

CONSTITUTIVE MODELING OF SUPERALLOY SINGLE CRYSTALS AND DIRECTIONALLY SOLIDIFIED MATERIALS

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A unified viscoplastic constitutive relation based on crystallographic slip theory is developed for the deformation analysis of nickel-base face-centered cubic superalloy single crystals at elevated temperature. The single crystal theory is then embedded in a self-consistent method to derive a constitutive relation for a directionally solidified material comprised of a polycrystalline aggregate of columnar cylindrical grains. One of the crystallographic axes of the cylindrical crystals points in the columnar direction whilst the remaining crystallographic axes are oriented at random in the basal plane perpendicular to the columnar direction. These constitutive formulations are currently being coded in FORTRAN for use in nonlinear finite element and boundary element programs. An experimental program to determine the biaxial tension-torsion behavior of PWA 1480 single crystal tubular specimens at 1600°F is also underway.

INTRODUCTION

This paper represents a first quarterly progress report on a program to develop anisotropic constitutive equations for use in modeling the multiaxial viscoplastic stress-strain response of single crystal and directionally solidified gas turbine alloys at elevated temperature. Two approaches are being pursued. The first approach consists of modeling the anisotropic response from a macroscopic continuum point of view, whilst the second approach consists of taking a micromechanics viewpoint using crystal plasticity concepts. Tubular specimens of the single crystal superalloy PWA 1480 are currently being machined. Tension-torsion experiments on tubular specimens of PWA 1480 will be conducted at 1600°F to provide a data base for exercising the theoretical formulations. The anisotropic viscoplastic theories will be incorporated into a nonlinear finite element code since the non-uniform stress distribution in the tubular specimens will require the solution of a boundary value problem for data reduction purposes.

SINGLE CRYSTAL ANALYSIS

An analysis of single crystal superalloys undergoing steady state creep deformation was presented by Paslay, Wells and Leverant [1] in 1970 using a theoretical formulation based on crystallographic slip theory of face-centered cubic materials. In 1971 the theory was applied by Paslay, Wells, Leverant and Burck [2] to describe the creep behavior of single crystal nickel-base superalloy tubes under biaxial tension. Steady state creep formulations suitable for the analysis of single crystals were used by Brown [3] in 1970 and by Hutchinson [4] in 1976 to predict the behavior of polycrystalline materials whose aggregate consists of randomly oriented single crystal grains. Recently, Weng [5] has developed a single crystal creep formulation which accounts for transient (primary) as well as steady state (secondary) creep. However, in order to describe the combined plastic and creep behavior of polycrystalline materials, Weng combines the rate-independent and rate-dependent components of crystal behavior in such a way that each component is governed by a separate constitutive relation. The averaging of the single crystal creep relations to obtain the overall macroscopic creep response of the polycrystalline aggregate is easily accomplished by using Kroner's self-consistent method [6]. In a general analysis the constitutive relations for the overall macroscopic plastic response of the polycrystalline aggregate must be obtained using Hill's self-consistent method [7]. Kroner's method for calculating the macroscopic creep properties of a polycrystalline aggregate of single crystals is explicit in nature; but Hill's method for calculating the macroscopic plastic properties is implicit in nature and requires lengthy iterative computations.

In the decade of the seventies the creep and plastic responses of materials were combined into unified viscoplastic formulations [8]. These formulations differ from steady state creep theories by introducing history dependent state variables to account for primary creep and plasticity. Most of these unified theories exhibit an elastic response under instantaneous deformation. This instantaneous elastic response occurs because the inelastic strain rate is assumed to depend only on stress, state variables and temperature and not on the rates of these variables. These unified theories may, therefore, be integrated in time by means of an explicit Euler forward difference method. Macroscopic properties of a polycrystalline aggregate, comprised of single crystal grains which are assumed to deform according to a unified viscoplastic slip process, can therefore be obtained by means of Kroner's explicit self-consistent method.

In the unit cell of the face-centered cubic crystal shown in Figure 1 we denote by \underline{m}_i a unit vector in the i^{th} slip direction (say of type $\langle 110 \rangle$), whilst \underline{n}_i is a unit vector in the normal direction to the slip plane (of type $\{111\}$) of which \underline{m}_i constitutes a slip direction. The four octahedral $\{111\}$ planes and the twelve corresponding $\langle 110 \rangle$ slip directions (three on each plane) are shown in Figure 1.

