AN INTERFACE MODEL BASED ON DAMAGE COUPLED TO SLIP AND DILATATION

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A constitutive model for material interfaces is presented. The model is based on damage, which is kinetically coupled to plastic (or viscoplastic) slip and dilatation. The constitutive relations are derived from a free energy for the interface surface with internal variables representing inelastic slip and dilatation, mixed hardening and scalar damage. The adopted (quasistatic) yield criterion and potential function are both of the Drucker-Prager type, representing internal friction and dilatancy effects. For the modelling of rate-dependent (including creep) effects, the Duvaut-Lions' formulation of viscoplasticity is adopted. The main application of the interface model is in the context of a mesomechanics analysis of a polycrystalline microstructure.

INTRODUCTION

Degradation and fracture processes occur in engineering materials which may be characterized as predominantly brittle (e.g. ceramics, concrete, powder compacts) or ductile (e.g. metals and alloys, soft geological materials). In both cases the material degradation on the microstructural level may be viewed as the successive evolution of microdefects which are part of the microstructure heterogeneity. To a large extent, such microdefects are located along material *interfaces*.

In this paper, we adopt a thermodynamically consistent framework as a counterpart of continuum damage mechanics, cf. Lemaitre (1), to include a variety of interfacial effects of rate-independent as well as rate-dependent type. This infers that "phenomenological" constitutive laws can be used for the interfacial behavior, regardless of whether such interfaces are truly macroscopic, (e.g. constituting a joint between two bodies) or microscopic (e.g. representing the interfacial contact between grain and matrix in a polycrystalline metal). The model assumes that the interfacial damage is coupled kinetically to inelastic relative slip and dilatation (separation) of the jointed surfaces. That slip is kinetically coupled to such separation, due to the frictional resistance, is important in order to get a sufficiently general generic model framework.

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INTERFACE MODEL

Kinematics

Let us consider an interface in the shape of a band of width δ, that is embedded between two mating bodies. The tangent plane (in a certain point) is defined by the Cartesian coordinates x_2 and x_3, whereas the normal direction is defined by the axis x_1.

As the point of departure, we consider the interface as a continuous medium, that is homogeneous across its thickness, whereby the "interfacial strains" ϵ_{1i} are obtained from the displacement field u_i as[2] $\epsilon_{1i} = \frac{1}{2}(u_{1,i} + u_{i,1})$. Upon introducing the assumption that the normal displacement component has a moderate variation along the band, i.e. $|u_{1,\alpha}| \ll |u_{\alpha,1}|$ and the approximation $u_{i,1} = v_i/\delta$, where v_i is the jump of u_i across the interface, then we obtain the relations

$$\epsilon_{1i} = A_{ij}\frac{v_j}{\delta} \quad \text{with} \quad [A_{ij}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix} \tag{1}$$

Thermodynamic basis

The free energy function ψ (per unit *area* of the interface) will be defined for the interface model, including a scalar damage parameter α. First, we introduce the elastic-plastic decoupling of ψ formally as

$$\psi = \psi^{\mathrm{e}} + \psi^{\mathrm{p}} \tag{2}$$

where ψ^{e} is the elastic part of the free energy, whereas ψ^{p} is the inelastic part. Particularizing the isotropic elastic response for a thin homogeneous layer with thickness δ, by setting $\nu = 0$ and using (1), we may express the elastic part as

$$\psi^{\mathrm{e}} = \frac{1}{2}E'\, v_i^{\mathrm{e}} M_{ik} A_{kj} v_j^{\mathrm{e}} + \frac{1}{2}\delta E\, \epsilon_{\alpha\beta}^{\mathrm{e}} \epsilon_{\alpha\beta}^{\mathrm{e}} \tag{3}$$

where $E' = E/\delta$ (interfacial elastic stiffness), $v_i^{\mathrm{e}} = v_i - v_i^{\mathrm{p}}$, and M_{ij} is defined as

$$[M_{ij}] = \begin{bmatrix} 1 - \mathcal{H}(v_1^{\mathrm{e}})\alpha & 0 & 0 \\ 0 & 1-\alpha & 0 \\ 0 & 0 & 1-\alpha \end{bmatrix} \tag{4}$$

where $\mathcal{H}(\cdot)$ is the Heaviside function. The reason behind this choice is that damage is not supposed to influence on the capability of the interface to sustain a compressive load. We now obtain the constitutive equations for q_i as

$$q_i = \frac{\partial \psi^{\mathrm{e}}}{\partial v_i} = E' M_{ik} A_{kj} v_j^{\mathrm{e}} \tag{5}$$

[2]We use the index convention that Latin letters take the values 1, 2 and 3, whereas Greek characters take the values 2 and 3, if not stated otherwise.

