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Strain gradient plasticity by internal-variable approach with normality structure

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Abstract

This paper presents a constitutive formulation for materials with strain gradient effects by internal-variable approach with normality structure. Specific micro-structural rearrangements are assumed to account for the inelasticity deformations for this class of materials, and enter the constitutive formulations in form of internal variables. It is further assumed that the kinetic evolution of any specific micro-structural rearrangement may be fully determined by the thermodynamic forces associated with that micro-structural rearrangement, by normality relations via a flow potential. Macroscopic gradient-enhanced inelastic behaviours may then be predicted in terms of the microscopic internal variables and their conjugate forces, and thus a micro–macro bridging formulation is available for strain-gradient-characterised materials. The obtained formulations are first applied to crystallographic materials, and a crystal gradient plasticity model is developed to account for the influence of microscopic slip rearrangements on the macroscopic gradient-dependent mechanical behaviour for this class of materials. Micro-cracked geomaterials are also treated with these formulations and a gradient-enhanced damage constitutive model is developed to address the impacts of the evolutions of micro-cracks on the macroscopic inelastic deformations with strain gradient effects for these materials. The available formulations are further compared with other thermodynamic approaches of constitutive developing.

Keywords: Strain gradient plasticity; Normality structure; Internal variable; Thermodynamics

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1. Introduction

Strain gradient plasticity has aroused increasing interest in the community of both solid mechanics and material science since the pioneering work of Aifantis (1984, 1987). A variety of gradient plasticity models have been developed with some success during the past decades to address a large range of problems unresolved by classic continuum theories for materials, such as localised failure, size effects in micro-level, mesh-dependency of finite element modelling, and shear band width determination (see, e.g., Fleck and Hutchinson, 1993, 1997; Aifantis, 2001; Fleck and Hutchinson, 2001, and references therein). The gradient effects have been related with

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underlying micro-scale mechanisms in the material such as crystal dislocation, particle rearrangement, and development of defects and imperfections including pre-existing micro-cracks and microvoids. These micromechanisms have been shown both theoretically and experimentally important to account for the irreversible deformation for a wide range of materials.

However, as may be found, most of these gradient models are constructed through phenomenological approaches. As a result, the micro-structural influence on the macroscopic behaviour is only expressed by incorporating one or more internal length scales into the constitutive relations. The assumption that the internal length scale(s) is related to the basic dimension of the micro-structures remains unverified against experiment results. Additionally, gradient constitutive relations have been developed in various ways (e.g., the principle of virtual power). So far, a fully systematic development of these theories within the framework of thermodynamics and which, at the same time, establishes of a direct link between the macroscopic mechanical behaviour and the underlying micro-scale mechanisms, are scarce in the literature. Hence, the attention here is focused on developing a thermodynamically consistent strain gradient plasticity theory with direct links to the micro-scale mechanisms, and applying it to crystallographic solids and micro-cracked geomaterials.

It is clear that thermodynamics and continuum mechanics are inseparable for most of the mechanical processes in materials, and in the vast majority of these cases, deformation of a continuum is an irreversible process. To address the irreversible processes, developing continuum constitutive relations by means of thermodynamics has long been adopted by scholars. The irreversible process for deformation of a continuum solid was first addressed by Onsager (1931), with his reciprocity relations for the symmetric tensors connecting velocities and forces. However, these functions are restricted to linear processes only, which is thus incapable of addressing the status of a physical law and many other non-linear processes in continuum mechanics. Later on, Ziegler (1958) proposed an orthogonality principle for irreversible processes, which included Onsager's theory as a special case. This orthogonality principle was later proved to be equivalent to the principle of maximal dissipation rate and the principle of maximal entropy production rate (Ziegler and Wehrli, 1987a). The orthogonality principle allows one to establish constitutive relations from a single pair of scalar functions characterizing the free energy and the dissipation rate function of a material, and a thermomechanical approach was developed based on this principle. A variety of developments and applications of this approach have been made through the past decades (see, e.g., Ziegler, 1983; Ziegler and Wehrli, 1987b; Houlsby, 1981; Germain et al., 1983; Collins and Houlsby, 1997; Houlsby and Puzrin, 2000; Puzrin and Houlsby, 2001). In addition, using thermodynamic concepts, Valanis (1971) proposed an endochronic theory of plasticity to deal with the plastic response of materials by means of memory integrals in terms of memory kernels. Non-linear visco-elasticity and visco-elasto-plasticity were later developed by using this theory (see, e.g., Valanis, 1980).

An internal-variable approach based on the normality structure, proposed by Rice (1971, 1975), will be introduced here with particular interest, as this approach provides an appealing constitutive framework for solids undergoing irreversible thermodynamic processes. Using a set of internal variables to characterise the state of internal changes, Rice (1971) originally developed such a normality structure to relate structural rearrangements of material elements on the micro-scale, by slip or diffusion, to corresponding increments of macroscopic plastic strain. The normality structure shares a similarity of the 'essential structure' proposed by Hill (1968). The central idea of normality structure is that, the rate of progression of any local micro-structural rearrangement within the material is dependent on the current stress state only through the thermodynamic force conjugate to the extent of that rearrangement. When the kinetics of the structural rearrangements is so characterised, Rice (1971) showed that there exists a scalar potential function of the macroscopic stress-state at each instant in the history of deformation, such that the inelastic part of the strain rate may be given by the derivatives of the function on corresponding stress components. When the behaviour may be adequately idealised as rate-independent, the theory reduces to a normality requirement of inelastic strain-increment with respect to a yield surface in stress space. This normality structure provides a good thermodynamic framework for linking the micro-structural changes in gradient theories with the macroscopic description, which will be adopted in this paper to develop strain gradient models in account for micro-structural influence for crystal solids and geomaterials. Inhomogeneous plastic deformations in crystal solids have been shown to be related closely to the micro-slip dislocations in these materials (Nye, 1953; Ashby, 1970), while geomaterials are usually weakened by micro-cracks or microvoids. These special features associated with the two classes of materials make them suitable for being described using the internal variables to describe their micro-structural evolution and rearrangement. By using the internal-variable approach with normality structure, it is easy to accommodate a direct link of the macroscopic, especially the gradient response, with their micro-scale mechanisms. This feature attracts the attention of the authors to use the approach to develop strain gradient models with micro-structural damage mechanism for micro-cracked geomaterials, and for crystallographic solids characterised by micro-dislocations, respectively.

This paper is organised in the following structure. In Section 2, a framework for strain gradient theory is constructed by the internal-variable approach with normality structure. The basic strain gradient concept follows the second-order gradient framework developed by Fleck and Hutchinson (1993, 1997), which may be further traced to earlier work by Mindlin (1965) and Germain (1973). Incremental constitutive relations are presented in both compound stress space and compound strain space. A specific free energy function and a flow function defined from the normality structure complete the base of the preceding formulations. Kinetic rate laws for the internal variables and their conjugate thermodynamic forces are discussed. In Section 3, the internal variable approach for gradient theories outlined in Section 2 are applied to the constitutive developing for crystallographic solids characterised by microscopic dislocation systems and geomaterials weakened by micro-cracks, respectively. Strain gradient-enhanced models with micro-structural mechanisms are obtained for the two classes of materials. Following Section 3 are the discussing and concluding remarks of this paper. Some comparisons between the currently obtained internal-variable approach with other thermodynamic methods of constitutive developing are made.

It is also noted that Einstein's summation convention is defaulted for repeated indexes unless stated otherwise. Dots, double dots and triple dots between tensors denote tensor operations having equivalents in indicial notation with Einstein's summation convention, illustrated by the following typical examples:

$$\mathbf{A}\cdot\mathbf{a} = A_{ij}a_j, \quad \mathbf{A}\cdot\mathbf{B} = A_{ij}B_{jk}, \quad \mathbf{A}:\mathbf{B} = A_{ij}B_{ji}, \quad \mathbf{A}\overset{\cdot}{:}\mathbf{B} = A_{ijk}B_{kji}$$

2. Internal-variable approach with normality structure for strain gradient models

A material sample with volume V in an unloaded reference state is considered. When it is subjected to boundary loadings, the resulting macroscopic deformation is assumed to be homogeneous. The mechanical response of the material is assumed to be governed by gradient-type descriptions as addressed by Fleck and Hutchinson (1993, 1997) after Mindlin (1965) and Germain (1973). The strain and strain gradient are denoted by a second-order symmetric strain tensor $\boldsymbol{\varepsilon}$ and symmetric third-order strain gradient tensor $\boldsymbol{\eta}$, respectively. In a Cartesian coordinates system, they may be related to displacement $\mathbf{u}$ as follows:

$$\begin{cases} \varepsilon_{ij} = (u_{i,j} + u_{j,i})/2 \\ \eta_{ijk} = (u_{k,ij} + u_{k,ji})/2 \end{cases} \tag{1}$$

It is further assumed the work conjugates to $\boldsymbol{\varepsilon}$ and $\boldsymbol{\eta}$ are denoted by the Cauchy stresses $\boldsymbol{\sigma}$ and the higher-order stresses (or couple stresses) $\boldsymbol{\tau}$ (which is a third-order symmetric tensor), respectively. That is, $\boldsymbol{\sigma}:\delta\boldsymbol{\varepsilon}$ and $\boldsymbol{\tau}\overset{\cdot}{:}\delta\boldsymbol{\eta}$ constitute the work per unit volume of the adopted reference state in any virtual deformation $\delta\boldsymbol{\varepsilon}$ and deformation gradient $\delta\boldsymbol{\eta}$.

