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MICROMECHANICALLY BASED CONSTITUTIVE MODELING OF CRYSTALLINE MATERIALS

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Abstract—Overall stress and strain rates for crystalline materials with an "internal structure" are considered. It has been shown that these measures are related to some kinematical constraints which govern the evolution of the internal structure such as development of slip or shear bands within grains and on grain boundaries, growth of voids or microcracks. The overall stress and strain rates provide a framework for a micromechanically based constitutive modeling.

1. INTRODUCTION

The objective of the paper is to focus on a micromechanically based constitutive description for crystalline materials. The approach is based on Taylor's averaging theorem (Taylor, 1938) in the form proposed by Bishop and Hill (1951), and subsequently generalized by Hill (1972). The theorem provides a suitable tool for studying incremental constitutive relations including the evolution of the internal structure for crystalline materials. Based on the methodology, Hill and Rice (1972) have concluded that "what is commonly called 'plastic' deformation is not generally the resultant of the slip alone". Subsequently, Asaro and Rice (1977) specified certain Schmid stress rates depending on the prediction of lattice distortion. Furthermore, Asaro (1983), Nemat-Nasser (1983), and Nemat-Nasser and Iwakuma (1985) have utilized this framework in constructing incremental relations for crystalline materials.

In this paper, the averaging theorem is adopted in a modified form (Zubelewicz, 1989) in which overall stress rates and plastic velocity gradients replace the traditionally used pairs of stress, strains or stress, velocity gradients. The weight of the constitutive modeling is transferred to the lower microscopic level of material. The matrix is assumed to be linear elastic, plastic sliding is considered in a power-law form, and microcracking, hardening and recovery parameters are incorporated into the evolution of the internal structure of the material.

2. TRANSITION FROM MICRO- TO MACROLEVEL

The current internal structure, if representative for crystalline materials, must involve a sufficient number of slip systems, grain boundaries, and other microstructural features. The elastic gradient of deformation $\mathbf{F}^*$ and the Cauchy stress $\boldsymbol{\sigma}$ are assumed to be smeared uniformly over the elastic matrix; they do not differ from grain to grain at the characteristic volume δV. Inelastic behavior, such as sliding, void growth, microcracking, is referred to the active discontinuity planes, which are defined by the current local orthogonal systems $(\mathbf{n}^\alpha, \mathbf{s}^\alpha, \mathbf{m}^\alpha)$ and by the fraction areas δS^α. The unit vectors $\mathbf{n}^\alpha$ and $\mathbf{s}^\alpha$ indicate normal and slip directions, the unit lateral vector $\mathbf{m}^\alpha$ supplements the local coordinate system, and together they all satisfy the identity equation

$$\mathbf{I} = \mathbf{n}^\alpha\mathbf{n}^\alpha + \mathbf{s}^\alpha\mathbf{s}^\alpha + \mathbf{m}^\alpha\mathbf{m}^\alpha. \tag{1}$$

The overall properties of the material are referred to a characteristic volume, which is a representative constant volume δV.

An evolution of the internal structure is effected by a rotation of the local systems $(\mathbf{n}^\alpha, \mathbf{s}^\alpha, \mathbf{m}^\alpha)$

$$\begin{Bmatrix}\dot{\mathbf{n}}^\alpha\\ \dot{\mathbf{s}}^\alpha\\ \dot{\mathbf{m}}^\alpha\end{Bmatrix} = \dot{\boldsymbol{\Omega}}^\alpha\begin{Bmatrix}\mathbf{n}^\alpha\\ \mathbf{s}^\alpha\\ \mathbf{m}^\alpha\end{Bmatrix}. \tag{2}$$

At the current configuration of the internal structure the coordinate systems should remain orthogonal with unit vectors; this characterization implies the additional conditions:

$$\begin{aligned}\dot{\mathbf{n}}^\alpha\cdot\mathbf{n}^\alpha &= 0\\ \dot{\mathbf{s}}^\alpha\cdot\mathbf{s}^\alpha &= 0\\ \dot{\mathbf{m}}^\alpha\cdot\mathbf{m}^\alpha &= 0\end{aligned} \tag{3a}$$

$$(\mathbf{n}^\alpha\mathbf{n}^\alpha+\mathbf{s}^\alpha\mathbf{s}^\alpha+\mathbf{m}^\alpha\mathbf{m}^\alpha)^{\cdot} = 0. \tag{3b}$$

