

New thermodynamic framework for microplane model

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ABSTRACT: A new thermodynamic framework for microplane formulations is summarized. A free-energy potential is defined at the microplane level, such that its integral over all orientations gives the standard macroscopic free energy. From this simple assumption it is possible to derive in a unique way consistent microplane stresses and their corresponding integral relation to the macroscopic stress tensor. These new relations are discussed and compared to the traditional approach to microplane model using intuitively defined stresses and the PVW.

1 INTRODUCTION

Since it was first proposed in 1983 by Bažant and Oh, the microplane approach has become progressively more popular for the description of the constitutive behavior of a number of engineering materials such as concrete, rock, ceramics, or ice (Bažant and Gambarova, 1984; Bažant and Oh, 1985; Bažant and Prat, 1987; Bažant and Prat, 1988a; Bažant and Prat, 1988b; Carol et al., 1991; Carol et al., 1992; Cofer, 1992; Cofer et al., 1992; Ožbolt and Bažant, 1992; Cofer and Cohut, 1994; Bažant et al., 1996a; Bažant et al., 1996b; Fichant, 1996; Ožbolt and Bažant, 1996; Kuhl et al., 1998; Bažant et al., 2000a, Bažant et al., 2000b).

Microplane constitutive formulations are based on the assumption that intrinsic material behavior may be defined as a relation between normal and shear components of stress and strain on microplanes of various orientations, rather than between stress and strain tensors and their invariants. These microplane stresses are then integrated over all possible directions in space. This idea is actually not new. The classical elasto-plastic failure envelopes such as Tresca and Mohr-Coulomb may be also derived from the idea of a limit σ - τ condition for a generic plane (Mohr, 1900). The slip theory of plasticity (Taylor, 1938; Batdorf and Budiansky, 1949) and the viscoplastic multilaminate model for fractured rocks and soils (Zienkiewicz and Pande, 1977; Pande and Sharma, 1983) were also based on similar concepts. The main difference between those formulations and the traditional microplane model is the kinematic constraint assumed

(previous formulation were in general based on the static constraint), and the principle of virtual work (PVW) applied to obtain the corresponding integral micro-macro relation for stresses. This is well documented in the literature, see for instance Carol and Bažant (1997).

However, although successfully implemented and extensively verified with experimental results (Bažant and Prat, 1988b; Carol et al., 1992, Bažant et al., 1996b, Bažant et al., 2000a), the traditional microplane models were to some extent based on intuitive arguments, and their thermodynamic consistency could not be guaranteed in all loading situations. The lack of full thermodynamic consistency (actually common to many constitutive models used in engineering practice) seems to have had little influence on the representation of available experimental data, given the excellent fits obtained under numerous different loading conditions. But no doubt, an approach in which conjugacy of variables and thermodynamical consistency is assured should always be preferable.

A first simple version of such consistent approach has recently been proposed (Carol et al., 2001; Kuhl et al., 2001) and is summarized and discussed in the present paper.

2 TRADITIONAL MICROPLANE FORMULATION

The orientation of each microplane is described by the unit normal vector, \mathbf{n} . The deformation and stresses on the microplane are characterized by the normal and

shear strains, ϵ_N, ϵ_T (with Cartesian components ϵ_{T_r}), and the corresponding microplane tractions, σ_N , and σ_T (with Cartesian components σ_{T_r}). With the exception of the earliest formulations (Bažant and Oh, 1983; Bažant and Gambarova, 1984), which worked very well for distributed multidirectional tensile cracking but could not cope with the nonlinearity under compression and shear, most versions of the model assume the normal components to be further split into their volumetric and deviatoric parts, ϵ_V and ϵ_D (or σ_V and σ_D). The *kinematic constraint* means that the normal and shear strains on the microplane are assumed equal to the projections of the macroscopic strain tensor ϵ_{ij} (as opposite to a static constraint in previous models based on similar ideas):