As a central assumption of Rice's internal-variable approach with normality structure, the macroscopic inelastic behaviour of the material is considered as a consequence of internal rearrangement of constitutive parts of the material sample. A discrete set of explicit internal variables $\xi_1, \xi_2, \ldots, \xi_n$ (collectively $\boldsymbol{\xi}$) is assumed to characterise the state of internal rearrangement within the material sample V. The following specific free energy ϕ and its Legendre transform ψ with respect to strain and strain gradient are introduced:

$$\phi = \phi(\boldsymbol{\varepsilon}, \boldsymbol{\eta}, \theta, \boldsymbol{\xi}) = U - \theta s, \quad \psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi}) = \boldsymbol{\varepsilon} : \frac{\partial\phi}{\partial\boldsymbol{\varepsilon}} + \boldsymbol{\eta}\overset{\cdot}{:}\frac{\partial\phi}{\partial\boldsymbol{\eta}} - \phi(\boldsymbol{\varepsilon}, \boldsymbol{\eta}, \theta, \boldsymbol{\xi}) \tag{2}$$

where U, θ and s denote the internal energy, temperature and entropy of the material sample, respectively. The current pattern of micro-structural rearrangement of material elements is expressed by $\boldsymbol{\xi}$, and at fixed $\boldsymbol{\xi}$, variations of $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$ and θ result necessarily in a purely elastic response. Constrained equilibrium states introduced by Rice (1971) are assumed here. That is, the internal variables could be held at any definite set of values by imposition of appropriate constraints, with the material sample attaining an equilibrium state corresponding to a prescribed stress $\boldsymbol{\sigma}$ (or strain $\boldsymbol{\varepsilon}$), couple stress $\boldsymbol{\tau}$ (or strain gradient $\boldsymbol{\eta}$), and temperature θ. The variables, $\boldsymbol{\sigma}$ (or strain $\boldsymbol{\varepsilon}$), $\boldsymbol{\tau}$ (or strain gradient $\boldsymbol{\eta}$) and θ, together with $\boldsymbol{\xi}$, are therefore thermodynamic state variables. Let $\delta\boldsymbol{\varepsilon}$ and $\delta\boldsymbol{\eta}$ be the difference in strain and strain gradient, respectively, between neighbouring constrained equilibrium states, differing by $\delta\boldsymbol{\sigma}$, $\delta\boldsymbol{\tau}$, $\delta\theta$, $\delta\boldsymbol{\xi}$. Then the first law of thermodynamics states

$$\boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon} + \boldsymbol{\tau} \vdots \delta\boldsymbol{\eta} - \frac{1}{V}\sum_{i=1}^{n} f_i\,\delta\xi_i + \theta\delta s = \delta U \tag{3}$$

Eq. (3) also defines the thermodynamic forces $f_1, f_2, \ldots, f_n$ (collectively $\mathbf{f}$) conjugate to internal variables. It leads to the usual thermoelastic constitutive structure when the internal variables are supposed as fixed

$$\boldsymbol{\sigma} = \frac{\partial\phi(\boldsymbol{\varepsilon}, \boldsymbol{\eta}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\varepsilon}}, \quad \boldsymbol{\tau} = \frac{\partial\phi(\boldsymbol{\varepsilon}, \boldsymbol{\eta}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\eta}} \tag{4}$$

Eq. (3) may be recast as the following form if in term of the complementary energy ψ:

$$\boldsymbol{\varepsilon} : \delta\boldsymbol{\sigma} + \boldsymbol{\eta} \vdots \delta\boldsymbol{\tau} + \frac{1}{V}\sum_{i=1}^{n} f_i\delta\xi_i + s\,\delta\theta = \delta\psi \tag{5}$$

Eq. (5) leads to the following conjugate relationships:

$$\boldsymbol{\varepsilon} = \frac{\partial\psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\sigma}}, \quad \boldsymbol{\eta} = \frac{\partial\psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\tau}} \tag{6}$$

In addition, from Eqs. (3) and (5), the forces associated with the internal variables may be derived as

$$f_\alpha = V\frac{\partial\psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\xi_\alpha} = -V\frac{\partial\phi(\boldsymbol{\varepsilon}, \boldsymbol{\eta}, \theta, \boldsymbol{\xi})}{\partial\xi_\alpha} \tag{7}$$

In view of (6), applying the generalised Maxwell relation to (7) leads to the following equations:

$$\frac{\partial\boldsymbol{\varepsilon}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\xi_\alpha} = \frac{1}{V}\frac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\sigma}}, \quad \frac{\partial\boldsymbol{\eta}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\xi_\alpha} = \frac{1}{V}\frac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\tau}} \tag{8}$$

Eq. (8) relates variations in the internal variables to corresponding variations in the macroscopic strain and strain gradients, and provides a starting point for the developing of the inelastic constitutive gradient theory.

The inelastic portion of the strain difference $(\delta\boldsymbol{\varepsilon})^{\mathrm{p}}$, and strain gradient difference $(\delta\boldsymbol{\eta})^{\mathrm{p}}$, is defined as that part which would result from the change in internal variables if stresses and higher-order stresses and temperature were held fixed. Accordingly, the elastic (or thermoelastic) portion of strain difference $(\delta\boldsymbol{\varepsilon})^{\mathrm{e}}$ and strain gradient difference $(\delta\boldsymbol{\eta})^{\mathrm{e}}$ is defined as that which would result from the change in stress, couple stress and temperature, if the internal variables were held fixed. And the inelastic portion and elastic part constitute the total strain and strain gradient (cf., e.g., Fleck and Hutchinson, 1997)

$$\delta\boldsymbol{\varepsilon} = (\delta\boldsymbol{\varepsilon})^{\mathrm{e}} + (\delta\boldsymbol{\varepsilon})^{\mathrm{p}}, \quad \delta\boldsymbol{\eta} = (\delta\boldsymbol{\eta})^{\mathrm{e}} + (\delta\boldsymbol{\eta})^{\mathrm{p}} \tag{9}$$

with the following formulations defining the elastic and inelastic portions of strain and strain gradient differences, respectively:

$$\begin{cases} (\delta\boldsymbol{\varepsilon})^{\mathrm{e}} = \dfrac{\partial^2\psi}{\partial\boldsymbol{\sigma}\partial\boldsymbol{\sigma}} : \delta\boldsymbol{\sigma} + \dfrac{\partial^2\psi}{\partial\boldsymbol{\sigma}\partial\boldsymbol{\tau}} \vdots \delta\boldsymbol{\tau} + \dfrac{\partial^2\psi}{\partial\boldsymbol{\sigma}\partial\theta}\delta\theta \\ (\delta\boldsymbol{\eta})^{\mathrm{e}} = \dfrac{\partial^2\psi}{\partial\boldsymbol{\tau}\partial\boldsymbol{\sigma}} : \delta\boldsymbol{\sigma} + \dfrac{\partial^2\psi}{\partial\boldsymbol{\tau}\partial\boldsymbol{\tau}} \vdots \delta\boldsymbol{\tau} + \dfrac{\partial^2\psi}{\partial\boldsymbol{\tau}\partial\theta}\delta\theta \end{cases} \tag{10}$$

$$\begin{cases} (\delta\boldsymbol{\varepsilon})^{\mathrm{p}} = \dfrac{\partial\boldsymbol{\varepsilon}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\xi_\alpha}\delta\xi_\alpha = \dfrac{1}{V}\dfrac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\sigma}}\delta\xi_\alpha \\ (\delta\boldsymbol{\eta})^{\mathrm{p}} = \dfrac{\partial\boldsymbol{\eta}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\xi_\alpha}\delta\xi_\alpha = \dfrac{1}{V}\dfrac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial\boldsymbol{\tau}}\delta\xi_\alpha \end{cases} \tag{11}$$