When making use of the geometrical conditions (3), the components $\dot{\boldsymbol{\Omega}}^\alpha$, which are relative to the basis $(\mathbf{n}^\alpha, \mathbf{s}^\alpha, \mathbf{m}^\alpha)$, can be given in terms of the three independent functions $\dot{\zeta}_1^\alpha$, $\dot{\zeta}_2^\alpha$ and $\dot{\zeta}_3^\alpha$ as

$$\dot{\boldsymbol{\Omega}}^\alpha = \begin{vmatrix}0 & \dot{\zeta}_1^\alpha & \dot{\zeta}_2^\alpha\\ -\dot{\zeta}_1^\alpha & 0 & \dot{\zeta}_3^\alpha\\ -\dot{\zeta}_2^\alpha & -\dot{\zeta}_3^\alpha & 0\end{vmatrix}. \tag{4}$$

The functions are specified by decomposing them into an elastic and plastic portion as

$$\begin{aligned}\dot{\zeta}_1^\alpha &= \mathbf{n}^\alpha\cdot\boldsymbol{\omega}^*\cdot\mathbf{s}^\alpha+\dot{\zeta}_0^\alpha\\ \dot{\zeta}_2^\alpha &= \mathbf{n}^\alpha\cdot\boldsymbol{\omega}^*\cdot\mathbf{m}^\alpha\\ \dot{\zeta}_3^\alpha &= \mathbf{m}^\alpha\cdot\boldsymbol{\omega}^*\cdot\mathbf{s}^\alpha\end{aligned} \tag{5}$$

in which the viscous-plastic rotation $\dot{\zeta}_0^\alpha$ occurs at the planes $(\mathbf{n}^\alpha, \mathbf{s}^\alpha)$, and $\boldsymbol{\omega}^*$ is the elastic spin. Furthermore, by this means the change of the fraction area δS^α, which in an average sense corresponds to microcracking, void growth, and an elastic distortion, is taken into account. Then

$$\delta\dot{S}^\alpha = (\dot{\eta}^\alpha/\eta^\alpha)\,\delta S^\alpha \tag{6}$$

and the function η^α is specified as

$$\eta^\alpha = (\rho_0^*/\rho^*)\eta_0^\alpha \tag{7}$$

where, ρ_0^* and ρ^* are the initial and the current densities of the elastic matrix and are selected to each other as $\rho_0^* = (\det \mathbf{F}^*)\rho^*$. Functions η_0^α are proposed in a multiplicative form $\eta_0^\alpha = \eta_D^\alpha\cdot\eta_H^\alpha\cdot\eta_R^\alpha$, where η_D^α, η_H^α and η_R^α are the damage, hardening and recovery functions, respectively.

The transition rule from the micro- to macrolevel is based on the virtual work principle in the form

$$\dot{\boldsymbol{\sigma}}^{ov} : (\mathbf{L}-\mathbf{L}^*)\,\delta V = \sum_{\alpha=1}^{N}(\mathbf{s}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{n}^\alpha\,\delta S^\alpha)^{\cdot}\,\dot{\gamma}^\alpha \tag{8}$$

where $\boldsymbol{\sigma}^{ov}$ is the overall stress smeared over the characteristic volume δV of the material. The overall kinematically admissible plastic velocity gradient $\mathbf{L}^p = \mathbf{L}-\mathbf{L}^*$ is given as

$$\mathbf{L}^p = \frac{1}{\delta V}\sum_{\alpha=1}^{N}(\mathbf{s}^\alpha\mathbf{n}^\alpha)\dot{\gamma}^\alpha\,\delta S_0^\alpha \tag{9}$$

and is the summation of the plastic sliding from all the "N" active slip planes. The term ($\dot{\gamma}^\alpha\delta S_0^\alpha/\delta V$) represents the usually known nondimensional sliding. The micro–macro transition rule (8) is placed at the current state of the internal structure of the material. It can be transformed into any other reference state, hence the rate of the shear force $(\mathbf{s}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{n}^\alpha\,\delta S^\alpha)^{\cdot}$ and the rate of plastic sliding $\dot{\gamma}^\alpha$ may vary with the change of the reference frame, but the product, the overall plastic dissipation ($\boldsymbol{\sigma}^{m}:\mathbf{L}^p$) remains constant.