From the geometry of the unit cubic cell in Figure 1 the unit vectors are given by

$$\underline{m}_1 = (\underline{i} - \underline{k})/\sqrt{2}, \quad \underline{m}_2 = (-\underline{j} + \underline{k})/\sqrt{2}, \quad \underline{m}_3 = (\underline{i} - \underline{j})/\sqrt{2}, \quad \underline{m}_4 = (\underline{i} - \underline{k})/\sqrt{2},$$

$\underline{m}_5 = (\underline{i} + \underline{j})/\sqrt{2}$, $\underline{m}_6 = (\underline{j} + \underline{k})/\sqrt{2}$, $\underline{m}_7 = (\underline{i} + \underline{j})/\sqrt{2}$, $\underline{m}_8 = (-\underline{j} + \underline{k})/\sqrt{2}$,
 $\underline{m}_9 = (\underline{i} + \underline{k})/\sqrt{2}$, $\underline{m}_{10} = (\underline{j} + \underline{k})/\sqrt{2}$, $\underline{m}_{11} = (\underline{i} - \underline{j})/\sqrt{2}$, $\underline{m}_{12} = (\underline{i} + \underline{k})/\sqrt{2}$,
 with

$$\underline{n}_1 = \underline{n}_2 = \underline{n}_3 = (\underline{i} + \underline{j} + \underline{k})/\sqrt{3} , \underline{n}_4 = \underline{n}_5 = \underline{n}_6 = (\underline{i} + \underline{j} - \underline{k})/\sqrt{3} ,$$

$$\underline{n}_7 = \underline{n}_8 = \underline{n}_9 = (\underline{i} - \underline{j} - \underline{k})/\sqrt{3} , \underline{n}_{10} = \underline{n}_{11} = \underline{n}_{12} = (-\underline{i} - \underline{j} + \underline{k})/\sqrt{3} ,$$

where \underline{i} , \underline{j} , \underline{k} are unit vectors along the x,y,z crystallographic axes.

Figure 2 shows a single crystal whose global axes are denoted by x^* , y^* , z^* and whose crystallographic axes are denoted by x,y,z. If Q denotes the orthogonal tensor which rotates the crystallographic (unstarred) axes into the global (starred) axes, viz., $x_i^* = Q_{ij}x_j$, then the stress tensor $\underline{\sigma}$ and the strain rate tensor $\underline{\dot{\epsilon}}$ in the crystallographic axes may be obtained from the stress tensor $\underline{\sigma}^*$ and the strain rate tensor $\underline{\dot{\epsilon}}^*$ in the global system from the usual transformation relations,

$$\underline{\sigma} = \underline{Q} \cdot \underline{\sigma}^* \cdot \underline{Q}^T \quad \text{and} \quad \underline{\dot{\epsilon}} = \underline{Q} \cdot \underline{\dot{\epsilon}}^* \cdot \underline{Q}^T . \quad (1)$$

The assumption is now made that any of the unified viscoplastic theories discussed in Reference [8], when specialized to the case of shear deformation, is a valid constitutive relation in each of the twelve crystallographic slip directions. In the r^{th} slip direction the resolved shear stress, π_{mn}^r , is obtained from the relation

$$\pi_{mn}^r = \underline{m}_r \cdot \underline{\sigma} \cdot \underline{n}_r \quad \text{for } r = 1, 2, \dots, 12 . \quad (2)$$

