that

$$\frac{\partial \mu_2}{\partial d} \leqslant 0, \quad \frac{\partial}{\partial d} [\mu_1 + \frac{1}{3} (\mu_2 + \mu_3) + \frac{1}{9} (\mu_4 + \mu_5)] \leqslant 0. \tag{5.14}$$

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Recall now the expression (4.1) for P along with the interpretation of  $\xi$  as the rate of dissipation per unit mass in the media. On the assumption that the dissipative processes which are responsible for  $\xi$  cannot add to the stored energy  $\psi$  of the body, it seems reasonable to require that  $\xi \geq 0$  for all admissible processes. It is noted that this inequality can also be obtained from various statements of the Second Law (see, for instance, eq. (5.2) of Green & Naghdi 1984) in the special case of an isothermal process. The expression (4.9)<sub>1</sub> for  $\xi$  may be used with the decomposition (5.9) and the form (5.3)<sub>2</sub> for  $g_A$  to write this inequality as

$$\xi = [\phi_0 + \phi_1 \operatorname{tr} \mathbf{E} + \phi_3 \mathbf{c} \cdot \mathbf{E} \mathbf{c} + \phi_2 \mathbf{E} \mathbf{c}] \cdot \overline{\mathbf{w}} \geqslant 0.$$
 (5.15)

It is convenient to recall now the definition of the deviatoric components of the strain  $E^d$ , namely

$$E^{d} = E - \frac{1}{3} (\operatorname{tr} E) I$$
,  $\operatorname{tr} E^{d} = 0$ . (5.16)

Then, recalling (3.26) and (4.13), together with  $(5.2)_1$ , we obtain the following restriction

$$\phi_0 + (\phi_1 + \frac{1}{3}\phi_2) \operatorname{tr} E + \phi_3 c \cdot Ec + \phi_2 \bar{\beta}^{(3)} \geqslant 0,$$
 (5.17)

where  $\bar{\beta}^{(3)}$  is the eigenvalue of the deviatoric strain  $E^{\mathrm{d}}$ , i.e.

$$\bar{\beta}^{(3)} = \mathbf{a}^3 \cdot (\mathbf{E}^{\mathrm{d}} \mathbf{a}^3). \tag{5.18}$$

Since (5.16) must hold for every choice of E and c with coefficients in (5.16) being independent of them, we may deduce the following results:

$$\begin{array}{ll} \phi_0 \geqslant 0, & \phi_1 + \frac{1}{3}\phi_2 + \frac{1}{3}\phi_3 = 0, \\ \phi_2 \geqslant 0, & -\phi_2 \leqslant \phi_3 \leqslant \frac{1}{2}\phi_2, \end{array}$$
 (5.19)

which are both necessary and sufficient for the satisfaction of (5.15) or equivalently (5.17); details of the proofs are given in Appendix B.

# 6. Illustrative examples

The main purpose of this section is to indicate the manner in which the basic theory of this paper can be utilized, and to illustrate its predictive capabilities by means of two simple examples with the use of the special constitutive equations of §5. However, first we make some comments regarding some of the features of the theory constructed in §§3–5 and provide an outline of the procedure by means of which the various equations and restrictions on material response may be used.

# 6.1. Remarks on the nature of the basic theory and its utilization

The system of governing equations consists of the mass conservation  $(3.16)_1$ , the ordinary linear momentum  $(3.16)_2$ , the local balance of crack number  $(3.21)_1$ , the director momentum in the form (3.30), and the constitutive results  $(4.11)_{1-3}$  and (5.4). Quantitatively this system, together with the crack initiation condition (4.19), formally may be viewed as analogous to those in the theory of elastic–plastic materials even though no use has been made here of any of the concepts from plasticity. Thus, given a material with certain distribution of stationary microcracks and a loading program (either in terms of strain or stress) and once the constitutive coefficients (such as those in (5.4) and (5.6)) are identified, the following procedure can be used for the determination of the response of the material:

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- 1. As the loading program is carried out, the crack initiation condition (4.19) must be checked to establish the beginning of microcracking. (Recall that as long as (4.19) is not satisfied, the microcracks remain stationary and the medium behaves elastically.)
- 2. Once the microcracks are initiated, in the context of the present theory the material behaviour may be classified as inelastic (in the sense that the process of crack growth is irreversible) and the various quantities of interest for microcrack growth can be determined from the system of equations mentioned earlier in this paragraph. This inelastic behaviour continues until the microcracks become stationary again.
- 3. The medium will sustain additional elastic deformation until the initiation condition (4.19) is again satisfied.

From a casual examination of the system of governing equations, it is evident that closed form analytical solutions are extremely difficult except possibly in some very special cases. For this reason, in the remainder of this section we consider a special class of constitutive equations and then illustrate the procedure outlined under (1)–(3) above with reference to two examples involving homogeneous deformation.

#### 6.2. Determination of the constitutive coefficients

Our chief interest in §5 was to consider a class of material response in which the constitutive equations for  $\xi$  and h are linear in the velocity  $\bar{w}$  and at the same time assume a simple form for the dependence of the scalar-valued function  $\psi$  and the vector-valued functions  $\xi$  and h on the lagrangian strain E (see equations (5.4)); the coefficients in these constitutive equations, however, may depend on the variable (5.1). Moreover, remembering the definition (4.2), the determinate response  $_{\bf R}\hat{k}$  is still rate dependent even though a part of it is clearly given by the right-hand side of (5.8).