The evolution equations (2–7), when substituted into the virtual work principle (8), become

$$\dot{\boldsymbol{\sigma}}^{m}:\mathbf{L}^p = \sum_{\alpha=1}^{N}\eta^\alpha\left\{\mathbf{s}^\alpha\cdot\left[\dot{\boldsymbol{\sigma}}-\boldsymbol{\omega}^*\boldsymbol{\sigma}+\boldsymbol{\sigma}\boldsymbol{\omega}^*+\mathrm{tr}\,(\mathbf{L}^*)\boldsymbol{\sigma}+\frac{\dot{\eta}_0^\alpha}{\eta_0^\alpha}\boldsymbol{\sigma}\right]\cdot\mathbf{n}^\alpha\right.$$
$$\left.-\dot{\zeta}_0^\alpha(\mathbf{n}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{n}^\alpha-\mathbf{s}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{s}^\alpha)\right\}\dot{\gamma}^\alpha\,\delta S_0^\alpha/\delta V. \tag{10}$$

Although the shear stress ($\mathbf{s}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{n}^\alpha$) can be considered as the maximum shear stress at each α-slip plane, the stress magnitude is not necessarily maximum at the plane ($\mathbf{n}^\alpha,\mathbf{s}^\alpha$). The angle of deviation ζ_0^α from the direction of the maximum shear stress is characteristic for crystalline materials and is given as

$$\mu^\alpha = \tan\,(\pi/2\mp 2\zeta_0^\alpha) = \frac{-2\mathbf{s}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{n}^\alpha}{\mathbf{n}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{n}^\alpha-\mathbf{s}^\alpha\cdot\boldsymbol{\sigma}\cdot\mathbf{s}^\alpha}. \tag{11}$$

The deviation disappears ($\zeta_0^\alpha=0$) when $\boldsymbol{\sigma}:(\mathbf{n}^\alpha\mathbf{n}^\alpha-\mathbf{s}^\alpha\mathbf{s}^\alpha)=0$. Substituting (11) into (10) gives

$$\dot{\boldsymbol{\sigma}}^{m}:\mathbf{L}^p = \sum_{\alpha=1}^{N}\eta_0^\alpha\left[\dot{\boldsymbol{\tau}}^*+\left(\frac{2\dot{\zeta}_0^\alpha}{\mu^\alpha}+\frac{\dot{\eta}_0^\alpha}{\eta_0^\alpha}\right)\boldsymbol{\tau}^*\right]:[(\mathbf{s}^\alpha\mathbf{n}^\alpha)\dot{\gamma}^\alpha\,\delta S^\alpha/\delta V] \tag{12}$$

where the stress rate $\dot{\boldsymbol{\tau}}^*$ is the Jaumann derivative of the Kirchhoff stress corotational with the elastic spin $\boldsymbol{\omega}^*$. For simplicity, the evolution functions ζ_0^α and η_0^α are assumed to be identical for the all α-active planes $\zeta_0^\alpha=\zeta_0$, $\eta_0^\alpha=\eta_0$, $\mu^\alpha=\mu$ and they are projected onto the average directions $\langle\mathbf{n}^\alpha\rangle$ and $\langle\mathbf{s}^\alpha\rangle$. Substituting for $\mathbf{L}^p$ from (9) and using the micro–macro transition rule (12)

$$\dot{\boldsymbol{\sigma}}^{m} = \eta_0\left[\dot{\boldsymbol{\tau}}^*+\left(\frac{2\dot{\zeta}_0}{\mu}+\frac{\dot{\eta}_0}{\eta_0}\right)\boldsymbol{\tau}^*\right]. \tag{13}$$

At the current configuration of the internal structure, the Cauchy and the Kirchhoff stresses are identical. In general, the parameters ζ_0 and η_0 are dependent on the size of the characteristic volume δV, and on the average directions $\langle n^\alpha\rangle$ and $\langle s^\alpha\rangle$, so that they describe the nonlocal properties of the materials.

3. CONSTITUTIVE RELATIONS

In this approach constitutive assumptions are postulated based on the microscopic level of material behavior. Moreover, the evolution of the internal structure, if correctly predicted, will allow the description of material nonlinearities such as kinematical structural hardening and softening due to rotation of the active planes, hardening-recovery and damage of the material due to the change of the areas δS^α. These nonlinearities are imposed on the constitutive description for components of the structure of the material.