It is further assumed, in a manner analogous to the unified isotropic viscoplastic models, that the applicable relation governing the inelastic shear strain rate in the r^{th} slip direction is

$$\dot{\gamma}_r = K_r^{-p} \left\{ (\pi_{mn}^r - \omega_{mn}^r) |\pi_{mn}^r - \omega_{mn}^r|^{p-1} + \alpha_{mn} (\pi_{mn}^r - \omega_{mn}^r) |\pi_{mn}^r - \omega_{mn}^r|^{p-1} \right. \\
+ \alpha_{nn} (\pi_{nn}^r - \omega_{nn}^r) |\pi_{nn}^r - \omega_{nn}^r|^{p-1} + \alpha_{zz} (\pi_{zz}^r - \omega_{zz}^r) |\pi_{zz}^r - \omega_{zz}^r|^{p-1} \\
\left. + 2\alpha_{mz} (\pi_{mz}^r - \omega_{mz}^r) |\pi_{mz}^r - \omega_{mz}^r|^{p-1} + 2\alpha_{nz} (\pi_{nz}^r - \omega_{nz}^r) |\pi_{nz}^r - \omega_{nz}^r|^{p-1} \right\} , \quad (3)$$

where K_r and ω_{pq}^r (with p and q = m,n,z) denote the drag stress and equilibrium (rest or back) stress in the r^{th} slip direction. The expression for π_{mn}^r is defined in equation (2). Terms such as π_{mz}^r denote, by analogy, expressions of the type

$$\pi_{mz}^r = \underline{m}_r \cdot \underline{\sigma} \cdot \underline{z}_r , \quad (4)$$

where \underline{z}_r denotes a unit vector perpendicular to the unit vectors \underline{m}_r and \underline{n}_r . The vector \underline{z}_r is in the slip plane containing the vector \underline{m}_r and the vectors \underline{m}_r , \underline{n}_r , \underline{z}_r form an orthogonal triad for the r^{th} slip system. In equation (3) the tensor α_{pq} represents the effect of the non-Schmid factors [9] upon the inelastic strain rate in the r^{th} slip direction.

For example, the term containing α_{mn} represents the effect of the resolved stress, normal to the slip plane containing the r^{th} slip direction, on the inelastic strain rate in the r^{th} slip direction. Such terms can represent the effect of a pressure dependent inelastic strain rate. The dominant term in equation (3) is the Schmid type term containing the expression π_{mn}^r ; estimates of the magnitude of the non-Schmid type terms containing the tensor α_{pq} have been given by Asaro and Rice in Reference [10].

To complete the constitutive formulation it is necessary to specify the growth relations for the equilibrium and drag stress state variables. The equilibrium stress in the r^{th} slip system may be assumed to evolve according to the evolution equation

$$\dot{\omega}_{pq}^r = g_{pq}^1 \dot{\gamma}_r - g_{pq}^2 |\dot{\gamma}_r| \omega_{pq}^r - g_{pq}^3 |\omega_{pq}^r|^{m-1} \omega_{pq}^r, \quad (5)$$

where $g_{pq}^1, g_{pq}^2, g_{pq}^3$ and m are temperature dependent material constants. A simplifying assumption is to take

$$\lim_{\substack{R_r \rightarrow \infty \\ \dot{\gamma}_r \rightarrow \infty}} \frac{\omega_{pq}^r}{\pi_{pq}^r} = \lim_{\substack{R_r \rightarrow \infty \\ \dot{\gamma}_r \rightarrow \infty}} \frac{\omega_{mn}^r}{\pi_{mn}^r} \quad \text{for } p, q = m, n, z, \quad (6)$$

where the cumulative inelastic strain is defined by

$$R_r = \int_0^t \left| \frac{d\gamma_r}{d\epsilon} \right| d\epsilon. \quad (7)$$

Equation (6) states that the ratio of the saturated equilibrium (back) stress, i.e. the equilibrium stress for continued inelastic straining ($R_r \rightarrow \infty$) under fast straining conditions ($\dot{\gamma}_r \rightarrow \infty$), to the resolved shear stress in the same direction, is equal for all the non-Schmid systems. Moreover, the ratio is equal to the ratio of the saturated equilibrium stress to the resolved shear stress for the Schmid-type components, ω_{mn}^r and π_{mn}^r . Under continued inelastic straining the equilibrium stress saturates and $\dot{\omega}_{pq}^r \rightarrow 0$. Under fast straining conditions ($\dot{\gamma}_r \rightarrow \infty$) equation (5) shows that the saturated equilibrium stress is given by the relation

$$\lim_{\substack{R_r \rightarrow \infty \\ \dot{\gamma}_r \rightarrow \infty}} \omega_{pq}^r = \frac{g_{pq}^1}{g_{pq}^2}, \quad (8)$$

since the thermal recovery term containing the material constant g_{pq}^3 can be neglected for $\dot{\gamma}_r \rightarrow \infty$. The material constants g_{pq}^2 must therefore satisfy the relation

$$\frac{g_{pq}^1}{g_{pq}^2 \pi_{pq}^r (R_r \rightarrow \infty)} = \frac{g_{mn}^1}{g_{mn}^2 \pi_{mn}^r (R_r \rightarrow \infty)}. \quad (9)$$

