# MICROMECHANICALLY BASED CONSTITUTIVE RELATIONS FOR POLYCRYSTALLINE SOLIDS*

S. Nemat-Nasser and T. Iwakuma
Northwestern University
Evanston, Illinois 60201

## ABSTRACT

A basic method is presented for the estimate of the overall mechanical response of solids which contain periodically distributed defects (inhomogeneities, regions undergoing inelastic flow, voids, cracks, etc.). This method is then applied to estimate the shape and growth pattern of voids that are periodically distributed over the grain boundaries in a viscous matrix. The interaction effects are fully accounted for, and the results are compared with calculations for a single void in an infinitely extended viscous solid, by Budiansky, Hutchinson, and Slutsky. Then, for a polycrystalline solid that undergoes relaxation by grain boundary sliding, the relaxed moduli are obtained, again fully accounting for the interaction effects. Finally, the overall inelastic nonlinear response at elevated temperatures is discussed in terms of a model which considers nonlinear power law creep within the grains, and linear viscous flow in the grain boundaries.

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## 1. INTRODUCTION

The inelastic response of polycrystalline solids stems from a variety of microstructural changes, depending on the temperature regime, as well as the stress history. At temperatures sufficiently below 50% melting point, the rate effects are not dominant. The deformation consists of plastic slip on crystallographic planes, accompanied by the accommodating elastic lattice distortion. At higher temperature regimes the rate effects become significant, and the intracrystalline flow can be modelled adequately by a power law. At higher temperatures, creep effects are the major components in the overall response. In this case, adequate micromodelling involves a power law flow within the grains, accompanied by linearly viscous grain boundary sliding.

Various micromechanical defects that may arise in the course of deformation, contribute differently to the failure mechanisms during different temperature regimes. At low temperatures, voids are generated because of plastic flow at second phase particles, and this may lead to a reduction in ductility. At higher temperatures, on the other hand, voids are nucleated on grain boundaries, and grow in response to the applied load, as the solid creeps. Depending on the load level and the temperature regime, the mechanism of such void growth varies. For example, cavity growth is essentially crack-like, when surface diffusion is much slower than the grain boundary diffusion, whereas at a high stress level the cavity grows essentially by intragranular power law diffusion.

Under NASA-Lewis sponsorship, theoretical and experimental work has been initiated at Northwestern University on the micromechanical modelling of nonlinear constitutive relations of superalloys at various temperature regimes, addressing all the above-mentioned microscopic features. The present report summarizes some of the theoretical results on the growth of voids in viscous metals, the effects of grain boundary defects on the overall response of the polycrystal, and, finally, the overall creep response of the polycrystal. Elasto-plastic (rate-independent) modelling is discussed in a separate report; Iwakuma and Nemat-Nasser (1982).

The calculation of the overall response of the polycrystal is based on some fundamental results on the effect of periodically distributed defects (inhomogeneities, regions undergoing inelastic deformation, etc.) on the overall response of the solid; Nemat-Nasser et al. (1982). These results are first briefly discussed, and then applied to the estimation of the shape and growth pattern of voids that are periodically distributed over the grain boundaries in a viscous matrix. The interaction effects are fully accounted for, and the results are compared with calculations for a single void in an infinitely extended viscous solid, by Budiansky, Hutchinson, and Slutsky (1982). Then, for a polycrystalline solid that undergoes relaxation by grain boundary sliding, the relaxed moduli are obtained, again fully accounting for the interaction effects. Finally, the overall inelastic nonlinear response at elevated temperatures is discussed in terms of a model which considers nonlinear power law creep within the grains.

## 2. FORMULATION OF THE BASIC PROBLEM

Consider a solid containing periodically distributed sets of inhomogeneities such that it can be regarded as a collection of identical unit cells. Let D be a typical cell of volume V and exterior surface S. For simplicity assume that D is a parallelepiped of dimensions $\Lambda_i$, measured along the rectangular Cartesian coordinate axes $x_i$, $i = 1,2,3$. The results also apply to a single cell subjected on its boundary to suitable displacement or velocity fields.

Neither the matrix nor the inhomogeneities are required to be linearly elastic or rate-independent, but, for the intended applications, only small strains and rotations are considered.

To be specific, let $\underset{\sim}{\sigma}$ be the Cauchy stress and set

$$d\varepsilon_{ij} = D_{ijk\ell} d\sigma_{k\ell}, \tag{2.1}$$

where repeated indices are summed over 1, 2, 3, $d\underset{\sim}{\sigma}$ is the stress increment, and $\underset{\sim}{D} = \underset{\sim}{D}(\underset{\sim}{\sigma})$ is the instantaneous compliance which may or may not depend on stress. For rate-independent applications, $\underset{\sim}{\varepsilon}$ in (2.1) is the strain tensor. For rate-dependent cases, on the other hand, $\underset{\sim}{\varepsilon}$ is the <u>strain</u> <u>rate</u> tensor. For example, for non-linear creep, the strain rate is $\underset{\sim}{\varepsilon} = \underset{\sim}{F}(\underset{\sim}{\sigma})$. In this case we consider the incremental relation

$$d\underset{\sim}{\varepsilon} = \frac{\partial \underset{\sim}{F}}{\partial \sigma_{ij}} d\sigma_{ij}. \tag{2.2}$$

In particular, if power law creep is assumed, $\underset{\sim}{\varepsilon}' = \eta J^n \underset{\sim}{\sigma}'$, we obtain

$$d\varepsilon'_{ij} = \eta J^n \{\delta_{ik}\delta_{j\ell} + \frac{n\sigma'_{ij}\sigma'_{k\ell}}{2J^2}\} d\sigma'_{k\ell}, \tag{2.3}$$

where prime denotes the deviatoric part, and

$$J = (\tfrac{1}{2}\,\sigma'_{ij}\sigma'_{ij})^{\frac{1}{2}} \tag{2.4}$$

is the effective stress; in (2.3) $n$ is a positive number and $\eta$ is a dimensional parameter. If an inhomogeneity is linearly elastic or linearly viscous, then $\underset{\sim}{D}$ in (2.1) would be a constant tensor with suitable usual symmetries.

Let $\underset{\sim}{C}$ be the inverse of $\underset{\sim}{D}$ and rewrite (2.1) as

$$d\sigma_{ij} = C_{ijk\ell}d\varepsilon_{k\ell}. \tag{2.5}$$

Again, $\underset{\sim}{C}$ may be a function of $\underset{\sim}{\sigma}$.

Assume now that the displacement (velocity) field $\underset{\sim}{u}^0$ is prescribed on S in such a manner that the average strain (strain rate) field $\underset{\sim}{\varepsilon}^0$ is obtained. Let the corresponding average stress field be $\bar{\underset{\sim}{\sigma}}$. Consider an incremental change, $d\underset{\sim}{u}^0$, in $\underset{\sim}{u}^0$, which produces the increments $d\underset{\sim}{\varepsilon}^0$ and $d\bar{\underset{\sim}{\sigma}}$ in the average strain (strain rate) and stress fields, respectively. We seek to calculate the overall moduli $\underset{\sim}{C}^*$, defined by

$$d\bar{\sigma}_{ij} = C^*_{ijk\ell}d\varepsilon^0_{k\ell}, \tag{2.6}$$

where, in general, $\underset{\sim}{C}^*$ depends on the average stress $\bar{\underset{\sim}{\sigma}}$, as well as on the micro-structure.