$$\begin{aligned} \epsilon_N &= n_i n_j \epsilon_{ij} \quad (\text{or, with split, } \epsilon_V = \frac{\delta_{ij}}{3} \epsilon_{ij} \\ &\quad \epsilon_D = \epsilon_N - \epsilon_V) \\ \epsilon_{T_r} &= \frac{1}{2} [n_i \delta_{jr} + n_j \delta_{ir} - 2n_i n_j n_r] \epsilon_{ij} \end{aligned} \quad (1a,b,c,d)$$

where the Latin lowercase subscripts refer to Cartesian coordinates x_i ($i=1,2,3$), and subscript repetition implies summation. The same relations may be expressed in compact notation as:

$$\begin{aligned} \epsilon_N &= \mathbf{N} : \boldsymbol{\epsilon} \quad (\text{or, with split, } \epsilon_V = \mathbf{V} : \boldsymbol{\epsilon} \\ &\quad \epsilon_D = \mathbf{D} : \boldsymbol{\epsilon}) \\ \epsilon_{T_r} &= \mathbf{T} : \boldsymbol{\epsilon} \end{aligned} \quad (2a,b,c,d)$$

where the projection tensors $\mathbf{N}, \mathbf{V}, \mathbf{D}$ (of second order) and \mathbf{T} (of third order) have the Cartesian components:

$$\begin{aligned} N_{ij} &= n_i n_j, \quad V_{ij} = \frac{\delta_{ij}}{3}, \quad D_{ij} = n_i n_j - \frac{\delta_{ij}}{3} \\ T_{rij} &= \frac{1}{2} [n_i \delta_{jr} + n_j \delta_{ir} - 2n_i n_j n_r] \end{aligned} \quad (3a,b,c,d)$$

Stress quantities σ_N , σ_D and σ_T are introduced for each microplane, as well as the corresponding material laws in the form of functions

$$\begin{aligned} \sigma_N &= \mathcal{F}_N(\epsilon_N) \quad (\text{or, with split, } \sigma_V = \mathcal{F}_V(\epsilon_V) \\ &\quad \sigma_D = \mathcal{F}_D(\epsilon_D)) \\ \sigma_{T_r} &= \mathcal{F}_{T_r}(\epsilon_{T_r}, \epsilon_V) \end{aligned} \quad (4a,b,c,d)$$

With the kinematic constraint and *general* microplane material laws, equilibrium between the macro- and micro-stresses is not possible in a 'strong' sense (i.e. the static constraint dual to (1) is *not* satisfied). The *weak* form of micro-macro equilibrium equations can

be constructed using the principle of virtual work,

$$\frac{4\pi}{3} \boldsymbol{\sigma} : \delta \boldsymbol{\epsilon} = 2 \int_{\Omega} [\sigma_N \delta \epsilon_N + \sigma_{T_r} \delta \epsilon_{T_r}] d\Omega \quad (5)$$

where Ω is the surface of a unit hemisphere (representing the set of all possible microplane orientations). Substituting $\delta \epsilon_N = \mathbf{N} : \delta \boldsymbol{\epsilon}$ and $\delta \epsilon_{T_r} = \mathbf{T} : \delta \boldsymbol{\epsilon}$ and taking into account the independence of individual components of the (symmetric) virtual strain tensor, we get the integral micro-macro equilibrium condition

$$\boldsymbol{\sigma} = \frac{3}{2\pi} \int_{\Omega} \sigma_N \mathbf{N} d\Omega + \frac{3}{2\pi} \int_{\Omega} \sigma_{T_r} \cdot \mathbf{T} d\Omega \quad (6)$$

or, in index notation

$$\begin{aligned} \sigma_{ij} &= \frac{3}{2\pi} \int_{\Omega} \sigma_N n_i n_j d\Omega + \\ &\quad + \frac{3}{2\pi} \int_{\Omega} \frac{\sigma_{T_r}}{2} [n_i \delta_{rj} + n_j \delta_{ri}] d\Omega \end{aligned} \quad (7)$$

(when rewriting the second integral, the last term in the definition of \mathbf{T} (3d) has been omitted because σ_{T_r} is a vector contained in the microplane and therefore $\sigma_{T_r} n_r = 0$).