First, one may presume that the matrix remains linear elastic, so that the Kirchhoff stress rate $\dot{\boldsymbol{\tau}}^*$ and the rate of the elastic deformation $\mathbf{D}^* = (\mathbf{L}^* + \mathbf{L}^{*T})/2$ obey the relation

$$\dot{\boldsymbol{\tau}}^* = \mathbf{E} : \mathbf{D}^* \tag{14}$$

where $\mathbf{E}$ is the elastic tensor. Furthermore, for materials such as lead-based alloys, the plastic velocity gradient $\mathbf{L}^p$ is found as

$$\mathbf{L}^p = \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} H_{\alpha\beta}^{-1}[(\mathbf{s}^\beta \mathbf{n}^\beta)(\dot{\tau}_n^\beta + k_{\alpha\beta}\tau_n^\beta)] \tag{15}$$

where $H_{\alpha\beta}^{-1}$ and $k_{\alpha\beta}$ are material functions. As has been suggested by Asaro and Rice (1977) rate of shear stress is equal, $\dot{\tau}_n^\beta = \mathbf{s}^\beta \cdot \dot{\boldsymbol{\tau}}^* \cdot \mathbf{n}^\beta$ and the rate of normal stress $\dot{\sigma}_n^\beta = \mathbf{n}^\beta \cdot \dot{\boldsymbol{\tau}}^* \cdot \mathbf{n}^\beta$. When no coupling between the slip systems is assumed, the matrices $H_{\alpha\beta}^{-1}$, $k_{\alpha\beta}$ are diagonal, and then

$$\mathbf{L}^p = \sum_{\alpha=1}^{N} \frac{1}{H_{\alpha\alpha}} [(\mathbf{s}^\alpha \mathbf{n}^\alpha)(\dot{\tau}_n^\alpha + k_{\alpha\alpha}\tau_n^\alpha)]. \tag{16}$$

The plastic velocity gradient can be incorporated explicitly into the constitutive relation (14). The plastic deformation rate $\mathbf{D}^p$ is found from

$$\mathbf{D}^p = \mathbf{M} : \dot{\boldsymbol{\tau}}^* + \mathbf{K} : \boldsymbol{\tau}^* \tag{17}$$

where the fourth order tensors $\mathbf{M}$ and $\mathbf{K}$ are symmetric and equal

$$\mathbf{M} = \sum_{\alpha=1}^{N} \left| \frac{1}{H_{\alpha\alpha}} (\mathbf{r}^\alpha \mathbf{r}^\alpha) \right| \tag{18a}$$

$$\mathbf{K} = \sum_{\alpha=1}^{N} \frac{k_{\alpha\alpha}}{H_{\alpha\alpha}} (\mathbf{r}^\alpha \mathbf{r}^\alpha) \tag{18b}$$

where $\mathbf{r}^\alpha = (\mathbf{s}^\alpha \mathbf{n}^\alpha + \mathbf{n}^\alpha \mathbf{s}^\alpha)/2$. When substituting (17) into the relation (14), the constitutive equations on the microlevel take the form

$$\dot{\boldsymbol{\tau}}^* = (\mathbf{E}^{-1} + \mathbf{M})^{-1} : (\mathbf{D} - \mathbf{K} : \boldsymbol{\tau}^*) \tag{19}$$

where the Jaumann rate of the Kirchhoff stress $\dot{\boldsymbol{\tau}}^*$ is given on the microlevel of the material. The rate of the overall stress $\dot{\boldsymbol{\sigma}}^m$ incorporates the elastic distortions of matrix as well as the irreversible evolution of the internal structure of the crystalline material. The constitutive relation (19) and the transition rule (13) make it possible to model the overall behavior of the material, and the relations are found as

$$\dot{\boldsymbol{\sigma}}^m = \eta_0 \left\{ (\mathbf{E}^{-1} + \mathbf{M})^{-1} : \mathbf{D} + \left[\left(\frac{2\dot{\zeta}_0}{\mu} + \frac{\dot{\eta}_0}{\eta_0} \right) \mathbf{I} - (\mathbf{E}^{-1} + \mathbf{M})^{-1} \mathbf{K} \right] : \boldsymbol{\tau}^* \right\} \tag{20}$$

in which $\mathbf{I}$ is the identity tensor. Note that at the current configuration of the internal structure $\boldsymbol{\sigma}^m = \eta_0 \boldsymbol{\tau}^*$. The constitutive equation (20) is composed of two terms. The first represents non-viscous elasto-plastic behavior of the crystalline material at the current state of the internal structure. The second term includes the viscous-plastic evolution of the internal structure and the microviscosity of the material itself. The microviscosity is principally addressed to the growth of cavities on grain boundaries (Rice, 1981). Such cavitation influences the local behavior at each active plane, while the global evolution of the average fraction areas δS^α also includes the current hardening-recovery processes and microcracking (fracturing).