Assuming the constants g_{mn}^1 and g_{mn}^2 and the limiting saturated value of the resolved shear stress π_{mn}^r are known for the Schmid-type terms, equation (9) determines the ratio of g_{pq}^1 to g_{pq}^2 for the non-Schmid terms. If it is further assumed that the initial hardening rate for the non-Schmid equilibrium stresses are all equal to the Schmid equilibrium stress hardening rate, then $g_{pq}^1 = g_{mn}^1$ for $\ell = 1, 2$ and $p, q = m, n, z$.

The drag stress may be assumed to grow according to the evolution equation

$$\dot{K}_r = \sum_{k=1}^n h_{rk} |\dot{\gamma}_k|, \quad (10)$$

in which the hardening moduli are given by

$$h_{rk} = [q + (1-q)\delta_{rk}] e^{-h \sum_{i=1}^n \int_0^t |\dot{\gamma}_i| d\tau} \quad (11)$$

The hardening moduli h_{rk} defined in equation (10) account for the latent hardening effects observed in single crystal materials, and equation (11) is similar in form to that proposed by Hutchinson [11], Asaro [12] and Peirce, Asaro and Needleman [13]. Numerous forms for the hardening moduli h_{rk} have been proposed in the literature and a review of hardening moduli may be found by consulting Havner's papers (cf. Reference [14]). The drag stress evolution equation does not contain thermal recovery terms, but these terms can easily be included in the formulation.

The shear slip strain rates may now be resolved into the crystallographic system and summed for each slip system to obtain the inelastic strain rate tensor with respect to the crystallographic axes in the form

$$\dot{\underline{\epsilon}} = \sum_{k=1}^n \frac{1}{2} \dot{\gamma}_k (\underline{n}_k \underline{m}_k + \underline{m}_k \underline{n}_k) \quad (12)$$

Finally, the stress rate tensor with respect to the crystallographic axes is determined from the relation

$$\dot{\underline{\sigma}} = \underline{D}^c : (\dot{\underline{\epsilon}} - \dot{\underline{\epsilon}}) \quad (13)$$

where \underline{D}^c is the anisotropic elasticity tensor for the face-centered cubic crystal referred to the crystallographic axes.

The variables can now be updated in the Euler forward difference form:

$$\begin{aligned} \underline{\sigma} &= \underline{\sigma} + \dot{\underline{\sigma}} \Delta t, \quad \underline{\epsilon} = \underline{\epsilon} + \dot{\underline{\epsilon}} \Delta t, \quad \omega_{pq}^r = \omega_{pq}^r + \dot{\omega}_{pq}^r \Delta t, \\ \underline{\gamma}_r &= \underline{\gamma}_r + \dot{\underline{\gamma}}_r \Delta t, \quad \underline{\sigma}^* = \underline{Q}^T \cdot \underline{\sigma} \cdot \underline{Q}, \quad \underline{\epsilon}^* = \underline{Q}^T \cdot \underline{\epsilon} \cdot \underline{Q}, \end{aligned} \quad (14)$$

where Δt is the current time increment. The process may then be repeated by integrating equations (1), (2), (3), (4), (5), (10), (11) for each time increment.