In previous models with volumetric-deviatoric split similar to (Bažant and Prat, 1988a), σ_N in the first term of the previous equation was directly replaced by $\sigma_V + \sigma_D$. Since, according to (4b), volumetric stress σ_V depends only on ϵ_V and therefore is the same for all microplanes, (6) was written as

$$\boldsymbol{\sigma} = \sigma_V \mathbf{I} + \frac{3}{2\pi} \int_{\Omega} \sigma_D \mathbf{N} d\Omega + \frac{3}{2\pi} \int_{\Omega} \sigma_{T_r} \cdot \mathbf{T} d\Omega \quad (8)$$

where $\mathbf{I} = 3\mathbf{V}$ is the second-order identity tensor (Kronecker delta).

3 NEW THERMODYNAMIC DERIVATION

The first standard assumption in a thermodynamically consistent constitutive framework is the existence of a free-energy potential per unit mass of material in isothermal conditions, $\Psi^{mac}(\boldsymbol{\epsilon}, \boldsymbol{\xi})$, where $\boldsymbol{\xi}$ is a given set of internal variables that fully define the state of the material at any point of the loading history. The fundamental assumption for the new, thermodynamically consistent microplane approach is that the macroscopic free energy may be written as the integral of some free energy defined at the microplane level, Ψ_{Ω}^{mic} :

$$\Psi^{mac} = \frac{3}{2\pi} \int_{\Omega} \Psi_{\Omega}^{mic}(\boldsymbol{\epsilon}_{\mathbf{n}}, \boldsymbol{\xi}) d\Omega \quad (9)$$

where $\boldsymbol{\epsilon}_{\mathbf{n}}$ is the vector collecting the normal and shear strain components for the microplane with normal \mathbf{n} .

If the material density is ρ_0 , it is a standard procedure (Coleman and Gurtin, 1967; Ilankamban and Krajcinovic, 1987) to obtain the stress conjugate to ϵ as the derivative of the free energy per unit volume:

$$\sigma = \frac{\partial[\rho_0 \Psi^{mic}]}{\partial \epsilon} \quad (10)$$

In our case, this formula may be applied to Eqn. (9). Using the chain rule of differentiation on the right-hand side, one obtains:

$$\begin{aligned} \sigma &= \frac{3}{2\pi} \int_{\Omega} \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon} d\Omega = \\ &= \frac{3}{2\pi} \int_{\Omega} \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_N} \cdot \frac{\partial \epsilon_N}{\partial \epsilon} d\Omega \end{aligned} \quad (11a,b)$$

Assuming that the strain components on the microplane are ϵ_N , and ϵ_T , and that they are related to the macroscopic strain via the kinematic constraint given by equations (1a,d) or (2a,d), we may expand the two terms of the product inside the integral, obtain the strain derivatives and express:

$$\begin{aligned} \sigma &= \frac{3}{2\pi} \int_{\Omega} \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_N} \mathbf{N} d\Omega + \\ &+ \frac{3}{2\pi} \int_{\Omega} \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_T} \cdot \mathbf{T} d\Omega \end{aligned} \quad (12)$$

This equation turns out to be equivalent to (6) if we define

$$\begin{aligned} \sigma_N &= \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_N} \\ \sigma_T &= \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_T} \end{aligned} \quad (13a,b)$$

This is actually a consistent definition of the microplane stresses σ_N and σ_T as the work-conjugate quantities of the microplane strains ϵ_N and ϵ_T .