Within the unit cell, neither the stress increment nor the strain (strain rate) increment is uniform. Let there be M inhomogeneities, $\Omega_r$, r = 1,2,...,M, and set

$$\begin{aligned} d\sigma^T_{ij} &= C_{ijk\ell}[d\varepsilon^0_{k\ell} + d\varepsilon_{k\ell}(\underset{\sim}{x})] \quad \text{in } D-\Omega_r \\ &= C^r_{ijk\ell}[d\varepsilon^0_{k\ell} + d\varepsilon_{k\ell}(\underset{\sim}{x})] \quad \text{in } \Omega_r, \quad r = 1,2,\ldots,M, \end{aligned} \tag{2.7}$$

where $d\underset{\sim}{\varepsilon}$ is the perturbation strain (strain rate) field due to inhomogeneities; $\underset{\sim}{C}$ is the modulus tensor of the matrix; and $\underset{\sim}{C}^r$ is that of the $r^{th}$ inhomogeneity.

As has been shown by Eshelby (1957) for an ellipsoidal inhomogeneity in a linearly elastic, unbounded solid, the nonhomogeneous body may be replaced by a homogeneous one, provided that suitable transformation strains are prescribed in the ellipsoid. In this case, the transformation strain tensor is constant. For periodically distributed inhomogeneities, or when the inhomogeneity is not ellipsoidal, the transformation strain tensor is no longer constant. The basic concept, however, still applies, and can be quite effective, as shown by Nemat-Nasser and Taya (1981) and Nemat-Nasser _et al_. (1982).

Hence, in place of (2.7), one writes

$$d\sigma_{ij}^{T} = C_{ijk\ell}[d\varepsilon_{k\ell}^{0} + d\varepsilon_{k\ell} - d\varepsilon_{k\ell}^{*r}], \tag{2.8}$$

where $d\underset{\sim}{\varepsilon}^{*r}$ is zero in $D - \Omega_r$, and seeks to express this transformation strain (strain rate) increment in terms of $d\underset{\sim}{\varepsilon}^{0}$. This is done by the use of the Fourier series representation of the incremental fields, as has been discussed by Nemat-Nasser et al. (1982). The final results for the present case are as follows:

$$d\varepsilon_{k\ell}^{0} = A_{k\ell mn}^{r} d\varepsilon_{mn}^{*r}(\underset{\sim}{x}) - d\varepsilon_{k\ell}(\underset{\sim}{x}) \quad \text{in } \Omega_r, \tag{2.9}$$

$$A_{k\ell mn}^{r} = [C_{k\ell pq} - C_{k\ell pq}^{r}]^{-1}\, C_{pqmn}, \tag{2.10}$$

$$d\varepsilon_{jk}(\underset{\sim}{x}) = \frac{1}{V} \sum_{n_p=0}^{\pm\infty}{}' \, g_{jkmn}(\underset{\sim}{\xi}) \sum_{r=1}^{M} \int_{\Omega_r} d\varepsilon_{mn}^{*r}(\underset{\sim}{x}') e^{i\underset{\sim}{\xi}\cdot(\underset{\sim}{x}-\underset{\sim}{x}')} d\underset{\sim}{x}', \tag{2.11}$$

$$\xi_j = \frac{2\pi n_j}{\Lambda_j} \text{ (no sum on j)}, \quad i = \sqrt{-1}, \tag{2.12}$$

and where $k,\ell,m,n,j = 1,2,3$. In (2.11), the fourth order tensor $g_{jkmn}(\underset{\sim}{\xi})$ depends on the matrix modulus tensor $\underset{\sim}{C}$. For an isotropic matrix,

$$C_{ijk\ell} = \mu(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}) + \lambda\delta_{ij}\delta_{k\ell}, \tag{2.13}$$

we have

$$g_{ijk\ell}(\underset{\sim}{\xi}) = \bar{\xi}_j(\delta_{i\ell}\bar{\xi}_k + \delta_{ik}\bar{\xi}_\ell) + \bar{\xi}_i(\delta_{j\ell}\bar{\xi}_k + \delta_{jk}\bar{\xi}_\ell) - \frac{1}{1-\nu}\bar{\xi}_i\bar{\xi}_j\bar{\xi}_k\bar{\xi}_\ell + \frac{\nu}{1-\nu}\bar{\xi}_i\bar{\xi}_j\delta_{k\ell}, \tag{2.14}$$

$$\bar{\xi}_i = \xi_i/\xi, \qquad \xi = (\xi_k\xi_k)^{\frac{1}{2}}, \qquad \nu = \frac{\lambda}{2\lambda + 2\mu}.$$

In (2.13) and (2.14), $\lambda$, $\mu$, and $\nu$ are material parameters for the matrix, which may depend on stress $\underset{\sim}{\sigma}$. For a linearly elastic matrix, these are the usual Lamé constants and Poisson's ratio, respectively. In the general formulation that will follow, we shall assume an anisotropic matrix. In Section 3, however, we assume an isotropic matrix, and hence use (2.14). In Section 4, on the other hand, a nonlinear creep law is considered, and this makes the tensor $\underset{\sim}{C}$ dependent on the current stress state; then (2.14) cannot be used, and hence a more general expression is obtained.

Let $f_r$ be the volume fraction of the $r^{th}$ inhomogeneity,

$$f_r = V_r/V, \tag{2.15}$$

where $V_r$ is the volume of $\Omega_r$, and denote by $d\bar{\underset{\sim}{\varepsilon}}^{*r}$ the average value of $d\underset{\sim}{\varepsilon}^{*r}$ taken over $\Omega_r$,

$$d\bar{\underset{\sim}{\varepsilon}}^{*r} = \frac{1}{V_r}\int_{\Omega_r} d\underset{\sim}{\varepsilon}^{*r}(\underset{\sim}{x})d\underset{\sim}{x}; \tag{2.16}$$

note that $d\underset{\sim}{\varepsilon}^{*r}$ is zero outside of $\Omega_r$. Averaging (2.8) over D, and using (2.6) we obtain

$$(C_{ijk\ell} - C^*_{ijk\ell})d\varepsilon^0_{k\ell} = C_{ijk\ell} \sum_{r=1}^{M} \beta^r_{k\ell}, \tag{2.17}$$

where the notation

$$f_r\, d\bar{\varepsilon}^{*r}_{k\ell} \equiv \beta^r_{k\ell} \tag{2.18}$$

is used. We now substitute from (2.11) into (2.9), average the resulting equation over $\Omega_r$ to arrive at

$$f_r\, d\varepsilon^0_{jk} = A^r_{jkmn}\beta^r_{mn} - \sum_{n_p=0}^{\pm\infty}{}' g_{jkmn}(\underset{\sim}{\xi})f_r Q^r(\underset{\sim}{\xi}) \sum_{s=1}^{M}\int_{\Omega_s} d\varepsilon^{*s}_{mn}(\underset{\sim}{x}')e^{-i\underset{\sim}{\xi}\cdot\underset{\sim}{x}'}\, d\underset{\sim}{x}', \tag{2.19}$$

where

$$Q^r(\underset{\sim}{\xi}) = \frac{1}{V_r}\int_{\Omega_r} e^{i\underset{\sim}{\xi}\cdot\underset{\sim}{x}}\, d\underset{\sim}{x}. \tag{2.20}$$

It has been shown by Nemat-Nasser and Taya (1981) that good accuracy is obtained if the transformation strain (strain rate) increment in the integrand in (2.19) is replaced by its average value. This then leads to

$$f_r\, d\varepsilon^0_{jk} = A^r_{jkmn}\beta^r_{mn} - \sum_{s=1}^{M} S^{rs}_{jkmn}\beta^s_{mn}, \tag{2.21}$$

where

$$S^{rs}_{jkmn} = \sum_{n_p=0}^{\pm\infty}{}' \, g_{jkmn}(\underset{\sim}{\xi}) f_r Q^r(\underset{\sim}{\xi}) Q^s(-\underset{\sim}{\xi}). \tag{2.22}$$

Equations (2.21) are now solved for $\beta^r_{mn}$, results substituted into (2.17), and since $d\underset{\sim}{\varepsilon}^0$ is arbitrary, the following general result is obtained:

$$C^*_{ijk\ell} = C_{ijk\ell} - C_{ijmn} \sum_{s=1}^{M} f_s \Big\{ \sum_{r=1}^{M} [A^r_{mnk\ell} \delta^{rs} - S^{rs}_{mnk\ell} f_r \Big\}^{-1}, \tag{2.23}$$

where $\delta^{rs}$ is the Kronecker delta.