The purpose of this subsection is to provide estimates for various constitutive coefficients in (5.4), (5.7) and (5.8) in terms of their dependence on the set of variables (5.1) Although some of these estimates are based on highly idealized (cartoon-like) processes which occur on the microscopic level, they do incorporate many of the basic features of microcracking and at the same time suppress the effect of some of the terms (in the constitutive equations) that do not appear to be significant for use in the illustrations discussed below in §6.4.

We begin our task for simplification of the constitutive equations by considering first the function  $\psi$ . To this end, consider (on the microscopic scale) a fixed volume  $\mathscr{V}_0^*$  of the material and suppose that in its current configuration at time t it possesses  $n^*$  cracks, all of them having the same orientation and the same area  $a^{*2}$ . Remembering the discussion following (A 6) of Appendix A, the magnitude  $\bar{d}$  of the kinematic variable  $\bar{d}$  can be regarded as corresponding to the effect of total area (=  $n^*a^{*2}$ ) of all cracks in  $\mathscr{V}_0^*$ . We assume that the surface energy  $\mu_0$  is proportional to the total crack area  $\bar{d}^2$  and is independent of E. Then, for a material which is free of cracks in its reference configuration, the strain energy of the medium is  $\psi - \mu_0$  and this would correspond to the energy of the 'uncracked' solid which is isotropic in the reference configuration. Moreover, the change in the strain energy ( $\psi - \mu_0$ ) due to the effect of microcracks on the material immediately surrounding them is proportional to the total volume influenced by the cracks in the limiting case when the cracks are few and well separated. This suggests assuming a dilute concentration of aligned cracks, as has been frequently utilized in the literature; see, in this connection, a

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paper by Piau (1980) which contains an exact solution within the scope of a linear isotropic elastic solid. Also, to accommodate the possibility that some of the microcracks may not be aligned with the direction of  $\bar{d}$  in the reference configuration, we introduce a measure of the degree of alignment by a scalar constant  $\bar{d}_0$  such that

$$\overline{d}_{\mathbf{0}} = \begin{cases} 0 & \text{if the microcracks are fully aligned,} \\ \|\overline{\boldsymbol{d}}\| & \text{if the microcracks are random.} \end{cases}$$

The preceding background discussion suggests the following choices for  $\mu_0$  and for coefficients  $\mu_1, ..., \mu_5$  in (5.6):

$$\mu_0 = \nu_0 \, n \bar{d}^2, \quad \mu_1 = \lambda - \nu_1 \, \bar{d}^\gamma n^\delta, \quad \mu_2 = 2(\mu - \nu_2 \, \bar{d}^\gamma n^\delta), \\ \mu_3 = -2\nu_3 (\bar{d} - \bar{d}_0)^\gamma n^\delta, \quad \mu_4 = -2\nu_4 (\bar{d} - \bar{d}_0)^\gamma n^\delta, \quad \mu_5 = -\nu_5 (\bar{d} - \bar{d}_0)^\gamma n^\delta.$$
 (6.1)

In the expression (6.1), the coefficients  $\lambda$  and  $\mu$  could be identified with the Lamé constants for the 'uncracked' material,  $\nu_0, ..., \nu_5$  are additional material constants and the exponents  $\gamma$  and  $\delta$  have the values  $\gamma=3$ ,  $\delta=-\frac{1}{2}$  corresponding to a dilute concentration of cracks. (A plausible explanation regarding the choice of values for the exponents  $\gamma$  and  $\delta$  in (6.1) is contained in a paper by Eshelby (1957, p. 394) and further explored by Bristow (1960, eqs (8)).)

We now turn attention to those constitutive coefficients in (5.8) that are associated with the effect of energy dissipation due to microcracking. Such effects occur mainly along the edge of microcracks due to breaking of the bonds and also in the annular region surrounding the crack usually referred to as fracture process zone (FPZ) (see, for example, Hutchinson 1983, fig. 5 and pp. 1045, 1046). The dissipation in the FPZ is primarily due to plasticity effects at the microscopic level. We suppose here that the volume of the FPZ, as well as the length of the crack edge, is proportional to the size of the crack. (To avoid undue complications, we do not account for the possible dependence of the size of the FPZ on the macroscopic strain E.) Further, the energy dissipation may depend upon the macroscopic strain E, since the rate of plastic dissipation does. Based on these background considerations, we choose the following forms for the coefficients  $\phi_0, \ldots, \phi_3$  for the dissipation response function  $\xi$  in  $(5.4)_2$ :

$$\phi_0 = \omega_0 \, \overline{d}, \quad \phi_2 = -3\phi_1 = \omega_2 \, \overline{d}, \quad \phi_3 = 0.$$
 (6.2)

By requiring that the constants  $\omega_0$  and  $\omega_2$  are non-negative, the restriction (5.15), i.e.  $\xi \ge 0$ , is also satisfied.