If, on the other hand, we consider the formulation *with split*, in which the microplane strains are ϵ_V , ϵ_D and ϵ_T , developing (11b) leads to:

$$\begin{aligned} \sigma &= \frac{3}{2\pi} \int_{\Omega} \sigma_V \mathbf{V} d\Omega + \frac{3}{2\pi} \int_{\Omega} \sigma_D \mathbf{D} d\Omega + \\ &+ \frac{3}{2\pi} \int_{\Omega} \sigma_T \cdot \mathbf{T} d\Omega \end{aligned} \quad (14)$$

with the consistent microplane stresses σ_V , σ_D and σ_T defined as:

$$\begin{aligned} \sigma_V &= \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_V} \\ \sigma_D &= \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_D} \\ \sigma_T &= \frac{\partial[\rho_0 \Psi_{\Omega}^{mic}]}{\partial \epsilon_T} \end{aligned} \quad (15a,b,c)$$

4 DISCUSSION

Formulas (12) and (14) obtained by differentiation of the free energy may now be compared to their counterparts in the traditional microplane formulation, (6) and (8).

For the formulation *without volumetric-deviatoric split*, the thermodynamic derivation leads to an integral equation (12) which is identical to the one obtained in the traditional formulation (6). This means that, in spite of being derived in an intuitive manner, the traditional microplanes models without split do not seem to contradict thermodynamic principles. In particular, the microplane stresses defined in that way σ_N , σ_T , indeed correspond to the conjugate quantities to their strain counterparts ϵ_N and ϵ_T .

In contrast, for the *formulation with split of normal components*, the two derivations lead to different expressions. Comparing equations (8) and (14), there are two differences:

- (a) the simple term $\sigma_V \mathbf{I}$ in (8) is replaced by the integral involving the volumetric term (first on the right-hand side) in (14), and
- (b) the factor \mathbf{N} multiplying σ_D in the deviatoric integral of (8) is replaced by $\mathbf{D} = \mathbf{N} - \mathbf{V}$ in (14).

The first difference (a) only vanishes if σ_V may be assumed to be a function of ϵ_V but not of ϵ_D and ϵ_T . In that case, σ_V would be the same for all microplanes and could be taken out of the integral in (14), because of the simple relation

$$\frac{3}{2\pi} \int_{\Omega} \mathbf{V} d\Omega = \mathbf{I} \quad (16)$$

Since $\sigma_V = \partial[\rho_0 \Psi_{\Omega}^{mic}]/\partial \epsilon_V$, (Eqn 15a), having σ_V independent of ϵ_D and ϵ_T implies that the mixed derivatives $\partial^2[\rho_0 \Psi_{\Omega}^{mic}]/\partial \epsilon_V \partial \epsilon_D$ and $\partial^2[\rho_0 \Psi_{\Omega}^{mic}]/\partial \epsilon_V \partial \epsilon_T$ vanish, but then (because of the remaining definitions 15b,c) neither σ_D nor σ_T can depend on ϵ_V either. In this situation, the microplane free energy *must* have the following decoupled form:

$$\begin{aligned} \Psi_{\Omega}^{mic}(\epsilon_V, \epsilon_D, \epsilon_T, \xi) &= \Psi_1^{mic}(\epsilon_V, \xi) + \\ &+ \Psi_2^{mic}(\epsilon_D, \epsilon_T, \xi) \end{aligned} \quad (17)$$

Note that the very assumption of a microplane free energy Ψ_{Ω}^{mic} which depends on the strains on the same microplane exclusively, may be in itself quite restrictive. For instance, the latest practical formulation for concrete M4 (Bažant et al., 2000b), and also its predecessor M3 (Bažant et al., 1996a), use a procedure to calculate σ_V and σ_D on each microplane which makes

them actually dependent on deviatoric strains ϵ_D on *all other* microplanes. That was a way to combine the advantages of the model without split in tension, with those of the split in compression, and allowed a much better fit of experimental data for concrete. That same feature, however, makes those formulations more general than the thermodynamic framework considered in this paper, and for them the question of work conjugacy must be addressed in a different way (Bažant et al., 2000b).