In (2.23) the tensors $\underset{\sim}{C}$, $\underset{\sim}{A}^r$, and $\underset{\sim}{S}^{rs}$ may depend on the stress, $\underset{\sim}{\sigma}$, in the matrix as well as in each corresponding inhomogeneity. The estimate of the stress variation throughout the solid is indeed a formidable task. For our purposes, it seems adequate to use the overall average stress $\bar{\underset{\sim}{\sigma}}$ instead. Then the overall stress-strain (strain rate) relation can be obtained incrementally with the aid of (2.23) and (2.6). Some specific results are presented in subsequent sections. On the other hand, when necessary the local strain (strain rate) increment in, say, $\Omega_r$ can be obtained from (2.9),

$$d\varepsilon^0_{k\ell} + d\varepsilon_{k\ell}(\underset{\sim}{x}) = A^r_{k\ell mn} \, d\varepsilon^{*r}_{mn}(\underset{\sim}{x}), \tag{2.24}$$

and hence the local stress increment can be estimated from (2.7),

$$d\sigma^T_{ij}(\underset{\sim}{x}) = C^r_{ijk\ell} \, A^r_{k\ell mn} \, d\varepsilon^{*r}_{mn}(\underset{\sim}{x}) \quad \text{in } \Omega_r. \tag{2.25}$$

In a similar manner, the stress increment within the matrix can be obtained from (2.11) and (2.7).

## 3. GROWTH OF PERIODICALLY DISTRIBUTED VOIDS IN VISCOUS METALS

### 3.1 Background

At elevated temperatures, voids are nucleated at grain boundaries in polycrystalline solids. Depending on the deformation and temperature histories, the arrangement of these voids relative to the orientation of the principal applied stresses can vary considerably. For example, experiments show that voids can be concentrated on grain boundaries perpendicular to the direction of maximum tension, see, e.g., Garofalo (1965). For superalloys that are plastically deformed at room temperature, on the other hand, Dyson et al. (1976) have shown and Kikuchi and Weertman (1980) and Saegusa et al. (1980) have conclusively verified that after annealing, voids are generated at grain boundaries parallel to the direction of maximum tension. The mechanisms giving rise to the formation of these cavities are different, but their presence has similar adverse effects on the life expectancy of the structural components. An account of diffusive cavitation in polycrystalline solids is given by Chuang et al. (1979) and by Argon et al. (1981); see also Rice (1981). Here, however, a different approach is used, which considers the growth of periodically distributed cavities within a viscous metal. We make contact with the work by Budiansky et al. (1982) who examine the growth of a single cavity in an unbounded viscous medium, as well as with an earlier contribution by McClintock (1968) on the same subject.

### 3.2 Formulation

For a linearly viscous matrix, we have

$$\sigma_{ij} = C_{ijk\ell}\varepsilon_{k\ell}, \tag{3.1}$$

where

$$C_{ijk\ell} = 2\mu(I_{ijk\ell} + \frac{\nu}{1-2\nu}\,\delta_{ij}\delta_{k\ell}), \tag{3.2}$$

$$D_{ijk\ell} = C^{-1}_{ijk\ell} = \frac{1}{2\mu}(I_{ijk\ell} - \frac{\nu}{1+\nu}\,\delta_{ij}\delta_{k\ell}). \tag{3.3}$$

In (3.2), $I_{ijk\ell}$ is the fourth order identity tensor; in (3.1) $\underset{\sim}{\varepsilon}$ is the <u>strain rate</u>.

Consider a unit cell of dimensions $\Lambda_i$, and let it include an ellipsoidal void of (principal) semi-axes $a_i$, oriented along the coordinate axes $x_i$, $i = 1,2,3$. Define

$$\alpha = \frac{a_2}{a_1}, \quad \beta = \frac{a_3}{a_1}, \quad \gamma = \frac{\Lambda_2}{\Lambda_1}, \quad \zeta = \frac{\Lambda_3}{\Lambda_1}, \quad f = \frac{4\pi}{3}\frac{a_1 a_2 a_3}{\Lambda_1\Lambda_2\Lambda_3}. \tag{3.4}$$

Since (3.1) is linear, all the <u>incremental</u> relations in Section 2 can be replaced by the <u>total</u> ones, i.e. all the relations apply if $d\underset{\sim}{\varepsilon}^0$, $d\bar{\underset{\sim}{\sigma}}, \ldots$, are replaced by $\underset{\sim}{\varepsilon}^0$, $\bar{\underset{\sim}{\sigma}}, \ldots$, respectively.

From (2.8) it follows that[†]

$$\underset{\sim}{\varepsilon}^* = \underset{\sim}{\varepsilon}^0 + \underset{\sim}{\varepsilon} \tag{3.5}$$

within the void, and from (2.21) we obtain

$$\varepsilon^0_{ij} = [I_{ijk\ell} - S_{ijk\ell}]\bar{\varepsilon}^*_{k\ell}, \tag{3.6}$$

where, in view of (2.22) and (2.14),

$$\begin{aligned}
S_{1111} &= -\frac{1}{1-\nu}S_4 + \frac{2-\nu}{1-\nu}S_1, & S_{1133} &= -\frac{1}{1-\nu}S_8 + \frac{\nu}{1-\nu}S_1,\\
S_{2222} &= -\frac{1}{1-\nu}S_5 + \frac{2-\nu}{1-\nu}S_2, & S_{1122} &= -\frac{1}{1-\nu}S_9 + \frac{\nu}{1-\nu}S_1,\\
S_{3333} &= -\frac{1}{1-\nu}S_6 + \frac{2-\nu}{1-\nu}S_3, & S_{2211} &= -\frac{1}{1-\nu}S_9 + \frac{\nu}{1-\nu}S_2,\\
S_{2233} &= -\frac{1}{1-\nu}S_7 + \frac{\nu}{1-\nu}S_2, & S_{2323} &= \tfrac{1}{2}(S_2 + S_3) - \frac{1}{1-\nu}S_7,\\
S_{3322} &= -\frac{1}{1-\nu}S_7 + \frac{\nu}{1-\nu}S_3, & S_{3131} &= \tfrac{1}{2}(S_3 + S_1) - \frac{1}{1-\nu}S_8,\\
S_{3311} &= -\frac{1}{1-\nu}S_8 + \frac{\nu}{1-\nu}S_3, & S_{1212} &= \tfrac{1}{2}(S_1 + S_2) - \frac{1}{1-\nu}S_9.
\end{aligned} \tag{3.7}$$

The infinite series $S_\ell = S_\ell(\alpha,\beta,\gamma,\zeta,f)$ in (3.7) is defined by

$$S_\ell = \sum_{n_p=0}^{\pm\infty}{}' P(\eta)h_\ell(\underset{\sim}{\xi}), \qquad \ell = 1,2,\ldots,9, \tag{3.8}$$

where

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[†]Since M = 1, the superscript r = 1 is dropped.