# 6.3. A simplified system of equations

We record in this subsection a simplified system of equations obtained from the nonlinear theory of §§ 3–5 and the constitutive results of §6.2. Thus, in the absence of body force and director body force it will suffice to set (in view of the constrained condition (3.26))

$$\boldsymbol{b} = 0, \quad \boldsymbol{l} \cdot \boldsymbol{a}^3 = 0, \tag{6.3}$$

and after substituting the constitutive equations for S, K,  $\xi$  and h in terms of special coefficients discussed in §6.2, the final form of the governing equations may be written as

$$\rho_0 \, \dot{n} = \alpha \boldsymbol{h} \cdot \boldsymbol{a}^3, \quad \rho_0 \, \dot{\boldsymbol{v}} = \mathrm{Div} \, \{ \boldsymbol{F}(\boldsymbol{\mathscr{C}}[E]) \}, \quad \rho_0 \, \dot{\overline{y}} = -\,_{\mathrm{R}} \boldsymbol{k} \cdot \boldsymbol{a}^3, \tag{6.4}$$

where  $_{\mathbf{R}}\mathbf{k}\cdot\mathbf{a}^{3}$  on the right-hand side of  $(6.4)_{3}$  is determined by (4.2) and  $(4.20)_{2}$  and the scalar  $\alpha$ , which originally occurs in  $(3.26)_{1}$ , is determined by  $(6.4)_{1,3}$ .

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In view of the constitutive results of §5 and §6.2, the restriction (4.19) can be reduced to

$$\phi[R_1 \, \bar{d} + R_2 \, \bar{d}^{(\gamma - 1)} + R_3 (\bar{d} - \bar{d}_0)^{\gamma - 1}] + [R_4 \, \bar{d}^\gamma + R_5 (\bar{d} - \bar{d}_0)^\gamma] \, \mathbf{h} \cdot \mathbf{a}^3 \geqslant 0, \tag{6.5}$$

where the coefficients  $R_1, ..., R_5$  are given by

$$\begin{split} R_1 &= \nu_0 + \omega_0 + \omega_3 (\beta^{(3)} - \frac{1}{3} \operatorname{tr} \pmb{E}), \\ R_2 &= -\gamma n^\delta \psi_1, \quad R_3 = -\gamma n^\delta \psi_2, \\ R_4 &= -\delta n^{\delta - 1} \psi_1, \quad R_5 = -\delta n^{\delta - 1} \psi_2, \end{split}$$
 (6.6)

the scalar  $\phi$ , which is related to c in (5.2), is defined by

$$\phi = c \cdot a^3, \tag{6.7}$$

 $\beta^{(3)}$  defined by (3.8) is the eigenvalue associated with  $a^3$  and the coefficients  $\psi_1$  and  $\psi_2$  in (6.6) are defined in terms of other coefficients by

$$\psi_{1} = \frac{1}{2} [\nu_{1}(\operatorname{tr} E)^{2} + 2\nu_{2} \operatorname{tr} (E^{2})], \psi_{2} = \frac{1}{2} [2\nu_{3}(\operatorname{tr} E) (c \cdot Ec) + 2\nu_{4}(c \cdot E^{2}c) + \nu_{5}(c \cdot Ec)^{2}].$$
(6.8)

6.4. Uniform extensive and compressive straining of a microcracking material

In this subsection we apply the system of equations (6.4) and the restriction (6.5) to two simple problems pertaining to uniform extensive and compressive straining of a material, with cracks fully aligned ( $\bar{d}_0 = d_0 = 0$ ) along the direction of maximum principal strain. To keep the discussion that follows as simple as possible, we need to introduce a further simplifying assumption associated with a certain idealization in regard to one of the two independent variables which occur in the equations of motion (6.4)<sub>1-3</sub> and the constitutive equations, namely n and  $\bar{d}$ . For this purpose, we may assume: either (1) constant average crack area per unit volume, hereafter abbreviated as CACA, or (2) constant crack number, hereafter abbreviated as ccn. Thus in the discussion that follows we invoke either (1) or (2) in obtaining the desired solutions. The consequences of the two special assumptions, each of which represents an additional assumption in regard to the initial and final stages of microcracking, will be examined separately in the solutions sought.

Before considering our main objective in this subsection, it is expedient to examine the effect of the assumptions (1) and (2) on the constitutive coefficients.

1. Constant average crack area. Since  $d/\sqrt{n}$  is a measure of average area of microcracks at any material point in the macroscopic theory, the special assumption of constant average crack area can be stated as

$$\bar{d}/\sqrt{n} = \text{const.} = \kappa_0 \quad \text{(say)}$$
 (6.9)

and this, in turn, with the help of (5.4)<sub>3</sub> implies that

$$\boldsymbol{h} \cdot \boldsymbol{c} = (2/\kappa_0^2) \, \bar{d},\tag{6.10}$$

where  $\kappa_0$  is a material constant. It then follows from the constitutive equation  $(5.4)_3$  for h that the coefficients  $\epsilon_0, \epsilon_1, \ldots, \epsilon_3$  have the values

$$\epsilon_0 = (2/\kappa_0^2)\, \bar{d}, \quad \epsilon_1 = \epsilon_2 = \epsilon_3 = 0. \eqno(6.11)$$

2. Constant crack number. By this assumption we have  $\dot{n} = 0$  and then from  $(6.4)_1$  and  $(5.4)_3$  it follows that

$$\epsilon_0 = \epsilon_1 = \epsilon_2 = \epsilon_3 = 0. \tag{6.12}$$

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Clearly either of the above two special assumptions considerably reduce the complexity of the constitutive equation for the rate of crack production h.