Note that here in this paper, effects of local inertia terms, temperature gradients, etc, within the material sample are not considered. If the classical theory of irreversible processes applies, all the preceding relations may be rewritten by replacing the difference between neighbouring constrained equilibrium states with rate form terms with respect to time. For example, $(\delta\boldsymbol{\varepsilon})^{\mathrm{e}}$, $(\delta\boldsymbol{\eta})^{\mathrm{e}}$, $(\delta\boldsymbol{\varepsilon})^{\mathrm{p}}$ and $(\delta\boldsymbol{\eta})^{\mathrm{p}}$ by $(\dot{\boldsymbol{\varepsilon}})^{\mathrm{e}}$, $(\dot{\boldsymbol{\eta}})^{\mathrm{e}}$, $(\dot{\boldsymbol{\varepsilon}})^{\mathrm{p}}$ and $(\dot{\boldsymbol{\eta}})^{\mathrm{p}}$, respectively, accordingly, in term of $\dot{\boldsymbol{\sigma}}$, $\dot{\boldsymbol{\tau}}$ and $\dot{\theta}$. Or alternatively, all of the these variables may be just denoted by their respective incremental forms: $d(\cdot)$. Two neighbouring patterns of micro-structural rearrangement, $\boldsymbol{\xi}$ and $\boldsymbol{\xi} + \mathrm{d}\boldsymbol{\xi}$, are considered, with $\mathrm{d}\xi_\alpha(\alpha = 1,2,\ldots,n)$ (or alternatively $\dot{\xi}_\alpha$) being the specific local rearrangements. It should also be noted that, due to the increment taking at constrained constant stress and couple stress, the physical dimensional change of the material sample, corresponding to the inelastic strain increment $(\delta\boldsymbol{\varepsilon})^{\mathrm{p}}$ and inelastic strain gradient increment $(\delta\boldsymbol{\eta})^{\mathrm{p}}$, are not independent of the particular strain measure represented by the symbol $\boldsymbol{\varepsilon}$ and $\boldsymbol{\eta}$, respectively. The changes in forces applied to the boundary of the material sample so as to keep $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ constant will, of course, depend on the stress measure, and this will bear different relations to the boundary forces according to the adopted strain and strain gradient measures.

The key foundation of the Rice's internal-variable approach is an assumption termed 'unifying normality structure'. This normality structure assumes that the kinetic rate laws of the internal variables are fully determined by the thermodynamic force associated with the internal micro-structural rearrangements within the material sample

$$\dot{\xi}_\alpha = \dot{\xi}_\alpha(f_\alpha, \theta, \boldsymbol{\xi}), \quad (\alpha = 1, 2, \ldots, n) \tag{12}$$

Eq. (12) may be recast to be

$$\dot{\xi}_\beta = \frac{\partial}{\partial f_\beta} \int_0^{\mathbf{f}} \dot{\xi}_\alpha(f_\alpha, \theta, \boldsymbol{\xi})\, \mathrm{d}f_\alpha \tag{13}$$

where at fixed values of θ and $\boldsymbol{\xi}$ the integral is carried out, and defines a point function of $\mathbf{f}$ since each term in the integrand is an exact differential. A flow potential Q may then be related to the kinetic rate laws

$$Q = Q(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi}) = \frac{1}{V} \int_0^{\mathbf{f}(\boldsymbol{\sigma},\boldsymbol{\tau},\theta,\boldsymbol{\xi})} \dot{\xi}_\alpha(\mathbf{f}, \theta, \boldsymbol{\xi})\, \mathrm{d}f_\alpha \tag{14}$$

Then (13) may be further recast as

$$\dot{\xi}_\beta = V \frac{\partial Q}{\partial f_\beta} \tag{15}$$

where the integral is carried out at fixed values of θ and $\boldsymbol{\xi}$, and defines a point function of $\mathbf{f}$ since each term in the integrand is an exact differential. The thermodynamic forces are viewed as functions of the macroscopic stresses $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$, θ and $\boldsymbol{\xi}$. Consequently, the following normality structure holds:

$$(\dot{\boldsymbol{\varepsilon}})^{\mathrm{p}} = \frac{\partial Q(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial \boldsymbol{\sigma}}, \quad (\dot{\boldsymbol{\eta}})^{\mathrm{p}} = \frac{\partial Q(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial \boldsymbol{\tau}} \tag{16}$$

In view of (14), the above equations may be recast as

$$\begin{cases} (\dot{\boldsymbol{\varepsilon}})^{\mathrm{p}} = \dfrac{\partial Q}{\partial \boldsymbol{\sigma}} = \dfrac{1}{V} \dot{\xi}_\alpha(\mathbf{f}, \theta, \boldsymbol{\xi}) \dfrac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial \boldsymbol{\sigma}} \\ (\dot{\boldsymbol{\eta}})^{\mathrm{p}} = \dfrac{\partial Q}{\partial \boldsymbol{\tau}} = \dfrac{1}{V} \dot{\xi}_\alpha(\mathbf{f}, \theta, \boldsymbol{\xi}) \dfrac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial \boldsymbol{\tau}} \end{cases} \tag{17}$$

If a complex (15-dimensional) stress space is defined by stresses and higher-order stresses, the preceding normality structure implies the inelastic portion of the strain-rate and strain gradient vector geometrically lie normal to surfaces of constant flow potential in this complex space. The complete constitutive formulation may be presented in terms of the complementary energy as

$$\begin{cases} \dot{\boldsymbol{\varepsilon}} = \dfrac{\partial^2 \psi}{\partial \boldsymbol{\sigma} \partial \boldsymbol{\sigma}} : \dot{\boldsymbol{\sigma}} + \dfrac{\partial^2 \psi}{\partial \boldsymbol{\sigma} \partial \boldsymbol{\tau}} \vdots \dot{\boldsymbol{\tau}} + \dfrac{\partial^2 \psi}{\partial \boldsymbol{\sigma} \partial \theta} \dot{\theta} + \dfrac{\partial Q}{\partial \boldsymbol{\sigma}} \\ \dot{\boldsymbol{\eta}} = \dfrac{\partial^2 \psi}{\partial \boldsymbol{\tau} \partial \boldsymbol{\sigma}} : \dot{\boldsymbol{\sigma}} + \dfrac{\partial^2 \psi}{\partial \boldsymbol{\tau} \partial \boldsymbol{\tau}} \vdots \dot{\boldsymbol{\tau}} + \dfrac{\partial^2 \psi}{\partial \boldsymbol{\tau} \partial \theta} \dot{\theta} + \dfrac{\partial Q}{\partial \boldsymbol{\tau}} \end{cases} \tag{18}$$

where ψ and Q are function of $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$, θ and $\boldsymbol{\xi}$. The inverted form of the constitutive rate law is readily shown to be

$$\begin{cases} \dot{\boldsymbol{\sigma}} = \dfrac{\partial^2 \phi}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \dfrac{\partial^2 \phi}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\eta}} \vdots \dot{\boldsymbol{\eta}} + \dfrac{\partial^2 \phi}{\partial \boldsymbol{\varepsilon} \partial \theta} \dot{\theta} - \dfrac{\partial Q}{\partial \boldsymbol{\varepsilon}} \\ \dot{\boldsymbol{\eta}} = \dfrac{\partial^2 \phi}{\partial \boldsymbol{\eta} \partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \dfrac{\partial^2 \phi}{\partial \boldsymbol{\eta} \partial \boldsymbol{\tau}} \vdots \dot{\boldsymbol{\eta}} + \dfrac{\partial^2 \phi}{\partial \boldsymbol{\eta} \partial \theta} \dot{\theta} + \dfrac{\partial Q}{\partial \boldsymbol{\eta}} \end{cases} \tag{19}$$

here the free energy ϕ and flow potential Q are viewed as functions of $\boldsymbol{\varepsilon}$, $\boldsymbol{\eta}$, θ, $\boldsymbol{\xi}$.

In addition, the following relation for the neighbouring patterns may be identified:

$$d^p\psi = -d^p\phi = \frac{1}{V} f_\alpha \, \mathrm{d}\xi_\alpha \tag{20}$$

where $d^p\psi = \psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi} + \mathrm{d}\boldsymbol{\xi}) - \psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})$, $d^p\phi = \phi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi} + \mathrm{d}\boldsymbol{\xi}) - \phi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})$. And also, the entropy production rate ϑ should be always non-negative according to the second law of thermodynamics

$$\vartheta = \frac{1}{\theta V} f_\alpha \dot{\xi}_\alpha \geqslant 0 \tag{21}$$

This restriction of the kinetic rate laws for normality structure actually corresponds to the requirement of the non-linear Onsager reciprocal relations (De Groot and Marur, 1962), as remarked by Rice (1971).