$$h_1 = (\bar{\xi}_1)^2,\quad h_2 = (\bar{\xi}_2)^2,\quad h_3 = (\bar{\xi}_3)^2,\quad h_4 = (\bar{\xi}_1)^4,\quad h_5 = (\bar{\xi}_2)^4,$$
$$h_6 = (\bar{\xi}_3)^4,\quad h_7 = (\bar{\xi}_2\bar{\xi}_3)^2,\quad h_8 = (\bar{\xi}_3\bar{\xi}_1)^2,\quad h_9 = (\bar{\xi}_1\bar{\xi}_2)^2, \tag{3.9}$$

and, for an ellipsoidal inhomogeneity,

$$P(\eta) = f\,\frac{9(\sin\eta - \eta\cos\eta)^2}{\eta^6}, \qquad \eta \neq 0, \tag{3.10}$$

$$\eta = 2\pi R\left[n_1^2 + \left(\frac{\alpha n_2}{\gamma}\right)^2 + \left(\frac{\beta n_3}{\zeta}\right)^2\right]^{\frac{1}{2}},$$
$$\xi = \frac{2\pi}{\Lambda_1}\left[n_1^2 + \left(\frac{n_2}{\gamma}\right)^2 + \left(\frac{n_3}{\zeta}\right)^2\right]^{\frac{1}{2}}. \tag{3.11}$$

In view of (3.5), the shape change can be defined by

$$\frac{\dot{a}_1}{a_1} = \bar{\varepsilon}^*_{11},\qquad \frac{\dot{a}_2}{a_2} = \bar{\varepsilon}^*_{22},\qquad \frac{\dot{a}_3}{a_3} = \bar{\varepsilon}^*_{33},\qquad \frac{\dot{V}_\Omega}{V_\Omega} = \bar{\varepsilon}^*_{kk}, \tag{3.12}$$

and we also note, from (3.4), that

$$\frac{\dot{\alpha}}{\alpha} = \bar{\varepsilon}^*_{22} - \bar{\varepsilon}^*_{11},\qquad \frac{\dot{\beta}}{\beta} = \bar{\varepsilon}^*_{33} - \bar{\varepsilon}^*_{11},$$
$$\frac{\dot{\gamma}}{\gamma} = \varepsilon^0_{22} - \varepsilon^0_{11},\qquad \frac{\dot{\zeta}}{\zeta} = \varepsilon^0_{33} - \varepsilon^0_{11},\qquad \frac{\dot{f}}{f} = \bar{\varepsilon}^*_{kk} - \varepsilon^0_{kk}. \tag{3.13}$$

To obtain the current dimensions and other geometric variables, we integrate (3.12) and (3.13) with respect to time. This, for example, yields

$$\ln\frac{a_1}{(a_1)_0} = \int_0^t \bar{\varepsilon}^*_{11}dt,\ \ldots,\quad \ln\frac{\alpha}{\alpha_0} = \int_0^t (\bar{\varepsilon}^*_{22} - \bar{\varepsilon}^*_{11})dt, \ldots, \tag{3.14}$$

where the subscript 0 denotes the initial value.

Since the transformation strain rate tensor, $\bar{\underset{\sim}{\varepsilon}}^*$, characterizes the rate of change of the void geometry in accordance with (3.12) and (3.13), Eq. (3.6) relates the void change parameters to the overall strain rate tensor $\underset{\sim}{\varepsilon}^0$. To make contact with results of Budiansky et al. (1982), we relate the overall strain rates to the average stresses by

$$\bar{\sigma}_{ij} = C^*_{ijk\ell}\,\varepsilon^0_{k\ell}, \tag{3.15}$$

and note that, unlike the case of a single void in an infinitely extended solid considered by Budiansky et al. (1982), here $\underset{\sim}{C}^*$ does not equal the matrix modulus tensor $\underset{\sim}{C}$. The overall modulus in the present case is obtained by specializing (2.23) or, equivalently, by equating the overall rate of energy loss per unit volume with the average rate of loss. This results in†

$$C^*_{ijk\ell}\varepsilon^0_{ij}\varepsilon^0_{k\ell} = C_{ijk\ell}\varepsilon^0_{ij}\varepsilon^0_{k\ell} - f\, C_{ijk\ell}\varepsilon^0_{ij}\bar{\varepsilon}^*_{k\ell} \tag{3.16}$$

which, for M = 1 and because of (3.6), implies (2.23). Since $\underset{\sim}{\varepsilon}^0$ is arbitrary, (3.16) and (3.15) yield

$$\bar{\sigma}_{ij} = C_{ijk\ell}[\varepsilon^0_{k\ell} - f\, \bar{\varepsilon}^*_{k\ell}]. \tag{3.17}$$

In the present case $\underset{\sim}{C}$ is isotropic, Eq. (3.2), and if we introduce

$$S^0_{ij} = \bar{\sigma}_{ij}/2\mu \tag{3.18}$$

and eliminate $\underset{\sim}{\varepsilon}^0$ between (3.17) and (3.6), we obtain

$$\frac{1}{1+\nu}\begin{bmatrix} 1 & -\nu & -\nu \\ -\nu & 1 & -\nu \\ -\nu & -\nu & 1 \end{bmatrix}\begin{Bmatrix} S^0_{11} \\ S^0_{22} \\ S^0_{33} \end{Bmatrix} = \begin{bmatrix} 1-f-S_{1111} & -S_{1122} & -S_{1133} \\ -S_{2211} & 1-f-S_{2222} & -S_{2233} \\ -S_{3311} & -S_{3322} & 1-f-S_{3333} \end{bmatrix}\begin{Bmatrix} \bar{\varepsilon}^*_{11} \\ \bar{\varepsilon}^*_{22} \\ \bar{\varepsilon}^*_{33} \end{Bmatrix},$$

$$\begin{aligned} S^0_{12} &= (1 - f - 2S_{1212})\bar{\varepsilon}^*_{12}, \\ S^0_{23} &= (1 - f - 2S_{2323})\bar{\varepsilon}^*_{23}, \\ S^0_{31} &= (1 - f - 2S_{3131})\bar{\varepsilon}^*_{31}. \end{aligned} \tag{3.19}$$

From (3.19) it follows that

$$\begin{aligned} \frac{1-2\nu}{1+\nu}(S^0_{11} + S^0_{22} + S^0_{33}) = &\{1 - S_{1111} - S_{2211} - S_{3311} - f\}\bar{\varepsilon}^*_{11} \\ &+ \{1 - S_{2222} - S_{1122} - S_{3322} - f\}\bar{\varepsilon}^*_{22} \\ &+ \{1 - S_{3333} - S_{1133} - S_{2233} - f\}\bar{\varepsilon}^*_{33}. \end{aligned} \tag{3.20}$$

†The calculation is essentially the same as in Nemat-Nasser et al. (1982).

