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How to enforce non-negative energy dissipation in microplane and other constitutive models for softening damage, plasticity and friction

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ABSTRACT: Material constitutive models must be formulated in such a way that the energy dissipation can never become negative during deformation increments within the range of intended applications. However, checking this obvious thermodynamic condition for complex models such as the microplane model (e.g. Bažant 1984, Bažant and Caner 2000) is not a trivial task and is often complicated by incomplete, ambiguous or unrealistic definition of unloading or reloading. Ignoring such incompleteness may result in a misleading appraisal of the performance of the model for monotonic loading. Here an attempt is made to clarify this problem and suggest a simple way of ensuring non-negativity of dissipation. The condition of non-negative increment of energy dissipation density at each continuum point of each loading step in an incremental computation of structural response is formulated in the context of the microplane model. If a negative dissipation is detected, the trial constitutive law is adjusted by a change in the unloading compliance and, if necessary, also by a change of the final stresses in the loading step. This adjustment represents an integral part of the constitutive law and must be considered in calibrating the model by test data. A similar correction is then formulated for tensorial constitutive models. Further it is pointed out that without specifying the unloading behavior, the dissipation inequality cannot be checked, and that by modifying the hypothesis about unloading, negative dissipation increments can be changed to positive. Thus the dissipation inequality is not too important for constitutive models intended only for monotonically applied loads, provided that unloading for the individual microplane strain components either does not occur or occurs only rarely. The dissipation check is very sensitive to the assumption about unloading, and so it makes no sense to get alarmed by a check of the dissipation inequality for constitutive models whose characterization of unloading is known to be simplistic and unrealistic. But for models intended for cyclic loading, this inequality is, of course, an essential criterion of soundness.

1 INTRODUCTION AND DEFINITIONS

In constitutive models intended to describe damage such as distributed microcracking, the elastic stiffness tensor E_{ijkl} as well as is inverse, the compliance tensor C_{ijkl}, is variable (the subscripts refer to Cartesian coordinates $x_i, i = 1, 2, 3$). Under isothermal conditions, the rate of energy dissipation density, $\dot{D}$, is the rate of work of stress tensor σ_{ij} on the rate of strain tensor, $\dot{\epsilon}_{ij}$, minus the rate of change of the stored strain energy U (e.g., Jirásek and Bažant 2002). Thus we have:

$$\dot{D} = \sigma_{ij}\dot{\epsilon}_{ij} - \dot{U} \geq 0 \tag{1}$$

where the superior dots denote the derivatives with respect to time t. Two expressions for U may be considered:

$$U = \frac{1}{2}\epsilon^{e}_{ij}E_{ijkl}\epsilon^{e}_{kl} \tag{2}$$

or, equivalently,

$$U = \frac{1}{2}\sigma_{ij}C_{ijkl}\sigma_{kl} \tag{3}$$

where ϵ^{e} = elastic part of strain tensor. Under isothermal conditions, the former represents the Helmholtz free energy density (or isothermal potential energy), and the latter the Gibbs free energy density (or the isothermal complementary energy).

In some works (e.g., Lubliner 2006), Eq. (1) is enhanced by the term $\Sigma_k\, Q_k\, \theta_k$ where θ_k are internal variables and Q_k are the thermodynamically associated internal forces. However, such an enhancement is appropriate only if some physically different types of work, e.g., the work of a muscle driven by chemical energy (Lubliner 2006), are present, which is not the case considered here. Alternatively, the internal forces may be considered as a partial or full replacement of the term $\sigma_{ij}\dot{\epsilon}_{ij}$; but this is appropriate only if the plastic work itself is described by a set of internal variables (Rice 1970). Otherwise the internal variables do not belong into Eq. (1).