Consider a homogeneous microcracking material whose microcracks are fully aligned along a direction c in its reference configuration  $\kappa_0$  and let the material be suddenly subjected to a homogeneous extensive strain, i.e.

$$E = E_{11} c \otimes c, \quad E_{11} > 0. \tag{6.13}$$

We assume here that the deformation process is such that the effect of part of the macroscopic kinetic energy involving v (but not  $\overline{w}$ ) in the equations of motion (6.4), may be neglected. Then, since the deformation is homogeneous, the ordinary momentum equation  $(6.4)_3$  is identically satisfied and the non-zero components of the stress S can be calculated from the constitutive equation (5.7) with coefficients (6.1), once the evolution of  $\bar{d}$  with time is known. Further by (6.13), the principal direction of the strain coincides with the direction of alignment of the microcracks for all time. It then follows that with the assumption (6.13) the direction of microcrack alignment remains unchanged throughout the evolution of microcracking.

We now proceed to examine several features of the solution for extensive straining as follows:

(i) Initiation of microcracking. Since the microcracks are initially stationary, microcracking will not begin unless the value of the strain  $E_{11}$  is such as to satisfy the crack initiation condition (6.5). It can be verified that for the material characterized by the constitutive results (5.7), (6.1) and (6.2) and either (6.11) or (6.12), the microcracking does not begin unless  $E_{11}$  satisfies a condition of the form

$$E_{11} \geqslant [-b + (b^2 - 4ac)^{\frac{1}{2}}]/2a,$$
 (6.14)

where a, b and c stand for

$$a = [(\nu_1 + \nu_5) + 2(\nu_2 + \nu_3 + \nu_4)] \{\frac{1}{2}\gamma n^{\delta}(\bar{D}_0)^{(\gamma - 2)} + \frac{1}{2}\delta n^{\delta - 1}(\bar{D}_0)^{(\gamma - 1)} \mathbf{h} \cdot \mathbf{c}\}, \}$$

$$b = -\frac{2}{3}\omega_3, \quad c = -(\nu_0 + \omega_0),$$

$$(6.15)$$

where  $\bar{D}_0 (= D_0)$  is the initial magnitude of  $\bar{d}$ .

A close examination of the expressions  $(6.15)_{1,3}$  reveals that while b and c represent only material constants, the quantity a depends strongly upon microcrack number n, the microcrack size  $D_0$ , and the rate of production of new cracks represented by  $h \cdot c$ in  $(6.15)_1$ .

With the values  $\gamma = 3$ ,  $\delta = -\frac{1}{2}$  (corresponding to a dilute crack concentration) in the coefficients (6.1); and if we now invoke an idealization pertaining to new crack production represented by either (6.11) or (6.12), then a defined by  $(6.15)_1$  will have a lower value by the assumption of caca than that for ccn. For given values of n and  $\bar{d}$ , the former is representative of the early stages of microcracking, while the latter is representative of the final stages of microcracking. Moreover, according to the crack initiation condition (6.14), microcracks initiate at a higher value of the strain  $E_{11}$  under the assumption of CACA than under the assumption of CCN.

(ii) Microcrack growth. If the value of  $E_{11}$  in (6.13) is higher than that estimated by (6.15), the microcracking occurs and the crack growth rate  $\overline{w}$  can be calculated from  $(3.26)_1$  and  $(6.4)_3$  with  $\mathbf{k} \cdot \mathbf{c}$  given by the right-hand side of  $(4.19)_2$  or the left-hand side of the inequality (6.5). We again examine the predicted growth by separate use of the idealization represented by either CACA or CCN. Thus, the rate of growth  $\alpha = \bar{d}$  is either

$$\alpha = \{ [\gamma^{-1}(R_2 + R_3) \, \bar{d}^{\gamma} - \frac{1}{2}R_1 \, \bar{d}^2] \, (2/\rho y) \}^{\frac{1}{2}}, \tag{6.16}$$

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or 
$$\alpha = \left[ \frac{1}{(2\delta + \gamma)} (R_2 + R_3) \, \bar{d}^{\gamma} - \frac{1}{2} R_1 \, \bar{d}^2 + \frac{R_4 + R_5}{2\delta + \gamma - 1} \, \bar{d}^{\gamma} \right] \left( \frac{2}{\rho y} \right)^{\frac{1}{2}}. \tag{6.17}$$

In the expression (6.16), which corresponds to the assumption CCN, the coefficients  $R_1, R_2, R_3$  are constants while in (6.17), which corresponds to the assumption CACA,  $R_2$ ,  $R_3, R_4, R_5$  are functions of  $\bar{d}$  through their dependence on n (see (6.4)<sub>1</sub>).

(iii) Crack arrest condition. As long as the first bracket on the right-hand side of either (6.16) or (6.17) is non-negative, cracks will continue to grow. However, microcrack arrest occurs at a value of  $\bar{d}$ , say  $\bar{d}_1$  (greater than the initial  $\bar{D}_0$ ), by setting the right-hand side of either (6.16) or (6.17) equal to zero. No additional microcracking will occur if  $E_{11}$  is less than that predicted by (6.14) provided that  $\bar{D}_0$  is replaced by  $\bar{d}_1$  in the coefficient a of (6.15). If no such root as  $\bar{d}_1$  exists, then the microcracks will grow indefinitely. (Actually under such situations, the microcracks will link up and become large enough so that the deformation can no longer be considered as homogeneous on the macroscopic scale and the results of the type (6.16) or (6.17) will not be applicable.) Such a continued growth of microcracks under uniform straining without the possibility of arrest may be regarded as 'unstable' microcracking. This completes our discussion of uniform extensive straining.