If v_i is purely elastic, i.e. $v_i = v_i^{\mathrm{e}}$, it can be concluded from (1) and the definition of E', that the stresses q_i will be independent of δ. From the CDI, we obtain the damage stress A as

$$A = -\frac{\partial \psi^{\mathrm{e}}}{\partial \alpha} = \frac{1}{2}\mathcal{H}(v_1^{\mathrm{e}})E'(v_1^{\mathrm{e}})^2 + \frac{1}{4}E' v_\alpha^{\mathrm{e}} v_\alpha^{\mathrm{e}} = \frac{1}{2E'}\mathcal{H}(\hat{q}_1)\hat{q}_1^2 + \frac{1}{E'}\hat{q}_\alpha \hat{q}_\alpha \tag{6}$$

To complete the definition of ψ, we need to define the hardening part ψ^{p}. In order to account for mixed isotropic and kinematic hardening, we propose

$$\psi^{\mathrm{p}} = \frac{1}{2}C_{\mathrm{b}}'\beta_i A_{ij}\beta_j + \frac{1}{2}C_{\mathrm{k}}'\kappa^2 \tag{7}$$

where β_i and κ are hardening variables, whereas C_{b}' and C_{k}' are the interfacial hardening moduli, and the corresponding dissipative stresses are defined as

$$b_i = -\frac{\partial \psi^{\mathrm{p}}}{\partial \beta_i} = -C_{\mathrm{b}}' A_{ij}\beta_j\ , \quad k = -\frac{\partial \psi^{\mathrm{p}}}{\partial \kappa} = -C_{\mathrm{k}}'\kappa \tag{8}$$

Clearly, b_i are back-stresses due to kinematic hardening, whereas k is the drag-stress due to isotropic hardening.

Quasistatic slip criterion and plastic potential of Drucker-Prager type

We may express a yield function Φ in the space of interface stresses $(\hat{q}_i, b_i, k)$ and define a convex set $\mathcal{B}$ of quasistatically admissible states. Let us first introduce the reduced (effective) traction vector $\hat{q}_i^{\mathrm{r}} = \hat{q}_i - b_i$. The reduced (effective) normal stress $\hat{\sigma}^{\mathrm{r}}$ and the reduced (effective) shear stress $\hat{\tau}^{\mathrm{r}}$ are defined as

$$\hat{\sigma}^{\mathrm{r}} = \hat{q}_1, \quad \hat{\tau}^{\mathrm{r}} = \sqrt{(\hat{q}_2^{\mathrm{r}})^2 + (\hat{q}_3^{\mathrm{r}})^2} \tag{9}$$

A Drucker-Prager criterion is chosen, and since it is non-smooth (with an apex), the set $\mathcal{B}$ is conveniently defined as $\mathcal{B}(\alpha) = \{(q_i, b_i, k) \mid \Phi^{(1)} \leq 0,\ \Phi^{(2)} \leq 0\}$ where

$$\Phi^{(1)} = \hat{\tau}^{\mathrm{r}} + \mu\hat{\sigma}^{\mathrm{r}} - k - \tau_{\mathrm{f}}, \quad \Phi^{(2)} = -\hat{\tau}^{\mathrm{r}} \tag{10}$$

with μ as the coefficient of internal friction and τ_{f} as the initial flow stress (in simple shear) for the interface. For the purpose of defining the dissipation rules, we also introduce the potential functions $\Phi^{*(1)}$ and $\Phi^{*(2)}$ as

$$\Phi^{*(1)} = \hat{\tau}^{\mathrm{r}} + \mu^*\hat{\sigma}^{\mathrm{r}} - k - \tau_{\mathrm{f}}, \quad \Phi^{*(2)} = -\hat{\tau}^{\mathrm{r}} \tag{11}$$

where $\mu^*(\leq \mu)$ is the dilatancy coefficient.