2 DISSIPATION IN DAMAGE MODELS

The contribution to U from the plane of stress σ_{ij} versus strain ϵ_{ij} is represented by the cross-hatched triangular areas in Fig. 1(a). Generally, the unloading from a damaged state cannot terminate at the origin. An exception is the special case of an isotropic damage model, for which unloading terminates at the initial stress-free state for which the residual stresses σ^0_{ij} vanish (which corresponds to perfect closing of all microcracks). In this special case Eqs. (2) and (3) may be written as

$$U = \frac{1-\omega}{2}\epsilon^e_{ij}E^0_{ijkl}\epsilon^e_{kl} \tag{4}$$

or

$$U = \frac{1}{2(1-\omega)}\sigma_{ij}C^0_{ijkl}\sigma_{kl} \tag{5}$$

where E^0_{ijkl} and C^0_{ijkl} are the fourth-order tensors of the initial elastic moduli and compliances.

In real materials, though, plastic frictional deformations always accompany microcracking. The consequence is that the material cannot unload to its initial stress-free state and, after unloading of the material, nonzero residual stresses σ^0_{ij} or strains ϵ^0_{ij} are always locked in. Thus U, as given by Eq. (2) or (3), represents the triangular area cross-hatched in Fig. 1(a).

Consider now the one-dimensional case, representing the uniaxial loading, or one pair of tensorial components, or one component of the microplane stress or strain vector. The increment of energy dissipation density is, according to Eq. (1)

$$\dot{D} = \sigma\dot{\epsilon} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}C\sigma^2\right) = \sigma(\dot{\epsilon} - C\dot{\sigma}) - \frac{1}{2}\sigma\dot{C}\sigma \tag{6}$$

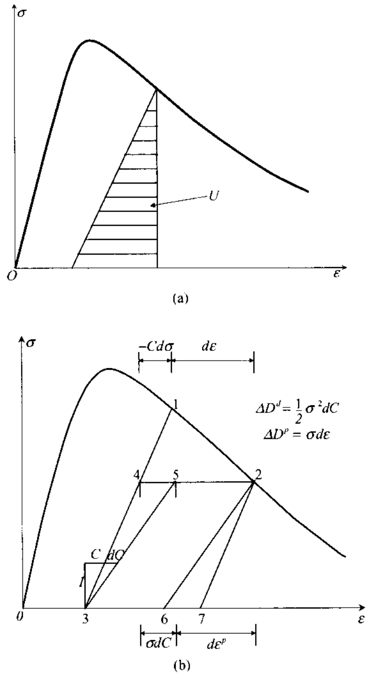

Figure 1. Areas representing various parts of work or energy dissipation in the one-dimensional case.

where σ, ϵ and C are the stress, strain and compliance. This equation may be rewritten as

$$\dot{D} = \frac{1}{2}\sigma\dot{C}\sigma + \sigma(\dot{\epsilon} - C\dot{\sigma} - \dot{C}\sigma) = \underbrace{\frac{1}{2}\sigma\dot{C}\sigma}_{\dot{D}^{\mathrm{d}}} + \underbrace{\sigma\dot{\epsilon}^{\mathrm{p}}}_{\dot{D}^{\mathrm{p}}} \tag{7}$$

where we have set $\dot{\epsilon}^p = \dot{\epsilon} - C\dot{\sigma} - \dot{C}\sigma$. Eq. (7) has a simple geometrical interpretation in the one-dimensional stress-strain diagram of Fig. 1(b) depicting an infinitesimal loading increment from point 1 to point 2 for the case of post-peak softening damage: The total energy dissipation increment $\dot{D}$ is represented by the area 42634 which is first-order small in terms of strain increment $\Delta\epsilon$ (cf. Bažant 1996), by subtracting the area of the triangular 2672 (i.e., the change of elastic strain energy, $\dot{U}$) from the area of parallelogram 42734 (i.e., the rate of work of stress, $\sigma\dot{\epsilon}$). The triangular area 1241 is second-order small and thus negligible in comparison. The first term of Eq. (7), $\dot{D}^d$, is equal to triangular area 4534 and represents the energy dissipation by damage alone. The second term, $\dot{D}^p$, corresponds to parallelogram area 52635 and represents the frictional-plastic energy dissipation.

The special case in which the second term vanishes for all load increments (i.e., area 52635 = 0, or length 36 = 0) represents the unloading to the origin, for which there is no plastic-frictional energy dissipation. In concrete, however, the plastic-frictional deformation in the fracture process zone generally dissipates more energy than the microcracking (Bažant 1996).