In the rest of this subsection we briefly discuss a parallel solution for the case of a uniform compressive straining. Again, consider a homogeneous microcracking material whose microcracks are fully aligned along a direction  $\bar{c}$  perpendicular to c in the reference configuration  $\kappa_0$  and let the material be suddenly subjected to a homogeneous compressive strain in the form

$$E = -E_{11} \bar{c} \otimes \bar{c}, \quad E_{11} > 0, \quad \bar{c} \cdot c = 0.$$
 (6.18)

The initiation of microcracking still takes place when  $E_{11}$  in (6.18) exceeds the value obtained from a condition of the form (6.14) with coefficients b and c the same as  $(6.15)_{2,3}$  but a is now different from  $(6.15)_1$  and is given by

$$a = \frac{1}{2}(\nu_1 + 2\nu_2)\left[\gamma n^{\delta}(\overline{d})^{\gamma - 2} + \delta(\overline{d})^{\gamma - 1} \mathbf{h} \cdot \mathbf{c}\right]. \tag{6.19}$$

Since the coefficient a has now a much smaller value than that in  $(6.15)_1$ , the value of the compressive strain required to initiate microcracking is considerably higher. The remainder of the analysis for compressive straining is similar to that of extensive straining. We omit details here but note that the coefficients  $\nu_3$ ,  $\nu_4$  and  $\nu_5$  which previously represented the effect of alignment of the microcracks in extensive straining are absent in the solution for compressive straining. (It is common in the rock mechanics literature to use different constitutive coefficients for compressive straining to account for the effect of the contact between the faces of the cracks. Materials exhibiting such an effect are sometimes referred to as bilinear. Here use has been made only of the same general constitutive equations.)

# 7. Concluding remarks

The construction of the theory of microcracking materials presented in §\$3–5 is motivated by the physical processes which occur at the microscopic level. Given the relatively simple structure of the theory for crack growth, it is reasonable to expect that the theory can predict—at least qualitatively—such phenomena as the initiation of microcracking and the gradual accumulation of 'damage' in the direction of the maximum principal strain. These qualitative characteristics, in turn,

can accommodate a wide range of features relevant to certain classes of fairly brittle materials. (For example, a detailed description of the operative dissipative mechanisms or the incorporation of the averaged effects of radiation of acoustic waves from the crack edges.) The quantitative nature of these features, as well as aspects of the predictive capabilities of the basic theory with the use of special constitutive equations, is brought out in §6.

It is of interest to briefly compare the present approach with that of Davison & Stevens (1973), who also introduce an additional vector-valued kinematical variable (identified by them as an 'internal' variable) to account for the effect of the microcracks. (Actually Davison & Stevens (1973) first introduce n 'internal state variables', but subsequently restrict their development to only one such variable.) However, while their identification of the crack area in the current configuration (Davison & Stevens 1973, eq. (6)) is formally analogous to  $(A 4)_1$  of Appendix A of the present paper, the precise nature of their internal variable (especially in the context of irreversible crack growth of the present paper in terms of our variable d defined by (3.4)), is open to ambiguities. Moreover, these authors (Davison & Stevens 1973) make no distinction between the two modes of 'damage' accumulation, namely the growth of pre-existing microcracks and the production of new microcracks; and thus their theory does not include the crack number n per unit volume and the corresponding balance law for crack number. (As is evident by the examples considered in subsection 6.4, the response of the material is significantly different for the two modes of damage accumulation inasmuch as they affect the specific free energy  $\psi$  and the rate of dissipation  $\xi$ .)

Aside from these and other details, the main difference between our theory and that of Davison & Stevens (1973) is that whereas these authors postulate a constitutive equation for the rate of their additional 'internal state variable' without any consideration of the inertia effect associated with microcracking, we have introduced an additional momentum-like balance law for the determination of the variable  $\bar{d}$ . This additional balance law includes terms representing the effects of inertia due to microcracking and the force maintaining the crack growth. Finally, it is worth emphasizing that the present developments easily permit the simplifications of the resulting dynamical equation by imposing several physically plausible restrictions on the constitutive equations without losing the ability to predict fairly complex non-trivial material behaviour.

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# Appendix A

The purpose of this appendix is to provide general background and motivation arising from microscopic considerations which enter parts of the macroscopic formulation of the theory used in the main text. In particular, emphasis is placed on identification of additional kinematical and kinetical quantities utilized in the construction of the macroscopic theory and the nature of their invariance properties.

A.1. Microscopic motivation for the use of an additional vector-valued kinematical variable and its invariance property

For simplicity, we consider in this appendix an idealized case of a *single* crack contained in a material part  $\mathscr{S}^*$  in the microscopic description of the body. Let the area of the crack and the volume occupied by  $\mathscr{S}^*$  be denoted respectively by  $a^*$  and  $\mathscr{V}^*$  in the current configuration  $\kappa^*$  and by  $A^*$  and  $\mathscr{V}^*_0$  in the reference configuration and by  $N^*$  in the current configuration and by  $N^*$  in the reference configuration, and for convenience we define two vectors  $a^*$  and  $A^*$  by

$$a^* = a^*n^*, \quad A^* = A^*N^*.$$
 (A 1)