The preceding discussion has focussed on slip which occurs on the $\{111\}$ octahedral planes in the $\langle 110 \rangle$ type directions of face-centered cubic nickel-base superalloys. Paslay, Wells, Leverant and Burck [1,2] also found that slip occurs under creep conditions on the $\{111\}$ planes in the $\langle 112 \rangle$ type directions. Cube slip on the crystallographic faces was also found to occur. For each different slip system the foregoing theory

is altered only by virtue of having different slip and normal vectors defining the triad \underline{m} , \underline{n} and \underline{z} . In general, the total inelastic strain rate may be written as the sum,

$$\dot{\underline{\epsilon}} = \sum_{i=1}^N \lambda_i \dot{\underline{\epsilon}}_i, \quad (15)$$

where $\dot{\underline{\epsilon}}_1$ is due to $\{111\} \langle 110 \rangle$ type slip, $\dot{\underline{\epsilon}}_2$ is due to $\{111\} \langle 112 \rangle$ type slip, $\dot{\underline{\epsilon}}_3$ is due to cube slip, etc. Such a combination was stated to be required to model primary creep behavior in Reference [1] by Paslay, Wells and Leverant. It is possible that $\{111\} \langle 112 \rangle$ type primary creep may evolve into $\{111\} \langle 110 \rangle$ type secondary creep as described by Leverant, Kear and Oblak in Reference [15]. In this instance it may be necessary to modify the theory so that the λ_i evolve with deformation, inelastic strain rate and temperature according to evolution growth equations similar to that employed for the equilibrium and drag stress state variables. This mixing of different slip systems to model the anisotropy of nickel-base superalloys was also stated by Ezz, Pope and Paidar [16] to be necessary in order to model tension-compression flow stress asymmetry observed in nickel-base superalloys.

DIRECTIONALLY SOLIDIFIED ANALYSIS

A model for directionally solidified alloys can be constructed by making use of a suitable self-consistent method to average the results of the single crystal viscoplastic constitutive theory. The directionally solidified material consists of aligned columnar single crystal grains which are oriented at random in the basal plane perpendicular to the cylindrical growth direction. This random orientation of the grains produces a material with transversely isotropic properties.

The directionally solidified material comprised of an aggregate of single crystal columnar grains may therefore be modeled in the following manner. We first choose a particular single crystal columnar grain and replace the aggregate of single crystal grains surrounding the chosen grain by a transversely isotropic material. The properties of this surrounding transversely isotropic material are found by averaging the properties of the chosen single crystal grain about its cylindrical growth axis. It is then possible to relate the stress and strain increments in the single crystal grain to those in the surrounding transversely isotropic matrix by means of the method proposed by Eshelby [17] in 1957.

Viscoplastic formulations which exhibit an instantaneous elastic response can be integrated by means of an Euler forward difference method. In physical terms this integration process consists of letting the material creep at constant stress at the level $\underline{\sigma}$ appropriate to the beginning of the increment for a time interval Δt . After the creep increment is completed the material is subjected to an instantaneous strain increment $\Delta \underline{\epsilon} - \Delta \underline{\epsilon}_c$, where $\Delta \underline{\epsilon}$ is the total strain increment during the time increment Δt and $\Delta \underline{\epsilon}_c$ is the completed creep strain increment. The instantaneous application of the strain increment $\Delta \underline{\epsilon} - \Delta \underline{\epsilon}_c$ induces an elastic stress increment given by Hooke's law in the form $\Delta \underline{\sigma} = \underline{D}:(\Delta \underline{\epsilon} - \Delta \underline{\epsilon}_c)$ where \underline{D} is the elasticity tensor for the material.

Let \mathcal{D}^c and \mathcal{D}^m denote the fourth rank cubic and transversely isotropic elasticity tensors for the single crystal and the surrounding matrix, respectively. In the cylindrical single crystal grain the inelastic strain increment is denoted by $\Delta \underline{\epsilon}$ and the corresponding quantity in the matrix is denoted by $\langle \Delta \underline{\epsilon} \rangle$. The quantity $\langle \Delta \underline{\epsilon} \rangle$ is obtained from $\Delta \underline{\epsilon}$ by averaging $\Delta \underline{\epsilon}$ over all angular orientations (viz. from 0 to 2π) in the basal plane perpendicular to the cylindrical growth axis. In the single crystal grain the constitutive relation has the form

$$\Delta \sigma_{ij} = D_{ijkl}^c (\Delta \epsilon_{kl} - \Delta c_{kl}), \quad (16)$$

whilst in the directionally solidified matrix the constitutive form is

$$\langle \Delta \sigma_{ij} \rangle = D_{ijkl}^m (\langle \Delta \epsilon_{kl} \rangle - \langle \Delta c_{kl} \rangle). \quad (17)$$