Constitutive relations

We may express the plastic flow and hardening rules for a non-smooth yield surface (consisting of smooth portions) as

$$\dot{v}_1^{\mathrm{p}} = \dot{\lambda}^{(1)}\frac{1}{1 - \mathcal{H}(\hat{q}_1)\alpha}\mu^*, \quad \dot{v}_\alpha^{\mathrm{p}} = \left(\dot{\lambda}^{(1)} - \dot{\lambda}^{(2)}\right)\frac{1}{1-\alpha}\frac{\hat{q}_\alpha^{\mathrm{r}}}{\hat{\tau}^{\mathrm{r}}} \tag{12}$$

and the hardening rules

$$\dot{\beta}_1 = -\dot{\lambda}^{(1)}\mu^*, \quad \dot{\beta}_\alpha = -\left(\dot{\lambda}^{(1)} - \dot{\lambda}^{(2)}\right)\frac{\hat{q}^{\mathrm{r}}_\alpha}{\hat{\tau}^{\mathrm{r}}}, \quad \dot{\kappa} = -\dot{\lambda}^{(1)} \tag{13}$$

We then propose the interface damage rule as

$$\dot{\alpha} = \dot{v}^{\mathrm{p}}_{\mathrm{e}}\frac{A}{S''(1-\alpha)^m}, \quad \dot{v}^{\mathrm{p}}_{\mathrm{e}} \stackrel{\mathrm{def}}{=} \sqrt{\dot{v}^{\mathrm{p}}_i\dot{v}^{\mathrm{p}}_i} = \sqrt{\left(\mu^*\dot{\lambda}^{(1)}\right)^2 + \left(\dot{\lambda}^{(1)} - \dot{\lambda}^{(2)}\right)^2} \tag{14}$$

where $\dot{v}^{\mathrm{p}}_{\mathrm{e}}$ is the length of $\dot{v}^{\mathrm{p}}_i$. The "damage modulus" $S'(= S''\delta)$ and the exponent m define the rate of damage development.

The viscoplastic flow and hardening rules are expressed in the spirit of Duvaut & Lions and we refer to Cannmo et al (2) for details.

Parameter identification

For given elastic stiffness E (that represents the material in the mating bodies), the stiffness $E' = E/\delta$ of the interface is determined by the *choice* of δ. The hardening moduli C'_{b} and C'_{k}, are related to the "effective" inelastic behavior in *simple shear* (at slow loading) as

$$C'_{\mathrm{b}} = 2(1-r)H', \quad C'_{\mathrm{k}} = [1-(1-r)(2\mu\mu^*+1)]H' \tag{15}$$

where H' is the hardening modulus, and where r is a scalar $(0 \leq r \leq 1)$ that represents the isotropic portion of hardening.

The damage characteristics (in terms of the damage modulus S' and the damage exponent m) are selected via a study of the mechanical dissipation in a suitable loading (deformation) mode. More specifically, these parameters are related to the *total amount of mechanical energy (plastic work)* that is dissipated during the process of completely damaging the interface (until $\alpha = 1$). Apparently, this work corresponds to the fracture energy release in the considered mode. A model calibrated in this fashion will be *dissipation-objective*.

APPLICATION: A POLYCRYSTALLINE MICROSTRUCTURE

The main application of the interface model is in the context of a mesomechanics analysis of a polycrystalline microstructure which may consist of two phases. A preprocessor code, which is based on Voronoi polygonization, is developed for the generation of the microstructure. The grains are either in direct contact (one-phase structure) and bonded to each other via interfaces, or embedded in a contiguous matrix (two-phase structure) and bonded to the matrix via interfaces.

FE-calculations are carried out for a unit cell of the microstructure, whereby the unit cell is defined by the number of grains ($n \times n$) contained in the cell, the area fraction of grain versus matrix, and the interface width parameter δ. The grain size defines the length scale of the microstructure.

Interface parameter study

From the damage rule (14) it follows that the "damage modulus" S' and the exponent m define the rate of damage development. Both parameters have significant influence on the macroscopic behavior of the composite. As shown in Figure 1a it is possible to design this behavior to be either extremely "brittle", referring to a very small value of S', or to be more and more "ductile" by successively increasing the value of S'.