In contrast, earlier versions of the model did conform to assumption (9), and most of them actually also to (17). This might not be apparent in some cases, in which the microplane law for the shear components involved some form of dependence on the volumetric strain in order to introduce the frictional effect of hydrostatic pressure on the deviatoric behavior. Nevertheless, the nature of that dependence is that of a shear yield limit that depends on normal stress, while unloading properties (which relate to stored energy) remain uncoupled. For this reason, this effect may be in general introduced via the history variables ξ , with the practical consequence that, for all those formulations included in the framework, difference (a) is only apparent and does not imply real inconsistency.

More essential, however, is the difference (b). In effect, by developing the second integral in (14) and because \mathbf{V} is the same for all microplanes, we can write

$$\int_{\Omega} \sigma_D \mathbf{D} d\Omega = \int_{\Omega} \sigma_D \mathbf{N} d\Omega - \mathbf{V} \int_{\Omega} \sigma_D d\Omega \quad (18a,b)$$

The second term on the right-hand side vanishes only if the average deviatoric stress is zero, and this is actually only satisfied for a very narrow class of models. The most important member of this class is isotropic linear elasticity, which is described by the microplane free-energy potential

$$\rho_0 \Psi_{\Omega}^{mic}(\epsilon_V, \epsilon_D, \epsilon_T) = \frac{3}{2} K \epsilon_V^2 + G [\epsilon_D^2 + |\epsilon_T|^2] \quad (19)$$

where K is the macroscopic bulk modulus and G is the macroscopic shear modulus of elasticity. The mean value of ϵ_D over all the microplanes is always zero, and as $\sigma_D = \partial[\rho_0 \Psi_{\Omega}^{mic}]/\partial \epsilon_D = 2G\epsilon_D$, the mean value of σ_D is zero as well. Note, however, that as soon as any nonlinear behavior is considered this condition is immediately violated except for very few special cases (Carol et al., 2001).

With regard to the traditional formulation of microplane model, difference (b) may be interpreted in the sense that, while total normal stress σ_N was always

conjugate to ϵ_N , its volumetric and deviatoric parts σ_V and σ_D were not necessarily one-to-one conjugates to their corresponding microplane strains ϵ_V and ϵ_D . This could result in spurious dissipation/generation of energy under certain load cycles, as shown in the example of section 5.

It is finally noted that the thermodynamically consistent formula (14) may also be derived from the PVW but only if the contribution of the normal microplane stresses to the virtual work in (5) is rewritten as $\int_{\Omega} [\sigma_V \delta \epsilon_V + \sigma_D \delta \epsilon_D] d\Omega$.

5 EXAMPLE OF SPURIOUS DISSIPATION

To illustrate the problem, consider a model with microplane laws in secant format proposed in (Bažant and Prat, 1988a), which was developed later in a damage format in (Kuhl et al., 1998). In such formulation, the microplane constitutive equations read

$$\begin{aligned} \sigma_V &= [1 - d_V] 3K \epsilon_V \\ \sigma_D &= [1 - d_D] 2G \epsilon_D \\ \sigma_T &= [1 - d_T] 2G \epsilon_T \end{aligned} \quad (20a,b,c)$$

where d_V , d_D and d_T are scalar damage parameters, initially set to zero. The simplest assumption is that d_V depends only on the history of ϵ_V , d_D depends only on the history of ϵ_D , and d_T only on the history of $|\epsilon_T|$. Parameter d_V is then the same on all microplanes while d_D and d_T in general vary as functions of the microplane orientation.