3 ENFORCING NON-NEGATIVE DISSIPATION IN MICROPLANE MODEL

The microplane model was conceived as a counterpart of the classical Taylor model (Taylor 1938, Batdorf and Budianski 1949), permitting the softening to be modeled. In this model, the total energy density dissipated, D, is the sum of the energies dissipated on all the microplanes. The contribution to D from each microplane can be positive or negative but the sum (or integral) of all these contributions must be non-negative. In the fitting of complex multiaxial data for complex loading histories, such as those for concrete, it is often not easy to ensure a priori that the dissipation inequality be always satisfied.

In microplane model M1 (Bažant and Oh 1986), in which only the normal and shear components of the stress and strain vectors on the microplanes are considered, the virtual work equation is given by

$$\delta W = \frac{3}{2\pi}\int_{\Omega}(\sigma_N \delta\epsilon_N + \boldsymbol{\sigma}_T \cdot \delta\boldsymbol{\epsilon}_T)\, d\Omega \tag{8}$$

and the energy dissipation density is

$$\dot{D} = \frac{3}{2\pi}\int_{\Omega}(\sigma_N \dot{D}\epsilon_N + \boldsymbol{\sigma}_T \cdot \dot{\epsilon}_T) d\Omega - \dot{U} \geq 0 \tag{9}$$

Therefore, it is proposed to make in each small loading step from time t_i to time t_j the following correction to the a priori assumed constitutive law: If a negative increment of the total ΔD is detected, the compliance increment or the stress increment, or both, are reset so as to be make ΔD non-negative. To this end, one may introduce, for an explicit finite element program, unknown parameters α and β as follows:

$$\begin{aligned}\Delta D = \frac{3}{2\pi}\int_{\Omega}\frac{1}{2}\Big[&(\beta\sigma_{N,j} + \sigma_{N,i})(\epsilon_{N,j} - \epsilon_{N,i}) \\ &+ (\beta\boldsymbol{\sigma}_{T,j} + \boldsymbol{\sigma}_{T,i})(\epsilon_{T,j} - \epsilon_{T,i}) \\ &- (\alpha C_{N,j}\cdot\beta\sigma^2_{N,j} - \alpha C_{N,i}\cdot\beta\boldsymbol{\sigma}^2_{T,i}) \\ &- (\alpha C_{T,j}\cdot\beta\boldsymbol{\sigma}^2_{T,j} - \alpha C_{T,i}\cdot\beta\boldsymbol{\sigma}^2_{T,i})\Big]\, d\Omega\end{aligned} \tag{10}$$

This equation represents a summation of the contributions defined by Eq. (7) over all the microplane stress components and all the microplanes. Subscripts i and j label the beginning and end of the loading step in which the strain increments are prescribed; subscripts N and T label the microplane normal and shear components; C_N and C_T are the normal and shear compliances specified by the microplane constitutive law; and σ_N and σ_T represent the normal component and the shear stress vector on each microplane. The use of averages such as $\frac{1}{2}(\beta\sigma_{N,j} + \sigma_{N,i})$ makes Eq. (6) a central difference approximation. In computations, the integral over the unit hemisphere surface Ω is approximated by a summation based on an optimal Gaussian integration formula.

At the end of computation of each small loading step (t_i, t_j), one evaluates ΔD from Eq. (8) assuming that $\alpha = \beta = 1$. If ΔD, no change is made. But if ΔD is detected, one solves a new value of α from the condition

$$\Delta D = 0 \tag{11}$$

still assuming that $\beta = 1$. This means that the unloading compliances are changed from C_N and C_T are changed to αC_N and αC_T.

However, if the new αC_N or new αC_T is greater than the initial elastic compliance for one or more microplanes (which is inadmissible), a revised α and a new β must be obtained from the condition that both $\alpha C_N - C_N^0 \geq 0$ and $\alpha C_T - C_T^0 \geq 0$ for all the microplane while $\Delta D > 0$. The minimum value of β satisfying these inequality conditions should be used, which is achieved by decreasing β in small steps until all the aforementioned inequalities are satsified.