Given a known strain increment $\langle \Delta \epsilon_{kl} \rangle$ in the directionally solidified matrix, the object is to determine the corresponding inelastic strain increment Δc_{kl} in the single crystal cylinder and then average this quantity by means of the relation

$$\langle \Delta c_{kl} \rangle = \frac{1}{2\pi} \int_0^{2\pi} \Delta c_{kl}(\theta) d\theta, \quad (18)$$

where θ is the angle between the crystallographic axes x, y in the specimen and the global axes x^*, y^* in the matrix, with the z, z^* axes aligned in the cylindrical crystal's growth direction. The stress increment in the directionally solidified matrix is then determined by equation (17).

The first step consists of determining the state of stress and strain in the cylindrical crystal grain when the matrix and crystal undergo creep for a time increment Δt . A preliminary step in this analysis consists of replacing the single crystal grain by a fictitious material which has elastic and inelastic properties which differ from those of the single crystal but in which the elastic properties are the same as that of the transversely isotropic matrix with elasticity tensor \mathcal{D}^m . Eshelby's cutting, straining and welding operations [17] are now applied to the fictitious crystal grain.

The fictitious cylindrical grain is now cut out of the matrix and the instantaneous shapes of the grain and resulting cylindrical hole in the matrix are maintained by appropriate equal and opposite surface tractions applied to the respective cylindrical surfaces of the grain and hole. The stress in the matrix is denoted by $\langle \underline{\sigma} \rangle$ and that in the fictitious grain by $\underline{\sigma}$, where $\underline{\sigma}$ is the stress state in the actual single crystal grain. From Eshelby's results, if the strain history in the matrix is homogeneous, the resulting stress in the actual and fictitious cylindrical grains will be constant throughout the cylindrical volume. This will be demonstrated subsequently. The fictitious cylindrical grain and the surrounding matrix are now assumed to undergo creep responses for a time increment Δt at their respective stress levels of $\underline{\sigma}$ and $\langle \underline{\sigma} \rangle$. In the grain the resulting creep strain increment is denoted by $\Delta \underline{\epsilon}^T$ and the corres-

ponding creep strain increment in the matrix is $\langle \Delta \underline{\underline{\epsilon}} \rangle$. If incremental surface tractions are instantaneously applied to the cylindrical surface of the fictitious grain so that it is elastically strained by an amount $-\Delta \underline{\underline{\epsilon}}^T$, it will regain the original size and shape which it had upon removal from the matrix prior to the creep response. If it is subsequently elastically strained by an amount $\langle \Delta \underline{\underline{\epsilon}} \rangle$ through the application of a further set of incremental tractions applied instantaneously to the cylindrical surface of the grain, it will fit back into the matrix from which it was removed. The fictitious grain and matrix now fit compatibly together, and the strain increment experienced by the grain is $-\Delta \underline{\underline{\beta}}$ where

$$\Delta \beta_{kl} = \Delta \epsilon_{kl}^T - \langle \Delta c_{kl} \rangle. \quad (19)$$

However, a layer of surface traction exists on the cylindrical surface boundary between the grain and the matrix. This layer of surface traction is given in magnitude by the relation

$$\Delta t_i = n_j \Delta \sigma_j = n_j D_{ijkl}^m (\langle \Delta c_{kl} \rangle - \Delta \epsilon_{kl}^T) = -n_j D_{ijkl}^m \Delta \beta_{kl},$$

and can be removed by the application of an equal and opposite layer of surface body force of magnitude

$$\Delta f_i = n_j D_{ijkl}^m \Delta \beta_{kl}. \quad (20)$$

The displacement increment Δu_i^c induced in the fictitious grain due to the application of surface tractions Δf_i over its cylindrical surface is given by

$$\Delta u_i^c = \iint_S \Delta f_j G_{ij}(\underline{r} - \underline{r}') dS(\underline{r}') \quad (21)$$