It should be noted that the aforementioned formulations are presented in case that $\boldsymbol{\xi}$ is one set of explicit state variables, and each variable describes a specific structural rearrangement occurring at a local site within the material sample. Otherwise, if there is no explicit set of internal variables available to characterise the internal rearrangement, one may need only to assume that any change in the pattern of internal rearrangement can be uniquely characterised. These possible rearrangements may be included by keeping within the simplicity of the present discrete variable description, by assuming that at any given pattern of internal rearrangement of the material sample, a set of discrete scalar infinitesimals characterises all possible infinitesimal variations in internal arrangement. It is not necessary to assume that any variable exists such that a change of the variable may be obtained, although the treatment may include this as a special case.

In addition, averaging variables that bear no relation to the size of the material size may be used to replace the size-dependent specific structural variables aforementioned. This may be easily done by introducing one set of much reduced internal variables $\boldsymbol{\zeta}$ to be average measurements of $\boldsymbol{\xi}$

$$\boldsymbol{\zeta} = \{\zeta_1, \zeta_2, \ldots, \zeta_m\}, \quad \zeta_\mu = \zeta_\mu(\xi_1, \xi_2, \ldots, \xi_n; V), \ \ (\mu = 1, 2, \ldots, m \ll n) \tag{22}$$

When both n and V are sufficiently large, Eq. (22) expresses a volume average of microscopic rearrangements whose value may be assumed to be independent of n and V. Compared with n, the number of averaging variables, m, will be refined to quite small for the necessity of an accurate description. A set of generalised thermodynamic force $g_1, \ldots, g_m$ (collectively $\mathbf{g}$) conjugate to the averaging variables may then be defined in analogy to (3)

$$\boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon} + \boldsymbol{\tau} \vdots \delta\boldsymbol{\eta} - g_\mu \delta\zeta_\mu + \theta \delta s = \delta U \tag{23}$$

In parallel to the proceeding formulations for the specific structural variables, the following relations may be obtained:

$$\begin{cases} \boldsymbol{\varepsilon} = \dfrac{\partial \psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\zeta})}{\partial \boldsymbol{\sigma}}, \quad \boldsymbol{\eta} = \dfrac{\partial \psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\zeta})}{\partial \boldsymbol{\tau}} \\ g_\alpha = \dfrac{\partial \psi(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\zeta})}{\partial \zeta_\alpha} \\ (\delta\boldsymbol{\varepsilon})^{\mathrm{p}} = \dfrac{\partial \boldsymbol{\varepsilon}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\zeta})}{\partial \zeta_\alpha} \delta\zeta_\alpha = \dfrac{\partial g_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\zeta})}{\partial \boldsymbol{\sigma}} \delta\zeta_\alpha \\ (\delta\boldsymbol{\eta})^{\mathrm{p}} = \dfrac{\partial \boldsymbol{\eta}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\zeta})}{\partial \zeta_\alpha} \delta\zeta_\alpha = \dfrac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\zeta})}{\partial \boldsymbol{\tau}} \delta\zeta_\alpha \end{cases} \tag{24}$$

At the level of a description in terms of averaging variables, it may be also assumed that $\dot{\boldsymbol{\zeta}}$ is derivable from a potential of $\mathbf{g}$ at fixed θ and $\boldsymbol{\xi}$, for an exact differential of $\dot{\xi}_\alpha \mathrm{d}f_\alpha$. Thus Eq. (14) may be rewritten as

$$Q = Q(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \mathbf{g}, \boldsymbol{\zeta}) = \frac{1}{V} \int_0^{\mathbf{f}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \mathbf{g}, \boldsymbol{\zeta})} \dot{\xi}_\alpha(\mathbf{f}, \theta, \boldsymbol{\xi})\, \mathrm{d}f_\alpha \tag{25}$$

then there is

$$\dot{\zeta}_\beta = \frac{\partial Q(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \mathbf{g}, \boldsymbol{\zeta})}{\partial g_\beta} \tag{26}$$

Note that the kinetic equation (15) or (26) for the internal variables has also been the starting point of many other thermomechanical theories (e.g., Ziegler, 1958; Lubliner, 1972; Collins and Houlsby, 1997).

Combination of (24) and (26) leads to

$$\begin{cases} (\dot{\boldsymbol{\varepsilon}})^{\mathrm{p}} = \dfrac{\partial Q}{\partial \boldsymbol{\sigma}} = \dot{\zeta}_\alpha \dfrac{\partial g_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial \boldsymbol{\sigma}} \\ (\dot{\boldsymbol{\eta}})^{\mathrm{p}} = \dfrac{\partial Q}{\partial \boldsymbol{\tau}} = \dot{\zeta}_\alpha \dfrac{\partial f_\alpha(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \boldsymbol{\xi})}{\partial \boldsymbol{\tau}} \end{cases} \tag{27}$$

which implies $\dot{\boldsymbol{\zeta}}$ lies in the outward normal direction of the yield surface in **g**-space at a smooth point, and within the limiting normal directions at a vertex.

In addition, the entropy production rate ϑ in Eq. (21) turns to be

$$\vartheta = \frac{1}{\theta} g_\alpha \dot{\zeta}_\alpha \geqslant 0 \tag{28}$$

which then restricts kinetic equations for the averaging variables.

The preceding formulated framework of an internal-variable approach with normality structure is sufficient for ascertaining certain broad structural features of macroscopic constitutive laws from only the most essential features of a broad class of micro-scale relations for the kinetics of process of micro-structural rearrangement. As one of its advantages, models following this approach may reflect at least approximately some of the real, complex features of gradient elasto-plasticity response when general state of combined stresses and non-proportional stress paths are examined in the compound stress space of stress and higher-order stress. It should be noted that, whenever those terms connecting with strain gradients and higher-order stresses are dropped out, the initial version of this approach by Rice (1971, 1975) for classic continuum mechanics will immediately be recovered.

3. Applications

3.1. Crystal materials with micro-scale dislocations

Plasticity analysis of metallic materials on a physically rigorous connection to its microscopic origins in the mechanics of defects has long been regarded to be difficult. The primary source of complexity arise in achieving an adequate theory that can describe the crystal dislocation distributions and evolutions on the micro-scale, and at the same time, can account for the interaction of the stress fields of these micro-defects as well as macroscopic applied loads. Dislocation theory was developed to address the plastic deformation mechanism of crystallographic slip in metals from early last century (Orowan, 1934; Nye, 1953; Ashby, 1970). Whenever a material is deformed, dislocations are always generated, slipped and stored. Stored dislocations are resulted either by inter-crystal trapping, named statistically stored dislocations (SSD), or by the requirement of compatible deformation of various parts of the material, named geometrically necessary dislocations (GND). Plastic strain gradients occur due to either the geometry of loading or inhomogeneous deformation in the material, and thus are closely related with dislocations, particularly with GND. A variety of strain gradient theories have thus been developed in account for experimental results of the size dependence of material mechanical properties on the higher-order strain gradients inherent in highly non-uniform zones of deformation at small length scales (see, e.g., Aifantis, 1984; Fleck and Hutchinson, 1993, 1997; Fleck et al., 1994; Nix and Gao, 1998; Gao et al., 1999; and references therein). One or more internal length scale was introduced into the formulations to scale the gradient terms in the strain gradient plasticity, and is thought of as an intrinsic material length related to the storage of GND.

Rice (1971) has previously applied his internal-variable approach with normality structure to developing a slip-model of metal plasticity, in which the plastic behaviour of metals arising as a consequence of slip rearrangements of crystallographic planes through dislocation motion and the stress dependence of slip is assumed to be characterised by Schmid law. Specifically, the micro-shear strain, $\gamma^{(\alpha)}$, over each single crystal is regarded to be the micro-structural rearrangement and is assumed to be able to fully describe the necessary pattern of internal rearrangement of the material. A set of thermodynamic shear stresses $\tau^{(\alpha)}$ are defined for each such operative slip system conjugate with the shear strain $\gamma^{(\alpha)}$, and the shear strain rate is dependent on $\tau^{(\alpha)}$ only.