(An idealized crack here could be thought of, for example, as being penny-shaped with vanishingly small thickness. The area of such a crack would then refer to the mean crack-sectional area (or one-half of the sum of the bottom and top surface areas). The normal to the crack surface refers to the normal of the surface of the cross section.) Also, let x and X defined in the paragraph preceding (3.1) be identified with the position of the centre of mass of  $\mathcal{S}^*$  in the current and reference configurations, respectively. This means that the entire part  $\mathcal{S}^*$  is associated with a single material point (or particle) X on the macroscopic scale; and, similarly, the macroscopic differential volumes dv and dV of the body associated with X may be identified with the volumes  $\mathcal{V}^*$  and  $\mathcal{V}_0^*$ , respectively. For a sufficiently small material volume in the microscopic description, we suppose that  $\mathcal{V}^*$  and  $\mathcal{V}_0^*$  are related by

$$\mathscr{V}^* = J\mathscr{V}_0^*, \tag{A 2}$$

with J interpreted to be the same as the jacobian of transformation associated with positions of the particle in the macroscopic description of the current and reference configurations. Since the area  $a^*$  in (A 1) is not necessarily associated with a material region, no relationship of the type (A 2) can be assumed between  $a^*$  and  $A^*$  in terms of the macroscopic quantities.

We now consider a process from the current configuration  $\kappa^*$  to some intermediate configuration  $\bar{\kappa}^*$  in which the deformation of the body is reversed (in the sense that the part  $\mathscr{S}^*$  is mapped back onto the same region that it occupied in the reference state) and during which we require that the bounding surface of the crack remains material. In the intermediate configuration, the crack area and the volume of  $\mathscr{S}^*$  are denoted by  $\bar{A}^*$  and  $\bar{\mathscr{V}}^*$ , respectively. Another vector  $\bar{A}^*$  is defined in terms of the scalar  $\bar{A}^*$  and the unit normal  $\bar{N}^*$  of the crack middle surface in the intermediate configuration by

$$\bar{A}^* = \bar{A}^* \bar{N}^*. \tag{A 3}$$

Since the motion between the intermediate configuration and the current configuration must be reversible, so that the bounding surface of the crack remains material, and noting that  $a^*$  and  $\bar{A}^*$  may be identified with differential areas in the current and reference configurations, respectively, on the macroscopic scale, we assume that  $\bar{A}^*$  and  $\bar{V}^*$  are related to  $a^*$  and  $V^*$  by

$$\boldsymbol{a}^* = J(\boldsymbol{F}^{-1})^{\mathrm{T}} \bar{\boldsymbol{A}}^*, \quad \mathscr{V}^* = J\bar{\mathscr{V}}^*, \tag{A 4}$$

where F is the deformation gradient in the macroscopic theory defined by  $(3.2)_2$ . Comparing (A 2) and (A 4)<sub>2</sub>, we find that  $\bar{\mathscr{V}}^* = \mathscr{V}_0^*$ ; however, in general no relationship of this kind can be established between  $A^*$  and  $\bar{A}^*$ . It is clear that the

difference  $A^* - \bar{A}^*$  is related to the crack growth and its orientation, as described in the second paragraph of §2.

Under a superposed rigid body motion on the microscopic scale from the current configuration  $\kappa^*$  to some configuration  $\kappa^{*+}$ , it is physically reasonable to assume that

$$a^{*+} = Qa^*, \quad \mathscr{V}^{*+} = \mathscr{V}^*, \quad F^+ = QF, \quad J^+ = J,$$
 (A 5)

where Q satisfies (3.11). Solving for  $\bar{A}^*$  from (A 4)<sub>1</sub> and examining the resulting expression under superposed rigid body motions with the help of (A 5)<sub>1,3</sub>, we obtain

$$\bar{A}^{*+} = (1/J^+)(F^{\mathrm{T}})^+ a^{*+} = (1/J)F^{\mathrm{T}}a^* = \bar{A}^*,$$
 (A 6)

so that  $\overline{A}^*$  is invariant under superposed rigid body motions. In the simple idealized case of a single crack under discussion the vector  $\overline{A}^*$  defined by  $(A \ 4)_1$  can be taken as a measure of the actual (or irreversible) crack size. Changes in  $\overline{A}^*$ , rather than in  $a^*$ , reflect the effect of fracture processes taking place in the material.

# A.2. Microscopic interpretation of the forces $_{\mathbf{R}}\mathbf{k}$ and $_{\mathbf{R}}\mathbf{m}$ and motivation of their invariance properties

We again consider the simple example introduced in §A.1 in which a single crack is contained in a particular microscopic material part  $\mathscr{S}^*$  of the body. It is well known that in the context of three-dimensional linear elasticity, along the curve forming the edge of an idealized crack there exists an integrable singularity in the stress. We suppose that such a stress singularity acts as a driving force for the crack growth in the simple example under discussion. In addition to this driving force, there exists a resistive force (somewhat analogous to a frictional force) which counteracts the growth of the crack. This resistive force is equal to the driving force until the latter reaches a critical value beyond which fracture begins and results in crack growth. During fracture, the rate of working of the driving force may be associated with the rate of decrease of the free energy due to crack growth in the region  $\mathscr{P}^*$  occupied by the part  $\mathscr{S}^*$  in  $\kappa^*$  and the rate of working of the resistive force corresponds to the rate of energy dissipated in  $\mathscr{P}^*$  as a consequence of fracture. The difference in the rate of working of these two forces is balanced by a corresponding increase in the kinetic energy of the microscopic particles immediately surrounding the crack edge.