Localization and shear bands

A (12×12)-cell is subjected to monotonic loading. At the peak of the macroscopic stress-strain curve, elastic unloading starts and localization of plastic deformation into a band begins. This localization process continues all through the softening range past peak until the final failure occurs. In Figure 1b, the development of plastic deformation close to final failure is shown. The shear band is inclined somewhere in the range $\theta = 40° - 45°$ to the major principal stress axis. Adopting von Mises plasticity, it can be shown that (for plane strain conditions with $\nu = 0.3$) the critical angle $\theta_{\mathrm{cr}} = 42.5°$. Hence, it may be concluded that the mesomechanics simulation presented here supports the analytical prediction.

Cyclic loading

A typical result of the macroscopic response (under strain control and pure kinematic hardening) is shown in Figure 2a. Due to the development of damage in the interfaces, the elastic stiffness is successively reduced in the following cycles. At the beginning of the sixth cycle the most critical interface reaches the criterion for local failure ($\alpha = 0.99$). Shortly after, several adjacent interfaces also fail, which leads to a significant drop of the macroscopic stress and, finally, macroscopic failure. Hence, the intrinsic behavior of low-cycle fatigue of the unit cell is simulated, and the well-known macroscopic behavior is verified.

Creep behavior

A unit cell is investigated for a constant uniaxial tensile stress. During the creep process, microscopic cavities nucleate and grow on the grain boundaries. The interface damage parameter, α, in the present constitutive theory, can be interpreted as the area fraction of the interface that is occupied by grain boundary cavities. Coalescence of these cavities leads to the occurrence of microcracks corresponding to complete decohesion ($\alpha = 1$). Intergranular creep fracture finally occurs as these microcracks link up, i.e. when complete decohesion has occurred along several adjoining interfaces. The results in Figure 2b show that the fracture strain increases (whereas the time to fracture decreases) with increasing stress level. The stages of primary (transient), secondary (stationary) and tertiary creep can be observed.

REFERENCES

(1) Lemaitre, J., "A Course on Damage Mechanics", Springer-Verlag, 1992.

(2) Cannmo, P., Mähler, L. and Runesson, K., Computational Mechanics, Vol. 20, No. 1/2, 1997, pp. 12-19.

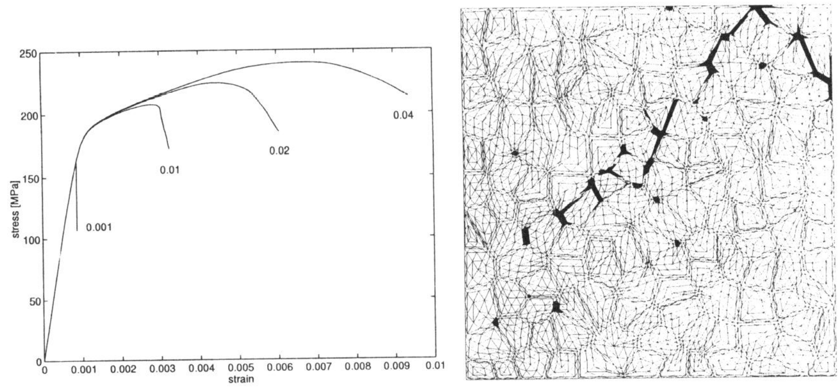

Figure 1: a) Macroscopic response of for different values of the damage modulus S' (in N/mm), and b) localization of plastic deformation close to final failure.

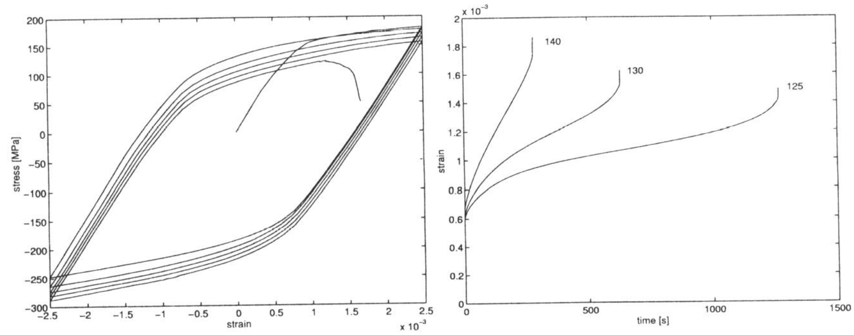

Figure 2: a) Macroscopic response in cyclic loading, and b) macroscopic response for different stress levels in creep: 140, 130 and 125 MPa.