However, major assumptions for the forgoing formulations are that the volume of the crystal and the relative orientation of crystallographic directions are assumed to be unaltered. As for many crystal experiments on small scales, such as micro-bending, twisting and micro-indentation tests, the case will be different and the crystallographic directions will generally be changed. To achieve a compatible configuration, GND is required and thus strain gradients are necessary to be included. Accordingly, the micro-structural rearrangement can no longer be represented only by the micro-shear strain as in Rice (1971), gradients of the shear strain should also be counted in. Thus in the following part of this section, the preceding strain gradient constitutive formulations by means of internal-variable approach is used to develop a micro–macro-scale interrelated strain gradient model for dislocation-characterised crystallographic materials.

Consider a sample volume of V for a continuous polycrystalline material. Each sub-element of the material is assumed to have a single-crystal slip structure indexed by α. The sample is subjected to boundary conditions and is deformed macroscopically homogeneous. $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$, $\boldsymbol{\varepsilon}$ and $\boldsymbol{\eta}$ are the macroscopic stress, higher-order stress, strain and strain gradients, respectively. Isothermal process is assumed such that thermal related terms may be dropped from the formulations. The slip systems α is characterised by orthogonal unit vectors $(\mathbf{s}^{(\alpha)}, \mathbf{t}^{(\alpha)}, \mathbf{m}^{(\alpha)})$ forming a right-handed set of orthogonal system and refer to the slip direction, the transverse direction and the normal direction to the slip plane, respectively (as shown in Fig. 1). Suppose the crystal is subject to a micro-shear of $\gamma^{(\alpha)}$, with slip strain gradients $(\gamma_{\mathrm{S}}^{(\alpha)}, \gamma_{\mathrm{T}}^{(\alpha)}, \gamma_{M}^{(\alpha)})$ in the three directions $(\mathbf{s}^{(\alpha)}, \mathbf{t}^{(\alpha)}, \mathbf{m}^{(\alpha)})$ respectively. As a comprehensive measurement of the micro-structural rearrangement to include the micro-shear as well as its gradients, an effective shear strain according to Shu and Fleck (1999) is adopted here

$$\dot{\gamma}_{\mathrm{e}}^{(\alpha)} = \left(\left|\dot{\gamma}^{(\alpha)}\right|^{\rho} + l\left|\dot{\gamma}_{\mathrm{S}}^{(\alpha)}\right|^{\rho} + l\left|\dot{\gamma}_{\mathrm{T}}^{(\alpha)}\right|^{\rho}\right)^{1/\rho} \tag{29}$$

where $\dot{\gamma}^{(\alpha)}$ is the microscopic shear strain rate. $\dot{\gamma}_{\mathrm{S}}^{(\alpha)}$ is the slip gradient in the slip direction and generates hardening via geometrically necessary edge dislocation and, $\dot{\gamma}_{\mathrm{T}}^{(\alpha)}$ is the slip gradient in the transverse direction and gives rise to hardening by geometrically necessary screw dislocations. Contribution of the normal direction to the geometrical necessary dislocations is assumed to be zero and thus $\dot{\gamma}_{M}^{(\alpha)}$ is excluded from the expression. l is an internal length scale and is introduced for dimensional consistency. ρ is a parameter describing the

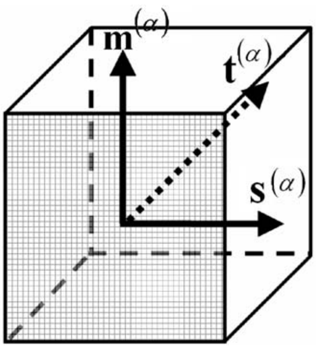

Fig. 1. A sketch of the local configuration of the slip system on the microscale.

interaction between slip rate and slip rate gradient, and in a loose sense it defines the interaction between SSD and GND.

Accordingly, an effective Schmid stress $\tau_{\mathrm{e}}^{(\alpha)}$ may be defined to be the thermodynamic conjugate stress to the effective strain $\gamma_{\mathrm{e}}^{(\alpha)}$. In this paper, we employ an expression from the Taylor hardening law to be the effective Schmid stress over a local slip system α

$$\tau_{\mathrm{e}}^{(\alpha)} = \alpha\mu b\sqrt{\rho_{\mathrm{S}}^{(\alpha)} + \rho_{\mathrm{G}}^{(\alpha)}} \tag{30}$$

where $\rho_{\mathrm{S}}^{(\alpha)}$ and $\rho_{\mathrm{G}}^{(\alpha)}$ denote the density of SSD and GND, respectively. μ is the shear modulus and α is an empirical constant. b denotes the Burgers vector length. The following expressions are adopted for $\rho_{\mathrm{S}}^{(\alpha)}$ and $\rho_{\mathrm{G}}^{(\alpha)}$, respectively (Ashby, 1970; Fleck et al., 1994):

$$\begin{cases} \rho_{\mathrm{S}}^{(\alpha)} = c\gamma^{(\alpha)}L^{(\alpha)}/b \\ \rho_{\mathrm{G}}^{(\alpha)} = \dfrac{1}{b}\sqrt{\left(\gamma_{\mathrm{S}}^{(\alpha)}\right)^2 + \left(\gamma_{\mathrm{T}}^{(\alpha)}\right)^2} \end{cases} \tag{31}$$

where $L^{(\alpha)}$ is the mean free path of dislocation on slip system α. c is a coefficient.

To seek a relation between the kinetic law of $\gamma_{\mathrm{e}}^{(\alpha)}$ and the effective shear stress $\tau_{\mathrm{e}}^{(\alpha)}$, as required by the normality structure, e.g., $\dot{\gamma}_{\mathrm{e}}^{(\alpha)} = \dot{\gamma}_{\mathrm{e}}^{(\alpha)}(\tau_{\mathrm{e}}^{(\alpha)}, \theta, \gamma_{\mathrm{e}})$, where, γ_{e} refers to a dependence on the current dislocated state over the material sampled, it is convenient to employ the following simple power law function in relation with slip resistance $g^{(\alpha)}$ (>0) from classical crystal plasticity theory (cf., e.g., Hutchinson, 1976; Peirce et al., 1983; Shu and Fleck, 1999)

$$\dot{\gamma}_{\mathrm{e}}^{(\alpha)}/\dot{\gamma}_0 = \left(\tau_{\mathrm{e}}^{(\alpha)}/g^{(\alpha)}\right)^{1/m} \tag{32}$$

where $\dot{\gamma}_0$ is a material parameter representing the reference plastic strain rate. m is the rate-sensitivity index which is generally between 0 (the rate-independent limit) and 1. The slip resistance increases from an initial value $g_0^{(\alpha)}$ for a crystallographic system according to (Fleck et al., 1994; Shu and Fleck, 1999):

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta}\left|\dot{\gamma}_{\mathrm{e}}^{(\beta)}\right| \tag{33}$$

where $\dot{\gamma}_{\mathrm{e}}^{(\beta)}$ is the effective slip rate defined by (29). $h_{\alpha\beta}$ is the so-called hardening matrix, and the second term in the summation denotes an effective slip rate accounting for the gradients. The hardening modulus is given by

$$h_{\alpha\beta} = h\delta_{\alpha\beta} + qh(1 - \delta_{\alpha\beta}) \tag{34}$$

where q denotes a latent hardening index and $\delta_{\alpha\beta}$ is the Kronecker delta symbol. h is the self-hardening modulus and is related to the effective slip accumulation over the whole loading history.

So far the internal variables $\dot{\gamma}_{\mathrm{e}}^{(\alpha)}$ with relation to their conjugate forces $\tau_{\mathrm{e}}^{(\alpha)}$ have been defined for the crystal materials. Thus Eq. (3) may be rewritten as

$$\boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon} + \boldsymbol{\tau}\vdots\delta\boldsymbol{\eta} - \frac{1}{V}\int_V \sum_{\alpha} \tau_{\mathrm{e}}^{(\alpha)}(\boldsymbol{\sigma}, \boldsymbol{\tau}, \theta, \gamma_{\mathrm{e}})\delta\gamma_{\mathrm{e}}^{(\alpha)}\,\mathrm{d}V + \theta\delta s = \delta U \tag{35}$$

As for each operative slip-system at each sub-element of the sample we have assumed $\dot{\gamma}_{\mathrm{e}}^{(\alpha)}$ to be a function in form of Eq. (32), the following flow potential thus may be reasonably defined over the chosen volume V:

$$Q = \frac{1}{V}\int_V \left\{\sum_{\alpha} \int_0^{\tau_{\mathrm{e}}^{(\alpha)}} \dot{\gamma}_{\mathrm{e}}^{(\alpha)} d\tau_{\mathrm{e}}^{(\alpha)}\right\}\mathrm{d}V \tag{36}$$

A free energy function is further required to furnish the constitutive relation development. Here we assume the following (cf., e.g., Shu and Fleck, 1999):

$$\psi = \frac{1}{2}D_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{2}\frac{1}{l^2}D_{ijpq}\eta_{ijk}\eta_{pqk} \tag{37}$$

where D_{ijkl} denote the elastic stiffness matrix and l the same internal length scale as in (29). In view of equations from (29) to (37), the rate form constitutive relations for gradient crystal materials may be readily derived in analogy to (19). Detailed formulations are not repeated here.