Now let the region  $\overline{\mathscr{P}}^*$  occupied by the part  $\mathscr{S}^*$  in the intermediate configuration be immersed in a somewhat larger material region with boundary  $\partial \overline{\mathscr{P}}^*$ . It is clear that both the driving and resistive forces will be influenced by the neighbouring cracks and their growth. Such effects may arise through the boundary  $\partial \overline{\mathscr{P}}^*$  of the part  $\overline{\mathscr{P}}^*$  as an additional net force on the crack which depends on the position and the orientation of the boundary  $\partial \overline{\mathscr{P}}^*$ . The effect of all these forces in the macroscopic theory are represented by the vector quantities  ${}_{\mathbf{R}}\mathbf{k}$  and  ${}_{\mathbf{R}}\mathbf{m}$  defined respectively per unit volume and per unit area of the reference configuration  $\kappa_0$ , while the body force  $\mathbf{l}$  may be thought of as representing the effect of surface tractions on the boundary surface of the crack. (The tractions on the boundary surface of the crack also contributes to the driving force, as does the stress concentration at the crack tip.) We also observe here that under superposed rigid body motions the kinetic energy of the microscopic particles surrounding the crack edge, the driving force and the resistive force remain unchanged since  $\overline{A}^*$  given by (A 3) is unchanged. This serves as the motivation for the invariance properties of  ${}_{\mathbf{R}}\mathbf{k}$  and  ${}_{\mathbf{R}}\mathbf{M}$  in (3.24).

From the interpretation of  $_{\mathbf{R}}\mathbf{m}$  in the preceding paragraph, it should be clear that

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when the size of the crack is much smaller than the region  $\overline{\mathscr{P}}^*$ , the force  ${}_{\mathbf{R}}\boldsymbol{m}$  does not significantly affect crack growth. Indeed, it is shown in §4 that when the response functions are assumed to be independent of the director gradient,  ${}_{\mathbf{R}}\boldsymbol{M}$  and hence also  ${}_{\mathbf{R}}\boldsymbol{m}$  must vanish identically. Of course, when the crack size becomes comparable with the typical dimension of  $\overline{\mathscr{P}}^*$ , the gradient of  $\overline{\boldsymbol{d}}$  may influence the response functions and  ${}_{\mathbf{R}}\boldsymbol{m}$  will play a significant role.

### Appendix B

The purpose of this appendix is to provide the details of the proof that the conditions (5.19) are both necessary and sufficient for satisfaction of (5.15) or equivalently (5.17). First, we note that substitution of  $(5.16)_1$  into (3.8) gives

$$E^{(d)}a^K = \bar{\beta}^{(K)}a^K$$
 (no sum on  $K, K = 1, 2, 3$ ), (B 1)

where  $a^{K}$  is now also the eigenvectors of  $E^{(d)}$  with eigenvalues  $\bar{\beta}^{(K)}$  defined by

$$\bar{\beta}^{(K)} = \beta^{(K)} - \frac{1}{3} \operatorname{tr} \mathbf{E}. \tag{B 2}$$

Since  $\operatorname{tr} E = \beta^{(1)} + \beta^{(2)} + \beta^{(3)}$  we also have

$$\sum_{K=1}^{3} \bar{\beta}^{(K)} = 0, \tag{B 3}$$

which is consistent with  $(5.16)_2$ .

Let  $\beta^{(3)}$  be the largest and  $\overline{\beta}^{(1)}$  the smallest eigenvalues of E associated with the eigenvectors  $a^3$  and  $a^1$ , respectively. Then, by (B 1) and (B 2),  $\overline{\beta}^{(3)}$  is the largest and  $\overline{\beta}^{(1)}$  the smallest eigenvalues of  $E^{(d)}$ . We now proceed to show that

$$\bar{\beta}^{(3)} \geqslant 0,$$
 (B 4)

and that

$$\bar{\beta}^{(1)} \geqslant -2\bar{\beta}^{(3)}.$$
(B 5)

The proofs (by contradiction) are as follows: suppose that  $\bar{\beta}^{(3)} < 0$ . Then, since  $\bar{\beta}^{(3)}$  is the largest eigenvalue, both  $\beta^{(1)}$  and  $\beta^{(2)}$  must also be negative and we may conclude that  $\operatorname{tr} E^{(d)} < 0$ . But this contradicts  $(5.16)_2$  and the proof of (B 4) is complete. Next, suppose that  $\bar{\beta}^{(1)} < -2\bar{\beta}^{(3)}$ . Then, introducing this assumption in  $\operatorname{tr} E^{(d)}$  yields

$$\operatorname{tr} \mathbf{E}^{(d)} = \bar{\beta}^{(1)} + \bar{\beta}^{(2)} + \bar{\beta}^{(3)} < -2\beta^{(3)} + \bar{\beta}^{(2)} + \beta^{(3)} = \bar{\beta}^{(2)} - \bar{\beta}^{(3)}. \tag{B 6}$$

But since  $\bar{\beta}^{(2)} - \bar{\beta}^{(3)} < 0$ , the right-hand side of the last expression implies tr  $E^{(d)} < 0$  and again this contradicts  $(5.16)_2$  and the proof of (B 5) is complete.