For the incompressible matrix, $\nu = 1/2$, and for (3.19) and (3.20) to yield non-trivial results, the matrix in the right-hand side of the matrix expression in (3.19) and the coefficients in the right-hand side of Eq. (3.20) should vanish.[†] With $\nu = 1/2$, this leads to

$$\begin{aligned}
&1 - 3S_1 - S_2 - S_3 + 2(S_4 + S_8 + S_9) = f,\\
&1 - S_1 - 3S_2 - S_3 + 2(S_5 + S_7 + S_9) = f, \qquad (3.21)\\
&1 - S_1 - S_2 - 3S_3 + 2(S_6 + S_7 + S_8) = f,
\end{aligned}$$

and, if only the infinite series $S_1$, $S_2$, and $S_3$ are retained, from (3.7) we deduce that

$$\begin{aligned}
&1 - S_{1111} - S_{2211} - S_{3311} - f = \frac{1 - 2\nu}{2(1-\nu)}\{1 - f - S_1 + S_2 + S_3\},\\
&1 - S_{2222} - S_{1122} - S_{3322} - f = \frac{1 - 2\nu}{2(1-\nu)}\{1 - f + S_1 - S_2 + S_3\}, \qquad (3.22)\\
&1 - S_{3333} - S_{1133} - S_{2233} - f = \frac{1 - 2\nu}{2(1-\nu)}\{1 - f + S_1 + S_2 - S_3\}.
\end{aligned}$$

With these and with $\nu = 1/2$, (3.19) yields

$$\begin{Bmatrix} \bar{\varepsilon}^*_{11} \\ \bar{\varepsilon}^*_{22} \\ \bar{\varepsilon}^*_{33} \end{Bmatrix} = [T_{ij}] \begin{Bmatrix} \frac{2}{3} s^0_{11} - \frac{1}{3} s^0_{22} - \frac{1}{3} s^0_{33} \\ -\frac{1}{3} s^0_{11} + \frac{2}{3} s^0_{22} - \frac{1}{3} s^0_{33} \\ -\frac{1}{3} s^0_{11} - \frac{1}{3} s^0_{22} + \frac{2}{3} s^0_{33} \end{Bmatrix}, \qquad (3.23)$$

where $[T_{ij}]$ is the inverse of the matrix

$$\begin{bmatrix} 1 - f - S_{1111} & -S_{1122} & -S_{1133} \\ -S_{2211} & 1 - f - S_{2222} & -S_{2233} \\ 1 - f - S_1 + S_2 + S_3 & 1 - f + S_1 - S_2 + S_3 & 1 - f + S_1 + S_2 - S_3 \end{bmatrix}. \qquad (3.24)$$

Equations (3.23) relate the void growth parameters to the overall stress components. In terms of the stress ratios

---

[†]Numerical tests for spherical, cylindrical, and ellipsoidal geometries show that to within the accuracy of the estimate of the infinite series, these conditions are almost satisfied.

$$\phi = \frac{S^0_{22}}{S^0_{11}} = \frac{\bar{\sigma}_{22}}{\bar{\sigma}_{11}}, \qquad \psi = \frac{S^0_{33}}{S^0_{11}} = \frac{\bar{\sigma}_{33}}{\bar{\sigma}_{11}}, \tag{3.25}$$

one obtains

$$\begin{aligned}
\frac{3\bar{\varepsilon}^*_{11}}{S^0_{11}} &= (2T_{11} - T_{12} + 2T_{13}) + (-T_{11} + 2T_{12} + 2T_{13})\phi + (-T_{11} - T_{12} + 2T_{13})\psi, \\
\frac{3\bar{\varepsilon}^*_{22}}{S^0_{11}} &= (2T_{21} - T_{22} + 2T_{23}) + (-T_{21} + 2T_{22} + 2T_{23})\phi + (-T_{21} - T_{22} + 2T_{23})\psi, \\
\frac{3\bar{\varepsilon}^*_{33}}{S^0_{11}} &= (2T_{31} - T_{32} + 2T_{33}) + (-T_{31} + 2T_{32} + 2T_{33})\phi + (-T_{31} - T_{32} + 2T_{33})\psi.
\end{aligned} \tag{3.26}$$

Finally, the components of $\underset{\sim}{\varepsilon}^0$ are obtained from (3.6) and (3.26).

## 3.3 Numerical Results

Table 1 lists the initial and the loading conditions for eight different cases which are reported here for illustration. It should be noted that even in high strength metals which undergo very small overall deformations, the local deformations close to inhomogeneities or at the tip of cracks can be quite large. For this reason in Fig. 1, results for rather large strains are included. This figure shows the void volume change as a function of the overall deformation measure, $L/L_0$ or $L_0/L$, for the indicated cases associated with Table 1. For comparison, an asymptotic and additional results of Budiansky et al. (1982) are also shown. [These are read off the figures in the published paper. In the final version of the present report, these will be recalculated in order to obtain a more accurate estimate of the effect of periodicity as compared with a single void in an extended solid.] Figure 2 shows the void shape changes for the indicated cases.

## 4. EFFECT OF GRAIN BOUNDARY SLIDING ON NONLINEAR STEADY CREEP

At elevated temperatures, creep of polycrystals involves nonlinear flow within grains accompanied by grain boundary sliding which can be modelled by a linearly viscous relation; see Kê (1947), Zener (1948), and McLean (1957). The problem of estimating the overall creep properties of a polycrystal on the basis of different constitutive relations for the grain and the grain boundary has been examined by a number of researchers using various models; see, e.g., Zener (1948), Budiansky and O'Connell (1976), and Chen and Argon (1979). Recently, Ghahremani (1980a,b) has studied a two-dimensional model of creep using a numerical approach. Except for his work, other studies do not include the full effect of the essentially periodic structure of the grain boundary geometry, and hence the corresponding interaction effects.

In this section we shall examine the creep of polycrystals on the basis of nonlinear transgranular and linear intergranular creep laws, using a two-dimensional (plane) model.

Figure 3 shows a typical unit cell of dimensions $\Lambda_1$ and $\Lambda_2$. Within the matrix, the flow is governed by constitutive relations (2.3) which, in conjunction with a linear creep in bulk, $d\varepsilon_{kk} = \kappa \, d\sigma_{mm}$, $\kappa$ = constant, yield

$$C_{ijk\ell} = \frac{1}{\eta J^n}\left[I_{ijk\ell} - \frac{n}{n+1}\frac{\sigma'_{ij}\sigma'_{k\ell}}{2J^2} - \frac{1}{2}\,\delta_{ij}\delta_{k\ell}\right] + \frac{1}{2\kappa}\,\delta_{ij}\delta_{k\ell}, \qquad (4.1)$$

so that $d\sigma_{ij} = C_{ijk\ell}d\varepsilon_{kk}$ holds for the incremental stress, strain-rate relation within the grains. In view of (4.1), Eq. (2.14) must be replaced by

$$g_{ijmn} = \tfrac{1}{2}(N_{ik}\xi_j + N_{jk}\xi_i)C_{\ell kmn}\xi_\ell, \qquad (4.2)$$

where, now, $N_{jk}$ is

$$N_{jk} = \frac{1}{D}\left[\frac{1}{\eta J^n}\left\{\frac{1}{2}\xi^2\delta_{k} + \frac{n}{n+1}\frac{\xi_i\xi_\ell\sigma'_{im}\sigma'_{n\ell}}{2J^2}(I_{jkmn} - \delta_{jk}\delta_{mn})\right\}\right.$$

$$\left. + \frac{1}{2\kappa}(\xi^2\delta_{jk} - \xi_j\xi_k)\right], \qquad (4.3)$$

where

$$D = \frac{1}{2\eta^2 J^{2n}}\left[\frac{1}{2}\xi^4 - \frac{n}{n+1}\xi^2\frac{\xi_k\sigma'_{ki}\sigma'_{i\ell}\xi_\ell}{2J^2}\right]$$

$$+ \frac{1}{2\kappa\eta J^n}\left[\frac{1}{2}\xi^4 - \frac{n}{n+1}(\xi^2\delta_{ij} - \xi_i\xi_j)\frac{\xi_k\sigma'_{ri}\sigma'_j\ \xi_\ell}{2J^2}\right] .$$