The α and β corrections are implemented at each integration point of each finite element at the end of calculation of each loading step. These corrections, which adjust the unloading moduli and the final microplane stresses, must be regarded as part of the microplane constitutive law.

Thus the initially assumed constitutive law of the microplane model represents only a trial constitutive law, and the α and β corrections based on Eq. (10) complete the definition of the constitute law. These corrections must, of course, be considered in data fitting and calibration of the microplane constitutive model.

4 ADAPTATION TO MICROPLANE MODEL WITH VOLUMETRIC-DEVIATORIC SPLIT

In microplane models M2 (Bažant and Prat 1988), M3 and M4 (Bažant et al. 2000), the normal strain and stress on the microplanes are split into the volumetric and deviatoric components. Upon substitution of the relations $\epsilon_N = \epsilon_V + \epsilon_D$ and $\sigma_N = \sigma_V + \sigma_D$ Eq. (10), based on the principle of virtual work, becomes

$$\delta W = \underbrace{\frac{3}{2\pi}\int_\Omega (\sigma_V \delta\epsilon_V + \sigma_D \delta\epsilon_D + \sigma_T \cdot \delta\epsilon_T)\, d\Omega}_{\delta W_m} + \underbrace{\frac{3}{2\pi}\int_\Omega \sigma_D \delta\epsilon_V d\Omega}_{\delta W_{VD}} \tag{12}$$

The microplane volumetric and deviatoric stress components are expressed separately in terms of the corresponding microplane strains ϵ_V and ϵ_D;

$$\sigma_V = f_V(\epsilon_V), \quad \sigma_D = f_D(\epsilon_D) \tag{13}$$

In microplane model M2, functions f_V and f_D are formulated as a microplane damage model, whereas in microplane models M3 and M4, these functions are implied by the strain and stress boundaries. In model M4, they are further constrained by the condition:

$$\sigma_V = \min\left(\frac{1}{2\pi}\int_\Omega \sigma_N d\Omega, f_V(\epsilon_V)\right) \tag{14}$$

In M4 (Bažant et al. 2000), only the first term, δW_m (Eq. 12), is considered in the virtual work equation, i.e.,

$$\delta W = \frac{3}{2\pi}\int_\Omega (\sigma_V \delta\epsilon_V + \sigma_D \delta\epsilon_D + \boldsymbol{\sigma}_T \cdot \delta\epsilon_T)\, d\Omega \tag{15}$$

The microplane volumetric stress σ_V is defined by the virtual work equation

$$\frac{\sigma_{kk}}{3}\delta_{mm} = \frac{3}{2\pi}\int_\Omega \sigma_V \epsilon_V d\Omega \tag{16}$$

which leads to $\sigma_V = \sigma_{kk}/3$. This is an equilibrium definition of microplane volumetric stress σ_V. As one can see from Eqs. (8), (12), (15) and (16), the stress tensor σ_{ij}, microplane normal stress σ_N and shear stress vector $\boldsymbol{\sigma}_T$ are an equilibrium system of forces, and can thus be used to calculate the first-order work and energy dissipation, which underlies Eq. (10).

One can, of course, introduce a postulate that the stress tensor σ_{ij}, the microplane volumetric stress σ_N, the deviatoric stress σ_D and the shear stress vector $\boldsymbol{\sigma}_T$, are also an equilibrium system of forces, but such a postulate is not consistent with the calculation of the dissipated work.

Therefore, the energy dissipation $\dot{D}$ in microplane models M2, M3 and M4 should be expressed as

$$\dot{D} = \dot{W} - \dot{U} = \underbrace{\dot{W}_m - \dot{U}}_{\dot{D}_m} + \dot{W}_{VD} \tag{17}$$