Note that, in case of GND are not appreciable, gradient terms will disappear from the formulations above. Only SSD in term of micro-shear $\gamma^{(\alpha)}$ and Schmid stress $\tau^{(\alpha)}$ may again be used for the internal variable and its conjugate force, and the formulations may fall into the category as outlined by Rice (1971). However, for a large range of metallic crystal materials, experimental results at small scale repeatedly prove the requirement of introducing GND and thus gradient terms into the constitutive description. In these cases, the constitutive relations as presented in this sub-section may demonstrate a convenient way to relate the microscopic dislocation mechanism with the macroscopic inelastic and gradient-enhanced behaviour. Note that there are also other models being developed in literature to address this problem, by means of either multi-scale framework or homogenisation approach (see, e.g., Gao et al., 1999; Shu and Fleck, 1999).

3.2. Micro-cracked geomaterials

It will be shown in this section, the internal-variable approach with normality structure for gradient characterised materials presented in Section 2 will be applied to the development of a gradient-enhanced anisotropic damage model for micro-cracked geomaterials, and this model is further compared with those presented by the authors previously (Zhou et al., 2002; Zhao et al., 2005). Note that in the following formulation, isothermal processes are assumed so that temperature and entropy can thus all be dropped from the formulations.

If rock-concrete-like geomaterials may be idealised as micro-cracked solids with distribution of Griffith cracks, and if the extension and healing of these micro-cracks may be regarded as the mechanism of inelastic deformation in this kind of materials, an internal variable description is thus possible. Consequently, the essential properties of normality structure will be suitable for formulating the constitutive relations for materials of this kind. Rice (1975, 1978) stated that the refined normality structure directly leads to the restriction on quasi-static extension of healing of Griffith cracks. Yang et al. (1999) further investigate the anisotropic damage revolution law within the normality structure by assuming kinking micro-cracks in solids. Here given the above-mentioned geomaterials are assumed to be micro-cracked solids, we try to apply the normality structure in preceding sections for gradient solids to derive constitutive relations covering the anisotropic case of gradient-enhanced damage model proposed by Zhou et al. (2002) and Zhao et al. (2005). It will be illustrated that, a general anisotropic damage tensor may be constructed from microscopic considerations within the normality structure, and thus serves as a bridge between microscopic and macroscopic mechanical descriptions of micro-cracked materials.

It is a good starting point by borrowing the anisotropic damage evolution laws of Yang et al. (1999) for micro-cracked solids. As the essential formulations of Yang et al. (1999) are constructed within the first-order theory of the normality structure approach, it will be convenient to introduce their results directly here. Nevertheless, this paper would rather derive micro-crack-damaged gradient constitutive relations than pure evolution laws for the damage tensor. A material sample of size V, which is weakened by n micro-cracks, is considered. The following set of internal variables may be used to characterise the micro-cracks in the material:

$$\boldsymbol{\xi} = \{\xi_1, \xi_2, \ldots, \xi_n\}, \quad \text{where } \xi_\alpha = \{\mathbf{n}^\alpha \quad r_\alpha\}, \ (\alpha = 1, 2, \ldots, n) \tag{38}$$

where $\mathbf{n}^\alpha$ and r_α are the normal vector and radius of αth micro-crack, respectively. Location of the micro-crack is neglected, hence the above expression by $\boldsymbol{\xi}$ is merely an approximation. Note in the following formulations, no summation for α is assumed unless specified. From (7), the thermodynamic conjugate force of each internal variable takes thus the following form:

$$f_\alpha = V\frac{\partial\psi}{\partial\xi_\alpha} = \{\mathbf{f}_n^{(\alpha)} \quad f_r^{(\alpha)}\} = V\left\{\frac{\partial\psi}{\partial\mathbf{n}^\alpha} \quad \frac{\partial\psi}{\partial r_\alpha}\right\} = -V\left\{\frac{\partial\phi}{\partial\mathbf{n}^\alpha} \quad \frac{\partial\phi}{\partial r_\alpha}\right\} \tag{39}$$

If the following second-order tensor is introduced:

$$\boldsymbol{\Omega} = \sum_{\alpha=1}^{n} \boldsymbol{\Omega}^{(\alpha)} = \sum_{\alpha=1}^{n} r_\alpha^3 \mathbf{n}^\alpha \mathbf{n}^\alpha \tag{40}$$

which characterises the overall influence of cracks in the sample and is usually termed as ‘damage tensor’ (Kawamoto et al., 1988), it is readily shown that

$$f_\alpha = \left\{\mathbf{f}_n^{(\alpha)} \quad f_r^{(\alpha)}\right\} = V\left\{\frac{\partial\psi}{\partial\mathbf{n}^\alpha} \quad \frac{\partial\psi}{\partial r_\alpha}\right\} = V\left\{\frac{\partial\psi}{\partial\boldsymbol{\Omega}} : \frac{\partial\boldsymbol{\Omega}}{\partial\mathbf{n}^\alpha} \quad \frac{\partial\psi}{\partial\boldsymbol{\Omega}} : \frac{\partial\boldsymbol{\Omega}}{\partial r_\alpha}\right\} = \mathbf{Y} : \left\{r_\alpha^3(\mathbf{I}\mathbf{n}^\alpha + \mathbf{n}^\alpha\mathbf{I})3r_\alpha^2\mathbf{n}^\alpha\mathbf{n}^\alpha\right\} \tag{41}$$

where $\mathbf{I}$ denotes the second-order identity tensor δ_{ij}. $\mathbf{Y}$ denotes the generalised thermodynamic force conjugate to the damage tensor $\boldsymbol{\Omega}$

$$\mathbf{Y} = \frac{\partial\psi}{\partial\boldsymbol{\Omega}} = -\frac{\partial\phi}{\partial\boldsymbol{\Omega}} \tag{42}$$

Eq. (12) now presents the following form:

$$\dot{\xi}_\alpha = \dot{\lambda}_\alpha\left\{(\mathbf{I} - \mathbf{nn}) \cdot \mathbf{f}_n^{(\alpha)} \quad \left(\frac{r_\alpha}{2}\right)^2 f_r^{(\alpha)}\right\} \tag{43}$$

where $\dot{\lambda}_\alpha$ denotes a flow multiplier and may be obtained as

$$\dot{\lambda}_\alpha = \frac{4\dot{r}_\alpha}{f_r r_\alpha^2} \tag{44}$$

In view of Eqs. (13), (41), (43) and (44), the following potential function may thus be obtained

$$Q = \frac{1}{2V}\sum_{\alpha=1}^{n} \dot{\lambda}_\alpha\left(\mathbf{f}_n^{(\alpha)} \cdot (\mathbf{I} - \mathbf{nn}) \cdot \mathbf{f}_n^{(\alpha)} + \left(\frac{1}{2} f_r^{(\alpha)} r\right)^2\right) \tag{45}$$