To apply Eq. (2.23), we must calculate the quantity $Q^r(\underset{\sim}{\xi})$ for the typical $r^{th}$ grain boundary segment. For a two-dimensional model, this is easily done and, if $\underset{\sim}{x}_0^r$ denotes the center of the segment, and $\theta^r$ its orientation relative to the $x_1$-axis, see Fig. 3, then we obtain

$$Q^r(\underset{\sim}{\xi}) = e^{i\underset{\sim}{\xi}\cdot\underset{\sim}{x}_0^r}\, h(\underset{\sim}{\xi},\theta^r),$$

$$h(\pm\underset{\sim}{\xi},\theta^r) = \frac{\sin z^r}{z^r}\ \frac{\sin y^r}{y^r}, \qquad (4.5)$$

$$z^r = \frac{\ell^r}{2}[\xi_1\cos\theta^r + \xi_2\sin\theta^r],$$

$$y^r = \frac{t^r}{2}[-\xi_1\sin\theta^r + \xi_2\cos\theta^r], \quad \text{no sum on } r,$$

where $\ell^r$ is the length and $t^r$ the thickness of the $r^{th}$ grain boundary segment. Note that Eq. (2.21) now becomes

$$d\varepsilon^0_{ij} = A^r_{ijk\ell}\,d\bar{\varepsilon}^{*r}_{k\ell} - \sum_{s=1}^{M} f_s \sum_{n_p=0}^{\pm\infty}{}' g_{ijk\ell}(\underset{\sim}{\xi})h(\underset{\sim}{\xi},\theta^r)h(\underset{\sim}{\xi},\theta^s)\cos\{\underset{\sim}{\xi}\cdot(\underset{\sim}{x}^r_0 - \underset{\sim}{x}^s_0)\}d\bar{\varepsilon}^{*s}_{k\ell}. \qquad (4.6)$$

Note also that when the thickness $t^r$ is small relative to the length $\ell^r$ of a segment, then $\sin y^r/y^r \simeq 1$ in $(4.5)_{2,4}$.

The unit cell shown in Fig. 3 includes a total of 9 grain boundary segments, so that M = 9 in Eq. (4.6) and in Eqs. (2.21). For each stress increment (or the strain rate increment), we first solve (2.21) to obtain $d\bar{\epsilon}^{*r}$, $r = 1,2,\ldots,9$. Then we calculate the stress increment and update the overall total stress. With this stress, we calculate the instantaneous moduli of the matrix from the nonlinear creep law (2.3). Equation (2.23) finally yields the overall instantaneous moduli.

Table 2 shows the geometrical data for the considered unit cell. It is easily seen that, in this case,

$$
\begin{aligned}
z^r &= \pi\, R^r\, [n_1 \cos\theta^r + \sqrt{3}\, n_2 \sin\theta^r] \,, \\
y^r &= \pi\, \frac{t_0}{3}\, [-\, n_1 \sin\theta^r + \sqrt{3}\, n_2 \cos\theta^r] \,,
\end{aligned}
\tag{4.7}
$$

where $t_0 = 3t/\Lambda_1$; note that

$$
f = \sum_{r=1}^{9} f_r = \frac{2t_0}{\sqrt{3}} \simeq t_0 \,. \tag{4.8}
$$

For the numerical calculations, we have assumed

$$
\begin{aligned}
&\frac{\kappa}{\bar{\kappa}} = 1.001 \qquad \text{so that} \quad \kappa \simeq \bar{\kappa} \,, \\
&\frac{\kappa}{\bar{\eta}} = 0 \qquad\quad\;\; \text{so that} \quad \bar{\eta} \gg 1 \,, \\
&n = 3 \,, \quad \text{and} \quad \rho = \frac{\bar{\sigma}_{22}}{\bar{\sigma}_{11}} = 0 \text{ (uniaxial tension).}
\end{aligned}
\tag{4.9}
$$

Detailed results are obtained for two cases: (1) $t_0 = 0.1$ which implies that $f \simeq 5.8\%$. We note that the model considers the linear viscous flow in a rather thick band about the grain boundary, and a nonlinear power law with n = 3 (in Eq. (2.3)) outside of this band. This model appears reasonable when we observe that instead of the local stress we have used the overall average stress in calculating the instantaneous moduli for the grains.

The results are presented in terms of the following nondimensional quantities:

$$S_{ij} = \left(\frac{\eta}{\kappa}\right)^{1/n} \sigma_{ij} , \qquad e_{ij} = \left(\frac{\eta}{\kappa^{1+n}}\right)^{1/n} \varepsilon_{ij} ,$$

$$dS_{ij} = \kappa\, C_{ijk\ell}\, de_{k\ell} , \qquad S_0 = \left(\frac{\eta}{\kappa}\right)^{1/n} \bar{\sigma}_{11} , \tag{4.10}$$

which together with

$$J = \frac{1-\rho}{2}\, S_0 \left(\frac{\kappa}{\eta}\right)^{1/n} \quad \text{and} \quad \nu \equiv (n+1) \left[ \frac{(1+\rho)S_0}{2} \right]^n , \tag{4.11}$$

leads to

$$\kappa\, C_{2222} = \kappa\, C_{1111} = \frac{1}{2} + \frac{1}{2\nu} ,$$

$$\kappa\, C_{1122} = \kappa\, C_{2211} = \frac{1}{2} - \frac{1}{2\nu} , \tag{4.12}$$

$$\kappa\, C_{1212} = \kappa\, C_{2121} = \frac{n+1}{2\nu} .$$

In Fig. 4, results are plotted in terms of non-dimensional axial stress and strain measures, instead of the effective stress and strain. At stress levels near $S_0 = 1$, the lateral strain, $\varepsilon_{22}$, is positive (extension) and larger than $\varepsilon_{11}$, and $\kappa C_{1122}$ is negative for smaller $S_0$. This anomalous result stems from the assumed power law creep for the matrix. Another peculiar phenomenon at this stress level is that some of the overall moduli are negative; the shear modulus remains positive. Another anomalous behavior for power law constitutive relations has been observed by Budiansky et al. (1982), in connection with void growth. These authors report examples in which, under axial tension larger than the lateral ones, a void in a power law matrix is predicted to extend more rapidly laterally than in the axial direction.

The results in Fig. 4 are tentative, as we are now examining this problem in more detail.