Substituting the microplane laws into the traditional stress-evaluation formula (8) and using (2), we obtain:

$$\begin{aligned} \boldsymbol{\sigma} &= [1 - d_V] 3K \mathbf{I} \epsilon_V + \frac{3G}{\pi} \int_{\Omega} [1 - d_D] \mathbf{N} \epsilon_D d\Omega + \\ &\quad + \frac{3G}{\pi} \int_{\Omega} [1 - d_T] \mathbf{T}^T \cdot \boldsymbol{\epsilon}_T d\Omega = \\ &= \left([1 - d_V] K \mathbf{I} \otimes \mathbf{I} + \frac{3G}{\pi} \int_{\Omega} [1 - d_D] \mathbf{N} \otimes \mathbf{D} d\Omega + \right. \\ &\quad \left. \frac{3G}{\pi} \int_{\Omega} [1 - d_T] \mathbf{T}^T \cdot \mathbf{T} d\Omega \right) : \boldsymbol{\epsilon} = \\ &= \mathbf{E} : \boldsymbol{\epsilon} \end{aligned} \quad (21a,b,c)$$

where \mathbf{T}^T satisfies $T_{ijr}^T = T_{rij}$, and

$$\begin{aligned} \mathbf{E} &= [1 - d_V] K \mathbf{I} \otimes \mathbf{I} + \frac{3G}{\pi} \int_{\Omega} [1 - d_D] \mathbf{N} \otimes \mathbf{D} d\Omega + \\ &\quad + \frac{3G}{\pi} \int_{\Omega} [1 - d_T] \mathbf{T}^T \cdot \mathbf{T} d\Omega \end{aligned} \quad (22)$$

is the secant macroscopic stiffness tensor.

Due to the presence of the term including $\mathbf{N} \otimes \mathbf{D}$ the stiffness tensor \mathbf{E} in general does not exhibit major symmetry. Only in the case of isotropic damage, in which $1 - d_D$ is the same for all microplanes, we can take that term out of the integral and taking advantage of the equation (Carol et al., 2001)

$$\int_{\Omega} \mathbf{N} \otimes \mathbf{D} \, d\Omega = \int_{\Omega} \mathbf{D} \otimes \mathbf{D} \, d\Omega \quad (23)$$

recover a symmetric secant stiffness.

The lack of major symmetry would not necessarily be in contradiction to the laws of thermodynamics if it were caused by frictional phenomena involving a unilateral condition. However, this is not the case here. During unloading and reloading below the maximal previously reached strain level, the damage parameters remain constant and the material responds as a linear elastic one with stiffness \mathbf{E} . The lack of major symmetry then implies that no elastic potential can exist, and the total work over a closed cycle is in general not zero. For certain loading cycles, energy is consumed, and for others it is extracted from the material spuriously (without changing the internal variables). A complete example of a specific loading cycle generating/dissipating energy (depending on the load direction) can be found in (Carol et al., 2001).

6 CONCLUDING REMARKS

A new, simple, thermodynamically-consistent framework for the formulation of microplane models has been described. The main assumption is that the macroscopic free energy may be obtained as the integral over all microplane orientations of a microplane free energy function, which depends on the microplane strains and the internal variables. This assumption does not contradict most of the early versions of microplane models for concrete with and without split of normal components (M1 and M2), but leaves out the more recent M3 and M4 models, for which the free energy of the various microplanes may not be written in a decoupled form.

The new formulation leads to a consistent definition of the microplane stresses which are conjugate to the microplane strains, and to the integral form of the micro-macro equilibrium equation which applies to those stresses.

A comparison with the previous microplane models not precluded by the new formulation leads to the conclusion that, while the earliest model without split (M1) was correct, the following version of microplane model with the split of normal components (M2) cannot be guaranteed to be thermodynamically consistent.

In that case, microplane stresses σ_V and σ_D are not work-conjugates to their strain counterparts ϵ_V and ϵ_D . The integral micro-macro relation for stresses does not coincide either with the one obtained from the thermodynamic derivation, and the model cannot be guaranteed to be free of spurious dissipation or generation of energy.

Further developments of the proposed framework by applying standard concepts such as the Coleman method and Clausius-Duhem inequality at both microplane and macroscopic levels, as well as some simple example models incorporating damage and plasticity concepts may be found in (Kuhl et al., 2001). Exploitation of this new framework for a general formulation of microplane models at finite strain is the object of a current research effort by the authors.

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