Since the deviatoric strain  $E^{(d)}$  is a real symmetric second-order tensor, the quadratic form  $(E^{(d)}V) \cdot V$ , where V is a unit vector, must satisfy the inequalities

$$\bar{\beta}^{(1)} \leqslant (E^{(d)}V) \cdot V \leqslant \bar{\beta}^{(3)} \quad \text{for all } V.$$
 (B 7)

The last result with the help of (B 5) can be rewritten in the useful form

$$-2\bar{\beta}^{(3)} \leq (E^{(d)}V) \cdot V \leq \bar{\beta}^{(3)} \quad \text{for all } V, \tag{B 8}$$

where both the lower and upper bounds involve only the same eigenvalue. Having obtained the foregoing preliminary results, we now turn to our main task in this appendix and note that the inequality (5.17) holds for all E and all c satisfying

$$\mathbf{c} \cdot \mathbf{a}^3 \geqslant 0. \tag{B 9}$$

B.1. Proofs of the necessary conditions

(a) With the choice E = 0, (5.17) at once yields the condition

$$\phi_0 \geqslant 0. \tag{B 10}$$

(b) With the choice E = eI, where e is an arbitrary scalar, both (tr E) and  $\bar{\beta}^{(3)}$  vanish by  $(5.16)_1$  and  $(B\ 1)$  and (5.17) reduces to

$$\phi_0 + [\phi_1 + \frac{1}{3}(\phi_2 + \phi_3)] e \geqslant 0. \tag{B 11}$$

Since the above inequality must hold for all arbitrary values of e, we must have

$$\phi_1 + \frac{1}{3}(\phi_2 + \phi_3) = 0, \tag{B 12}$$

for otherwise (B 11) could be violated for sufficiently large e.

(c) After substituting (B 12) into (5.17), we obtain

$$\phi_0 + \phi_3 c \cdot (E^{(d)}c) + \phi_2 \bar{\beta}^{(3)} \geqslant 0,$$
 (B 13)

which must hold for every c that satisfies (B 9). With the choice

$$c = \frac{1}{\sqrt{3}} \sum_{K=1}^{3} a^{K}, \tag{B 14}$$

 $c \cdot a^3 = \sqrt{\frac{1}{3}}$ , (B 9) is satisfied and it can easily be verified that  $c \cdot (E^{(d)}c) = 0$  so that (B 13) reduces to

$$\phi_0 + \phi_2 \, \overline{\beta}^{(3)} \geqslant 0. \tag{B 15}$$

The above inequality must hold for arbitrary positive values of  $\bar{\beta}^{(3)}$ . This, along with (B 10), implies that

$$\phi_2 \geqslant 0,$$
 (B 16)

for otherwise (B 15) could be violated for sufficiently large  $\bar{\beta}^{(3)}$ .

(d) Returning to (B 13), with the special choice  $c = a^3$  and using also (B 1) we obtain

$$\phi_0 + (\phi_3 + \phi_2) \, \bar{\beta}^{(3)} \geqslant 0,$$
 (B 17)

which must hold for arbitrary positive values of  $\bar{\beta}^{(3)}$  and we conclude that  $\phi_3 + \phi_2 \geqslant 0$  or

$$\phi_3 \geqslant \phi_2$$
. (B 18)

(e) With a choice of  $E^{(d)}$  such that the eigenvalues  $\bar{\beta}^{(3)}$  and  $\bar{\beta}^{(2)}$  are equal, it follows from (B 2) and (B 3) that  $\bar{\beta}^{(1)} = -2\bar{\beta}^{(2)}$  and after setting  $c = a^1$  the inequality (B 13) becomes

$$\phi_0 + (\phi_2 - 2\phi_3) \bar{\beta}^{(3)} \ge 0.$$
 (B 19)

Then, using a familiar line of argument we arrive at  $(\phi_2 - 2\phi_3) \ge 0$  or

$$\phi_3 \leqslant \frac{1}{2}\phi_2. \tag{B 20}$$

From the combination of (B 18) and (B 20) follows

$$-\phi_2 \leqslant \phi_3 \leqslant \frac{1}{2}\phi_2. \tag{B 21}$$

The results (B 10), (B 12), (B 16) and (B 21) are the desired necessary conditions. *Phil. Trans. R. Soc. Lond.* A (1991)

B.2. Proof of sufficiency

Consider the constant in the comment

$$\phi_3 \mathbf{c} \cdot (\mathbf{E}^{(d)} \mathbf{c}) + \phi_2 \, \overline{\beta}^{(3)},$$

which by virtue of (B 7) is bounded above and below by the eigenvalues  $\bar{\beta}^{(3)}$  and  $\bar{\beta}^{(1)}$  respectively. Hence, we may write

$$\phi_3 \bar{\beta}^{(1)} + \phi_2 \bar{\beta}^{(3)} \leqslant \phi_3 c \cdot (E^{(d)}c) + \phi_2 \bar{\beta}^{(3)} \leqslant (\phi_3 + \phi_2) \bar{\beta}^{(3)}. \tag{B 22}$$

With the help of (B 5), the last result can be rewritten as

$$(\phi_2 - 2\phi_3)\,\bar{\beta}^{(3)} \leqslant \phi_3\,c \cdot (E^{(d)}c) + \phi_2\,\bar{\beta}^{(3)} \leqslant (\phi_3 + \phi_2)\,\bar{\beta}^{(3)}. \tag{B 23}$$

By (B 16) and (B 21),

$$\phi_3 + \phi_2 \geqslant 0, \quad \phi_2 - 2\phi_3 \geqslant 0,$$
 (B 24)

and hence

$$\phi_3 \mathbf{c} \cdot (\mathbf{E}^{(d)} \mathbf{c}) + \phi_2 \bar{\beta}^{(3)} \geqslant 0. \tag{B 25}$$

The last result together with (B 10) and (B 12) imply that (5.17) is satisfied.

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