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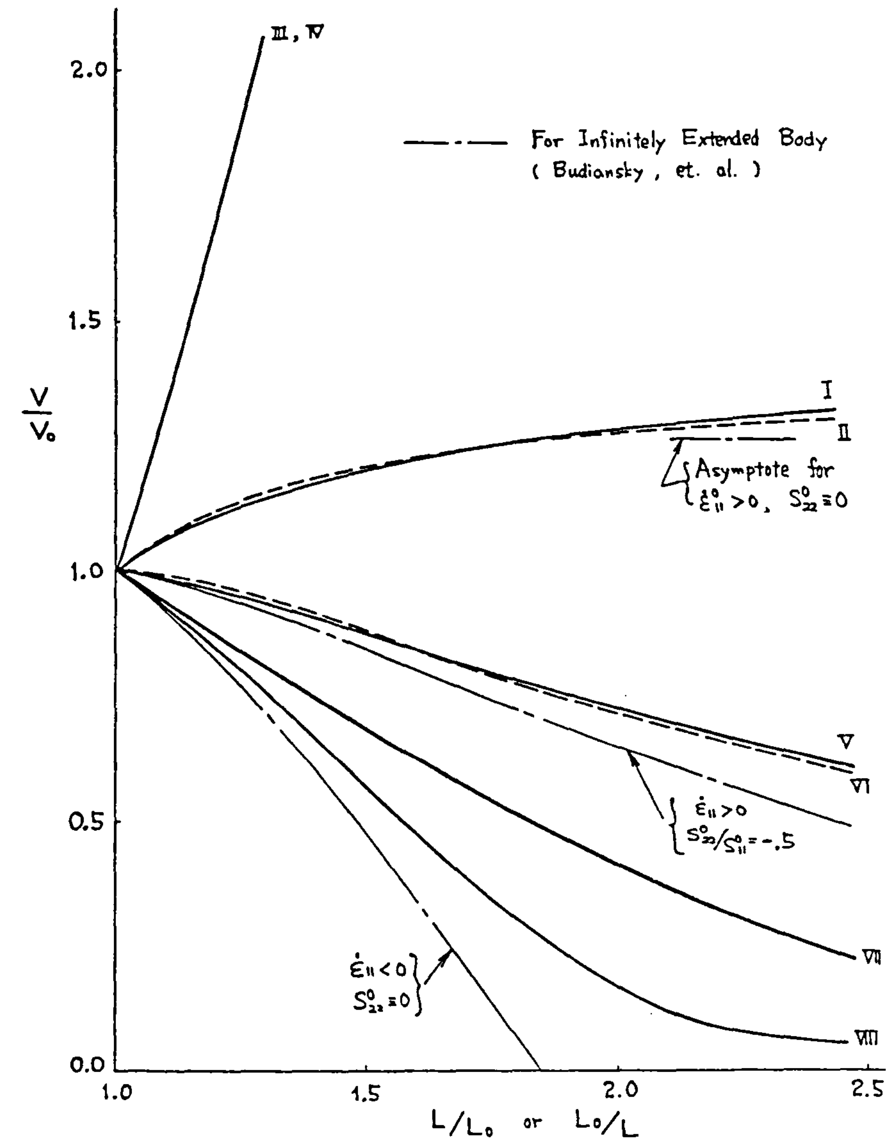
Table 1: Initial and loading conditions for considered cases of void growth problems; $\alpha_0 = \beta_0 = 1.0$, and $f_0 = .005$.

| Case | $\gamma_0$ | $\zeta_0$ | $S^0_{22}/S^0_{11}$ | $S^0_{33}/S^0_{11}$ | $\dot{\varepsilon}^0_{11}$ |
|---|---|---|---|---|---|
| I | 10 | 2 | 0 | 0 | .05 |
| II | 1 | 1 | 0 | 0 | .05 |
| III | 10 | 2 | .5 | .5 | .05 |
| IV | 1 | 1 | .5 | .5 | .05 |
| V | 10 | 2 | -.5 | -.5 | .05 |
| VI | 1 | 1 | -.5 | -.5 | .05 |
| VII | 10 | 2 | 0 | 0 | -.05 |
| VIII | 1 | 1 | 0 | 0 | -.05 |

Table 2: Geometrical data for grain boundary configuration in a unit cell.

| r | $\frac{x^r_{01}}{\Lambda_1}$ | $\frac{x^r_{02}}{\Lambda_2}$ | $\theta^r$ | $R^r$ | $f_r$ |
|---|---|---|---|---|---|
| 1 | $-\frac{7}{24}$ | $\frac{3}{8}$ | $\frac{\pi}{3}$ | $\frac{1}{6}$ | $\frac{t_0}{6\sqrt{3}}$ |
| 2 | $-\frac{5}{12}$ | $\frac{1}{4}$ | 0 | $\frac{1}{6}$ | $\frac{t_0}{6\sqrt{3}}$ |
| 3 | $-\frac{1}{4}$ | 0 | $-\frac{\pi}{3}$ | $\frac{1}{3}$ | $\frac{t_0}{3\sqrt{3}}$ |
| 4 | $-\frac{5}{24}$ | $-\frac{3}{8}$ | $\frac{\pi}{3}$ | $\frac{1}{6}$ | $\frac{t_0}{6\sqrt{3}}$ |
| 5 | 0 | $-\frac{1}{4}$ | 0 | $\frac{1}{3}$ | $\frac{t_0}{3\sqrt{3}}$ |
| 6 | $\frac{5}{24}$ | $-\frac{3}{8}$ | $-\frac{\pi}{3}$ | $\frac{1}{6}$ | $\frac{t_0}{6\sqrt{3}}$ |
| 7 | $\frac{1}{4}$ | 0 | $\frac{\pi}{3}$ | $\frac{1}{3}$ | $\frac{t_0}{3\sqrt{3}}$ |
| 8 | $\frac{5}{12}$ | $\frac{1}{4}$ | 0 | $\frac{1}{6}$ | $\frac{t_0}{6\sqrt{3}}$ |
| 9 | $\frac{7}{24}$ | $\frac{3}{8}$ | $-\frac{\pi}{3}$ | $\frac{1}{6}$ | $\frac{t_0}{6\sqrt{3}}$ |



III, IV
2.0
1.5
1.0
0.5
0.0
V/V₀
For Infinitely Extended Body
( Budiansky , et. al. )
I
II
Asymptote for
V
VI
VII
VIII
1.0
1.5
2.0
2.5
L/L₀ or L₀/L