Thus far, if an extra free energy function ψ or ϕ is defined, the entire constitutive structure may then be readily derived. Without loss of generality, the Holmholtz free energy function presented in Zhou et al. (2002) is used here (with omitting the terms with internal variables)

$$\phi = \frac{1}{2}\boldsymbol{\varepsilon} : \mathbf{D} : \boldsymbol{\varepsilon} + \frac{1}{2}\boldsymbol{\eta} \,\vdots\, \boldsymbol{\Lambda} \,\vdots\, \boldsymbol{\eta} \tag{46}$$

where $\mathbf{D}$ and $\boldsymbol{\Lambda}$ characterise the elasto-damage stiffness tensor higher-order elasto-damage stiffness tensor of the material, respectively. They present forms with damage tensor in the expressions as follows:

$$D_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - [\lambda\Omega_{ij}\delta_{kl} + \mu(\Omega_{ik}\delta_{jl} + \Omega_{il}\delta_{jk})] + (\lambda + 2\mu)\Omega_{ij}\Omega_{kl} \tag{47}$$

$$\boldsymbol{\Lambda}_{ijklmn} = l^2 D_{ijlm}\delta_{kn} \tag{48}$$

where λ and β are Lame constants of materials. δ_{ij} denotes the second-order Kronecker delta, and l represents a material length scale linking the micro-structures with the macroscopic mechanical response. The inclusion of damage tensor in the expressions makes it possible to account for the degradation due to accumulation of damage, and at the same time, addressing the influence of the micro-structures. As a result of (47) and (48), the following derivatives for the damage tensor $\boldsymbol{\Omega}$ may be obtained

$$\frac{\partial D_{ijkl}}{\partial\Omega_{mn}} = -\left(D^{\mathrm{e}}_{rjkl}\delta_{im}\delta_{nr} + D^{\mathrm{e}}_{ijkr}\delta_{rm}\delta_{nl}\right) + D^{\mathrm{e}}_{rjks}\Omega_{ir}\delta_{sm}\delta_{nl} + D^{\mathrm{e}}_{rjks}\Omega_{sl}\delta_{im}\delta_{nr} \tag{49}$$

$$\frac{\partial\Lambda_{ijklab}}{\partial\Omega_{mn}} = l^2\frac{\partial D_{ijla}}{\partial\Omega_{mn}}\delta_{kb} \tag{50}$$

where $D^{\mathrm{e}}_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ is the initial elasticity tensor.

The following intermediate relations for the tensor operations may be convenient for use in deriving the final constitutive relations:

$$\frac{\partial\phi}{\partial\boldsymbol{\varepsilon}} = \mathbf{D} : \boldsymbol{\varepsilon}, \quad \frac{\partial\phi}{\partial\boldsymbol{\eta}} = \boldsymbol{\Lambda} \vdots \boldsymbol{\eta}, \quad \frac{\partial\phi}{\partial\boldsymbol{\Omega}} = \frac{1}{2}\boldsymbol{\varepsilon} : \frac{\partial\mathbf{D}}{\partial\boldsymbol{\Omega}} : \boldsymbol{\varepsilon} + \frac{1}{2}\boldsymbol{\eta} \vdots \frac{\partial\boldsymbol{\Lambda}}{\partial\boldsymbol{\Omega}} \vdots \boldsymbol{\eta} \tag{51a}$$

$$\mathbf{Y} = -\frac{\partial\phi}{\partial\boldsymbol{\Omega}} = -\frac{1}{2}\boldsymbol{\varepsilon} : \frac{\partial\mathbf{D}}{\partial\boldsymbol{\Omega}} : \boldsymbol{\varepsilon} - \frac{1}{2}\boldsymbol{\eta} \vdots \frac{\partial\boldsymbol{\Lambda}}{\partial\boldsymbol{\Omega}} \vdots \boldsymbol{\eta}, \quad \frac{\partial\mathbf{Y}}{\partial\boldsymbol{\varepsilon}} = -\frac{\partial\mathbf{D}}{\partial\boldsymbol{\Omega}} : \boldsymbol{\varepsilon}, \quad \frac{\partial\mathbf{Y}}{\partial\boldsymbol{\eta}} = -\frac{\partial\boldsymbol{\Lambda}}{\partial\boldsymbol{\Omega}} \vdots \boldsymbol{\eta} \tag{51b}$$

$$\frac{\partial^2\phi}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}} = \mathbf{D}, \quad \frac{\partial^2\phi}{\partial\boldsymbol{\eta}\partial\boldsymbol{\eta}} = \boldsymbol{\Lambda}, \quad \frac{\partial^2\phi}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\eta}} = \mathbf{0}, \quad \frac{\partial^2\phi}{\partial\boldsymbol{\eta}\partial\boldsymbol{\varepsilon}} = \mathbf{0} \tag{51c}$$

$$\frac{\partial Q}{\partial\boldsymbol{\varepsilon}} = \frac{\partial Q}{\partial\mathbf{Y}} : \frac{\partial\mathbf{Y}}{\partial\boldsymbol{\varepsilon}}, \frac{\partial Q}{\partial\boldsymbol{\eta}} = \frac{\partial Q}{\partial\mathbf{Y}} : \frac{\partial\mathbf{Y}}{\partial\boldsymbol{\eta}} \tag{51d}$$

$$\frac{\partial\mathbf{f}_n^{(\alpha)}}{\partial\mathbf{Y}} = r_\alpha^3(\mathbf{I}\mathbf{n}^\alpha + \mathbf{n}^\alpha\mathbf{I}), \quad \frac{\partial f_r^{(\alpha)}}{\partial\mathbf{Y}} = 3r_\alpha^2\mathbf{n}^\alpha\mathbf{n}^\alpha \tag{51e}$$

$$\begin{aligned}\frac{\partial Q}{\partial\mathbf{Y}} &= \frac{1}{2V}\sum_{\alpha=1}^{n}\dot{\lambda}_\alpha\left(\left(\frac{\partial\mathbf{f}_n^{(\alpha)}}{\partial\mathbf{Y}} \cdot (\mathbf{I} - \mathbf{nn}) \cdot \mathbf{f}_n^{(\alpha)} + \mathbf{f}_n^{(\alpha)} \cdot (\mathbf{I} - \mathbf{nn}) \cdot \frac{\partial\mathbf{f}_n^{(\alpha)}}{\partial\mathbf{Y}}\right) + f_r^{(\alpha)} r \frac{\partial f_r^{(\alpha)}}{\partial\mathbf{Y}}\right) \\ &= \frac{1}{2V}\sum_{\alpha=1}^{n}\dot{\lambda}_\alpha(((\mathbf{n}^\alpha\mathbf{I} - \mathbf{nnn}) \cdot \mathbf{f}_n^{(\alpha)} + \mathbf{f}_n^{(\alpha)} \cdot (\mathbf{I}\mathbf{n}^\alpha - \mathbf{nnn})) + 3f_r^{(\alpha)}\mathbf{nn})\end{aligned} \tag{51f}$$

Generalisation from (38) to (51) with consideration of (17), the following incremental form constitutive relations for gradient-enhanced damage micro-cracked geomaterials may be obtained:

$$\begin{cases} \dot{\boldsymbol{\sigma}} = \mathbf{D} : \dot{\boldsymbol{\varepsilon}} + \sum\limits_{\alpha=1}^{n}\dot{\lambda}_\alpha\mathbf{S} \\ \dot{\boldsymbol{\tau}} = \boldsymbol{\Lambda} \vdots \dot{\boldsymbol{\eta}} + \sum\limits_{\alpha=1}^{n}\dot{\lambda}_\alpha\mathbf{T} \end{cases} \tag{52}$$

where

$$\mathbf{S} = \frac{1}{2V}\sum_{\alpha=1}^{n}\left[r_\alpha^3(((\mathbf{n}^\alpha\mathbf{I} - \mathbf{nnn}) \cdot \mathbf{f}_n^{(\alpha)} + \mathbf{f}_n^{(\alpha)} \cdot (\mathbf{I}\mathbf{n}^\alpha - \mathbf{nnn})) + 3f_r^{(\alpha)}\mathbf{nn}) : \frac{\partial\mathbf{D}}{\partial\boldsymbol{\Omega}} : \boldsymbol{\varepsilon}\right] \tag{53}$$

$$\mathbf{T} = \frac{1}{2V}\sum_{\alpha=1}^{n}\left[r_\alpha^3\big(((\mathbf{n}^\alpha\mathbf{I} - \mathbf{nnn}) \cdot \mathbf{f}_n^{(\alpha)} + \mathbf{f}_n^{(\alpha)} \cdot (\mathbf{I}\mathbf{n}^\alpha - \mathbf{nnn})\big) + 3f_r^{(\alpha)}\mathbf{nn}\big) : \frac{\partial\boldsymbol{\Lambda}}{\partial\boldsymbol{\Omega}} \vdots \boldsymbol{\eta}\right] \tag{54}$$

Thus from (52) we can see, the second terms $\sum_{\alpha=1}^{n}\dot{\lambda}_\alpha\mathbf{S}$ and and $\sum_{\alpha=1}^{n}\dot{\lambda}_\alpha\mathbf{T}$ may be deemed as the inelastic portions for stresses and higher-order stresses induced by the micro-cracks and their evolutions and are second-order and third-order tensor, respectively. Obviously, $\mathbf{S}$ and $\dot{\boldsymbol{\sigma}}$, $\mathbf{T}$ and $\dot{\boldsymbol{\tau}}$ are co-axial, respectively. $\mathbf{S}$ and $\mathbf{T}$ may be respectively called the accompanying stresses and higher-order accompanying stresses for αth micro-crack, as they both characterise the impacts of the previous micro-structural rearrangements of αth micro-crack, together with overall strain and strain gradient state and history, on the mechanical response of current loading step. $\dot{\lambda}_\alpha$ thus becomes a proportion coefficient of the αth accompanying stresses and higher-order accompanying stresses in contribution to the overall stress increments, in term of the radius growth of αth micro-crack. Also note that in both equations of (52), the involvement of damage tensor $\boldsymbol{\Omega}$ in both $\mathbf{D}$ and $\boldsymbol{\Lambda}$ in the first term also makes it possible to reflect the stiffness degradation due to accumulation of damage upon loading within the material.