It is easy to ensure that $\dot{D}_m = \dot{W}_m - \dot{U} \geq 0$. Therefore, it is only necessary to enforce the condition $\dot{W}_{VD} \geq 0$, i.e.,

$$\dot{W}_{VD} = \frac{3}{2\pi}\int_\Omega (\sigma_D \dot{\epsilon}_V)\, d\Omega = 3\bar{\sigma}_D \dot{\epsilon}_V \geq 0 \tag{18}$$

where $\bar{\sigma}_D$ is the average deviatoric stress over all microplanes

$$\bar{\sigma}_D = \frac{1}{2\pi}\int_\Omega \sigma_D\, d\Omega \tag{19}$$

Condition (18) requires that the sign of the average deviatoric stress $\bar{\sigma}_D$ be the same as that of $\Delta\epsilon_V$. If $\Delta\epsilon_V \geq 0$, the average deviatoric stress $\bar{\sigma}_D$ should be non-negative, i.e., the positive deviatoric stress on the microplanes under deviatoric tension should overall be greater in magnitude than the negative deviatoric stress on those under deviatoric compression. If $\Delta\epsilon_V < 0$, the average deviatoric stress $\bar{\sigma}_D$ should be negative (this property is necessary to describe the di-latancy exhibited under uniaxial and biaxial compression loadings).

5 ENFORCING NON-NEGATIVE DISSIPATION IN TENSORIAL FORM OF CONSTITUTIVE MODEL

For a constitutive law in the classical tensorial form, the increment of energy dissipation density loading step (t_r, t_s) is given by

$$\Delta D = \frac{1}{2}(\boldsymbol{\sigma}_r + \boldsymbol{\sigma}_s) : \Delta\epsilon - \frac{1}{2}\beta\boldsymbol{\sigma}_s : \alpha\mathbb{C}_s : \beta\boldsymbol{\sigma}_s + \frac{1}{2}\boldsymbol{\sigma}_r : \mathbb{C}_r : \boldsymbol{\sigma}_r \geq 0 \tag{20}$$

(now $\boldsymbol{\sigma}, \epsilon$ and $\mathbb{C}$ are all tensors). At the end of the computation of each load step, the procedure is as follows:

- Set first $\alpha = \beta = 1$.
- Check if $\Delta D \geq 0$.
- If satisfied, go to the next integration point. If not, find α from the condition $\Delta D = 0$, which amounts to adjusting the constitutive law for damage.

- But if $\frac{1}{2}\boldsymbol{\sigma}_s : \alpha\mathbb{C}_s : \boldsymbol{\sigma}_s < \frac{1}{2}\boldsymbol{\sigma}_s : \mathbb{C}^0 : \boldsymbol{\sigma}_s$, then reset also β so that, in this condition, '$<$' be changed to '$=$' while $\Delta D = 0$ would remain valid.

6 DISCUSSION

The material damage is in constitutive models often described by a reduction of secant compliance, with an unloading path that points to the origin. But often the unloading behavior might be considered beyond the scope of the model, or the unloading might be expected to follow some simple rule different from secant compliance, for example, the initial compliance or some nonlinear unloading rule.

This point needs to be realized in interpreting the example in Table 1 of Carol et al. (2001), which examined microplane model M2 (Bažant and Prat 1988). In this model, all the inelastic behavior is described by a variation of the secant compliance.

Under the hypothesis that unloading follows the secant compliance, Carol et al. (2001) demonstrated for M2 the existence of a loading cycle with negative energy dissipation. However, if the unloading is assumed to follow the initial compliance, the dissipation during this cycle would be positive, and so it would be for a certain range of intermediate unloading rules. The hypothesis of secant unloading was not followed in subsequent extension of model M2 for unloading and cyclic loading, and was replaced by a curved unloading path (Ožbolt and Bažant 1992).

It may thus be observed that, for constitutive models not intended to describe unloading, the dissipation inequality might not necessarily be an important consideration. If the loads are applied monotonically, the strains on the microplanes, of course, might not necessarily evolve monotonically, but it many application they do so, at least approximately.

On the other hand, for constitutive models intended to cover significant unloading and hysteretic loops, the dissipation inequality is an essential check.

Finally note that the checks for stability and bifurcation of the equilibrium path are a different matter. They deal with the positivity or vanishing of the second-order-small triangular area 1421 in Fig. 1(b), which is irrelevant for the dissipation inequality.

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