The evolution functions η_0 and ζ_0, the initial orientation of the α-active planes, and the material parameters $H_{\alpha\alpha}$, $k_{\alpha\alpha}$, E must be specified for each material separately.

4. CONCLUSIONS

Although the constitutive relations are derived in the framework of Taylor's theory, it is believed they capture the main physics of the processs of single crystals and of polycrystals at an advanced stage of deformation. The derivations provide some important results.

First, even though the plastic hardening on the microlevel of the material contributes to the overall behavior, the second order overall plastic dissipation ($\dot{\sigma}^{or} : \mathbf{L}^p$) given by eqn (12) does not necessarily need to be positive and depends heavily on the evolution of the internal structure described by the parameters ζ_0^α, μ^α, η_0^α. If such softening occurs it is a microstructural induced softening, i.e. due to a dynamic recrystallization.

The micro–macro stress transition rule (13) shows that the rate of the overall stress $\dot{\sigma}^{or}$ varies from the Jaumann rate of the Kirchhoff stress $\dot{\tau}^*$, and at the current configuration of the internal structure both the stresses correspond to each other through the relation $\sigma^{or} = \eta_0\tau^*$.

The overall constitutive relations given in the final form (20) are composed of two terms. The first represents the elasto-plastic properties of the material relative to the η_0 state of hardening-recovery and damage, while the second term describes solely the material and microstructural viscosity including the viscous damage of its internal structure.

Finally, the simplicity of the equations makes them very applicable, especially in studying the advanced damage of crystalline materials during thermomechanical cycling. The constitutive model has already been used successfully by Zubelewicz *et al.* (1988) in studying steady state of cycling of solder materials. The lifetime criteria for solder materials appeared not only to be well curve fitted but also predictive. For strain controlled cycling the formulae suggested that the life of the solders is significantly dependent on the stress versus plastic strain range relation. Subsequently, this finding has been confirmed experimentally.

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REFERENCES

Asaro, R. J. (1983). Crystal plasticity. *J. Appl. Mech.* **50**, 921–934.

Asaro, R. J. and Rice, J. R. (1977). Strain localization in ductile single crystals. *J. Mech. Phys. Solids* **25**, 309–338.

Bishop, J. F. W. and Hill, R. (1951). A theory of the plastic distortion of a polycrystalline aggregate under combined stresses. *Phil. Mag.*, Ser. 7 **42**, 414–427.

Hill, R. (1972). On constitutive macro-variables for heterogeneous solids at finite strain. *Proc. R. Soc. Lond.* **A326**, 131–147.

Hill, R. and Rice, J. R. (1972). Constitutive analysis of elasto-plastic crystals at arbitrary strain. *J. Mech. Phys. Solids* **20**, 401–413.

Nemat-Nasser, S. (1983). Micromechanically based finite plasticity. In *Proc. Symp. Plasticity Today* (Edited by A. Sawczuk). Elsevier, London.

Nemat-Nasser, S. and Iwakuma, T. (1985). Elasto-plastic composites at finite strains. *Int. J. Solids Structures* **21**, 55–65.

Rice, J. R. (1971). Inelastic constitutive relations for solids: an internal-variable theory and its application to metal plasticity. *J. Mech. Phys. Solids* **19**, 433–455.

Rice, J. R. (1981). Constraints on the diffusive cavitation of isolated grain boundary facets in creeping polycrystals. *Acta Metal.* **29**, 675–681.

Taylor, G. I. (1938). Plastic strain in metals. *J. Inst. Metals* **62**, 307–324.

Zubelewicz, A. (1989). Overall stress and strain rates for crystalline and frictional materials. *Int. J. Non-Linear Mech.* Accepted for publication.

Zubelewicz, A., Berriche, R., Keer, L. M. and Fine, M. E. (1988). Lifetime prediction of solder materials. *Proc. ASME Winter Annual Meeting*, Chicago, IL, November 27–December 2. Also *ASME J. Electronic Packaging*. Accepted for publication.