FIG. 1

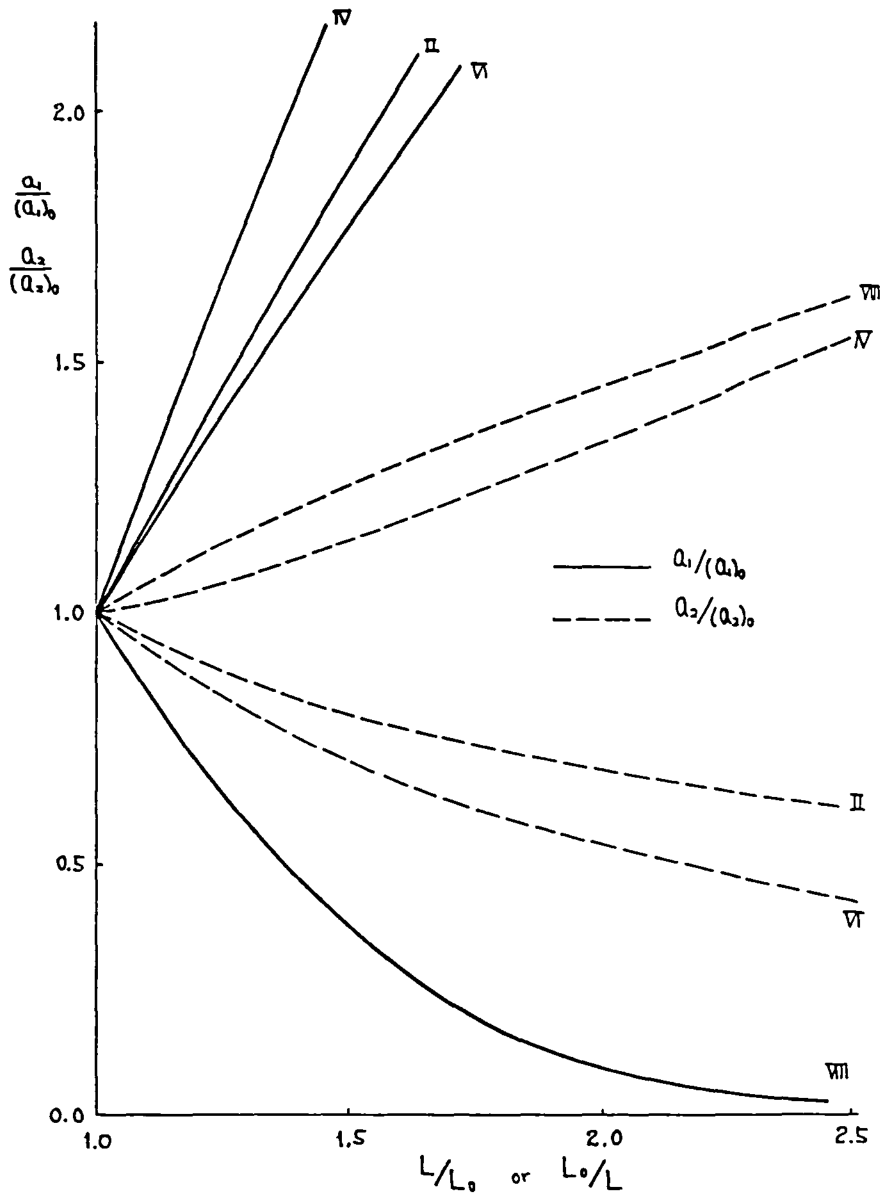



FIG. 2

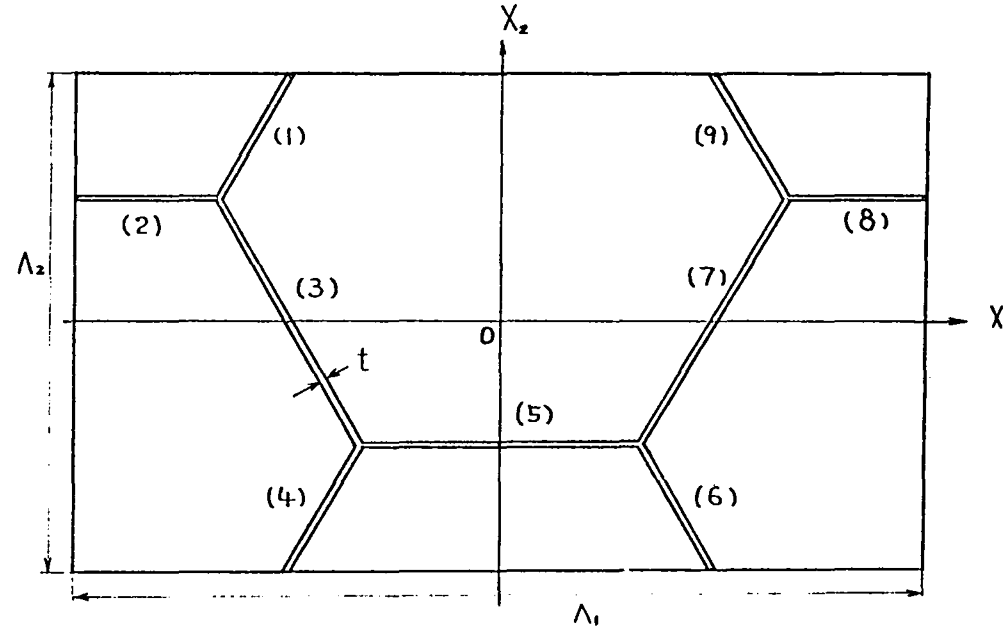



FIG. 3: A unit cell containing nine segments of grain boundary

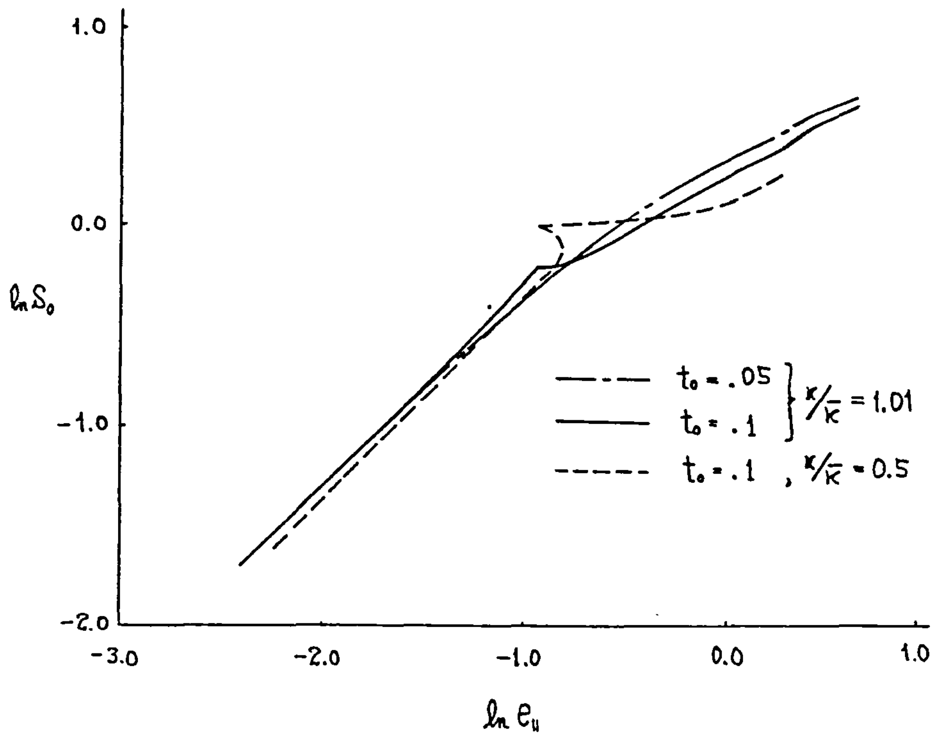



FIG. 4

A THEORY FOR THERMOVISCOPLASTICITY
FOR MECHANICAL AND THERMAL LOADING

E. Krempl
Rensselaer Polytechnic Institute
Troy, New York 12181

and

E.P. Cernocky
University of Colorado
Boulder, Colorado 80302

Abstract

A coupled isotropic thermoviscoplasticity theory for small strain is proposed. The theory consists of a mechanical constitutive equation and a constitutive assumption for the heat equation. These equations are separately postulated but are coupled through their common linear dependence upon stress rate and the mechanical strain rate tensors and the time rate of temperature. The equations depend nonlinearity on the stress and strain tensors through the overstress tensor which is the difference between the stress tensor and the equilibrium stress tensor (obtained as the loading rate approaches zero) and on the absolute temperature. The concept of a yield surface is not used and the transition from linear thermoelastic behavior to nonlinear inelastic behavior is smooth. Extensions of the theory to cyclic loading are under development.

The theory is first applied to conditions of homogeneous deformation where the temperature changes in the material are induced by deformation alone. For adiabatic conditions numerical experiments (the integration of the coupled nonlinear differential equations for the conditions employed in materials testing using postulated material functions) show that the theory reproduces initial thermoelastic behavior (cooling (heating) in uniaxial tension (compression), isothermal behavior in torsion) followed by inelastic heating in any state of stress during monotonic loading. The amount of deformation induced temperature change is negligible unless the loading is very fast. During cyclic plastic loading the temperature increase can be considerable and it is shown that the predictions of the theory compare very well with experiments performed at room temperature on Type 304 Stainless Steel and on a 3.5 Ni-Mo-V steel.

When large temperature changes are imposed the deformation induced temperature changes can be neglected. The numerical experiments involve in this case the uniformly changing temperature and the mechanical loading as inputs (no heat conduction is allowed). Although other possibilities exist only the elastic modulus is assumed to be a function of temperature. The response of the model is shown for heating and thermal cycling under mechanical constraint (thermal fatigue) and for combined thermal and mechanical cycling of a uniaxial bar. It is shown that the response depends on the rate of temperature application and on the temperature at which clamping occurs.

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