It is interest to make a comparison of the obtained model with the anisotropic case obtained in Zhou et al. (2002). Even though the anisotropic gradient damage model obtained by Zhou et al. introduces an involvement of micro-cracks by means of macroscopic damage tensor, it is essentially a phenomenological model. This is due to that the damage flow law is still controlled by macroscopically generalised variables which, by no means reflect the micro-structural rearrangements of the materials, as the model we just constructed by internal variable approach will do.

It also will be interest to make a comparison with another model developed by Zhao et al. (2005), which was a more generalised model of Zhou et al. (2002) with extra boundary conditions introduced. Recalling the obtained incremental constitutive relations in Zhao et al. (2005) (Eq. (39) therein)

$$\begin{cases} \dot{\sigma}_{ij} = \left(D_{ijkl} - \dfrac{1}{A} D_{ijab} \dfrac{\partial g}{\partial \sigma_{ab}} \dfrac{\partial f}{\partial \sigma_{cd}} D_{cdkl} \right) \dot{\varepsilon}_{kl} - \dfrac{1}{A} D_{ijpq} \dfrac{\partial g}{\partial \sigma_{pq}} \dfrac{\partial f}{\partial \tau_{rst}} l^2 D_{rsuv} \delta_{tw} \dot{\eta}_{uvw} \\ \dot{\tau}_{ijk} = \left(D_{ijlm} \delta_{kn} - \dfrac{1}{A} l^2 D_{ijab} \delta_{kc} \dfrac{\partial g}{\partial \tau_{abc}} \dfrac{\partial f}{\partial \tau_{xyp}} D_{xylm} \delta_{pm} \right) l^2 \dot{\eta}_{lmn} - \dfrac{1}{A} l^2 D_{ijqr} \delta_{ks} \dfrac{\partial g}{\partial \tau_{qrs}} \dfrac{\partial f}{\partial \sigma_{uv}} D_{uvwt} \dot{\varepsilon}_{wt} \end{cases} \tag{55}$$

In view of (52), it is readily to find that, relations in (52) are more appropriate to be called a decoupled model, while those in (55) a coupled one. Since we can see, in (55), increments of strain gradients contribute to the Cauchy stress, while increments of strain also emerge in the relations for the higher-order stress; whereas these coupling terms are not observed in (52). However, this is not to say the model obtained in this paper is absolutely decoupled for strains and strain gradients. Actually, the previous equilibrium state is built up by the combined rebalance of stress and higher-order stress, which then jointly influence the kinetic evolution of micro-cracks and damage tensor. Consequently, no real sense of decoupling for (52) exists. In fact, if other damage term is defined, for example: $\mathbf{\Omega} = \mathbf{\Omega}(\boldsymbol{\varepsilon}, \boldsymbol{\eta}, \boldsymbol{\xi})$, then the interchanged derivatives of free energy function will no longer be zero

$$\frac{\partial^2 \phi}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\eta}} \neq \mathbf{0}, \quad \frac{\partial^2 \phi}{\partial \boldsymbol{\eta} \partial \boldsymbol{\varepsilon}} \neq \mathbf{0}$$

Then coupled terms will emerge in (52).

The gradient-enhanced anisotropic damage model may be completed by the following governing equations and extra boundary conditions induced by the introduction of gradient terms into the constitutive relations:

$$\sigma_{ij,i} - \tau_{ijk,ik} + f_j = 0 \tag{56}$$

$$\dot{t}_k = n_i(\dot{\sigma}_{ik} - \partial_j \dot{\tau}_{ijk}) - D_j(n_i \dot{\tau}_{ijk}) + n_i n_j (D_l n_l) \dot{\tau}_{ijk} \tag{57}$$

$$\dot{r}_k = n_i n_j \dot{\tau}_{ijk} \tag{58}$$

where f_i denotes body forces. n_i is the norm of the boundary surface. $\dot{t}_k$ and $\dot{r}_k$ denote the traction and double force vector on the surface respectively. Detailed deduction of (56)–(58) for strain gradient theories may be referred to Zhao et al. (2005).

4. Discussion and conclusions

Rice's (1971, 1975) internal-variable approach with normality structure is used to developed strain gradient constitutive relations that are capable of accounting for the micro–macro interrelation. The obtained formulations are applied to crystal materials deformed by micro-scale dislocations and micro-cracked geomaterials degraded by damage accumulation. It is demonstrated strain gradient plasticity for materials characterised by micro-structures may be developed by this approach without difficulty. Kinetic rate laws for the internal variables are defined and related to the inelastic portions in the strain gradient constitutive relations. For the crystallographic materials, effective measures for shear strains and their gradients are used to comprehensively interpret the micro-structural rearrangements, and an effective shear stress defined by Taylor hardening law is used as the thermodynamic force to account for the non-Schmid effects in polycrystallines under complex experimental conditions on small scale. The application of developing the gradient-enhanced anisotropic damage model for micro-cracked geomaterials well demonstrated the advantages of the internal-variable approach. The obtained damage model relates the size, orientation and evolution of the micro-cracks with a material sample with the macroscopic mechanical behaviour reasonably. Decoupled formulations of incremental constitutive relations for stress and higher-order stress are found. Contribution from the micro-cracks accounts for the inelastic portions of the stress response. The damage-coupled stiffness tensors in the constitutive relations enable the characterisation of stiffness degradation due to damage accumulation typically observed in micro-cracked geomaterials.

Note that the current formulations are different from the gradient theory of internal variables proposed by Valanis (1996) (later extended by Walsh and Tordesillas (2004) to micro-polar model for granular materials) in that the latter assumes the internal variables are non-local and thus gradients terms are accounted for, while the current approach assumes the existence of macroscopic strain gradients. Though in name of micro-structure, the gradient theory developed by Germain (1973) treats the strain gradients as a macroscopic representation with micromorphic origin, which makes it essentially a phenomenological one and thus differ distinctively from the current work. However, it should be noted that the work of Germain (1973) may recover that of Mindlin (1965) with its second gradient theory, which was used in the beginning of this paper. Other works of gradient thermodynamics type include the strain gradient crystal plasticity formulations by Forest et al. (2002) in term of thermomechanical approach, and the gradient elastoplasticity model of Shizawa and Zbib (1999) by using dislocation density tensor. The distinctive difference of these works with the current work is their incapability of developing direct linkage of micro–macroscopic interaction even with gradients considered, while the current work can achieve this good.

In particular, it is worthy of noting that, the approach as formulated in this paper shares many similarities with the thermomechanical approach (Ziegler, 1983; Ziegler and Wehrli, 1987a,b; Collins and Houlsby, 1997; Houlsby and Puzrin, 2000). Differing from the general routine for conventional constitutive development approaches of proposing constitutive relations first and then imposing the laws of thermodynamics to these relations, both the current approach and the thermomechanical approach develop constitutive models by guaranteeing the fulfillment of the thermodynamic laws firstly. Additional internal variables other than the general state variables, either microscopic or macroscopic variables, will then be used to characterise the material. It is suggested the total constitutive relations may be merely determined by two thermodynamic functions in both approaches: a specific free energy function and one other function (a flow potential function in the current approach and a dissipation function in the thermomechanical approach). In addition, the underling orthogonality condition for the thermomechanical approach exhibits similar form as the normality structure in Eq. (15). Both the orthogonality condition and the normality structure may recover the Onsager's reciprocity relations for linear case as well as non-linear cases. However, the equivalence of the normality structure with the orthogonality condition and other extremum principles, such as the principle of maximal dissipation rate and the principle of maximal entropy production rate, merits further investigations. Moreover, as suggested in Collins and Houlsby (1997) and Collins (2005), the thermomechanical approach is capable of addressing non-associated flow cases typically shown by geomaterials, by using a normal flow law in dissipative stress space instead of true stress space. Therefore, it will be a future interest on relaxing of the normality conditions for the internal-variable approach to address such non-associated cases for frictional geomaterials.

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