where $G_{ij}(\underline{r} - \underline{r}')$ is the elastic Green's function for the transversely isotropic matrix and the fictitious grain. Application of Gauss' divergence theorem to the surface integral produces the result

$$\begin{aligned} \Delta u_p^c &= \iint_S n_i D_{ijkl}^m \Delta \beta_{kl} G_{pj}(\underline{r} - \underline{r}') dS(\underline{r}') \\ &= D_{ijkl}^m \Delta \beta_{kl} \iiint_V \frac{\partial G_{pj}(\underline{r} - \underline{r}')}{\partial x_i} dV(\underline{r}') \\ &= -D_{ijkl}^m \Delta \beta_{kl} \frac{\partial}{\partial x_i} \iiint_V G_{pj}(\underline{r} - \underline{r}') dV(\underline{r}'). \end{aligned} \quad (22)$$

The resulting strain increment $\Delta \epsilon_{ip}^c$ in the fictitious grain due to this annihilation of the incremental surface traction built up during the creep response of the fictitious grain and the matrix is

$$\Delta \epsilon_{ip}^c = \frac{1}{2} \left(\frac{\partial (\Delta u_i^c)}{\partial x_p} + \frac{\partial (\Delta u_p^c)}{\partial x_i} \right) = S_{iplm} \Delta \beta_{lm}, \quad (23)$$

where the Eshelby tensor $\underline{\underline{S}}$ is defined by the relation

$$S_{iplm} = -\frac{1}{2} D_{kijm}^m \left\{ \frac{\partial^2}{\partial x_i \partial x_k} \iiint_V G_{pj}(\underline{r} - \underline{r}') dV(\underline{r}') + \frac{\partial^2}{\partial x_p \partial x_k} \iiint_V G_{ij}(\underline{r} - \underline{r}') dV(\underline{r}') \right\}. \quad (24)$$

The strain increment induced in the fictitious grain in order to make it fit compatibly in the matrix is given by $-\Delta \beta_{ij}$, whilst the additional

strain induced in the grain by removing the unwanted surface traction increment Δt_i is given by $\Delta \epsilon_{ij}^c$. At the end of the creep increment the total strain increment induced in the fictitious grain is given by $\Delta \epsilon_{ij}^c - \Delta \beta_{ij}$, or from equation (23), by $S_{ijkl} \Delta \beta_{kl} - \Delta \beta_{ij}$. The stress increment in the grain is therefore

$$\Delta \sigma_{ij} = D_{ijkl}^m (S_{klmn} - I_{klmn}) \Delta \beta_{mn}, \quad (25)$$

where I is the fourth rank identity tensor. Note that the strain increment responsible for changing the size of the cylindrical grain from the size it had when it was placed back into the matrix is $\Delta \epsilon_{ij}^c = S_{ijkl} \Delta \beta_{kl}$, since the change in size is due to the annihilation of the surface traction increment Δt_i by the equal and opposite traction increment Δf_i .

Now consider the actual situation where the cylindrical grain has its own anisotropic elastic constant tensor with cubic symmetry, D^c . We remove the cylinder from the matrix, as before, and let the cylindrical grain undergo a creep strain increment $\Delta \epsilon$ in time Δt and the matrix undergo a creep strain increment $\langle \Delta \epsilon \rangle$. If we now apply surface traction increments instantaneously to the cylindrical boundary so that the cylinder is elastically strained by an amount $\langle \Delta \epsilon \rangle - \Delta \epsilon$, it will fit back into the matrix from which it was removed. Moreover, since the matrix creep strain increment $\langle \Delta \epsilon \rangle$ is the same as that in the problem with the fictitious cylinder, the cylindrical grain will have the same size and shape as the fictitious cylinder had when it was put back into the matrix. The strain increment responsible for changing the size of the cylindrical grain from the size it had when it was placed back into the matrix to the size in its final configuration is $S_{klmn} \Delta \beta_{mn}$. Hence, if the actual cylindrical grain is strained by the increment $S_{klmn} \Delta \beta_{mn} + \langle \Delta \epsilon_{kl} \rangle - \Delta \epsilon_{kl}$, it will have the same final size as the previously considered fictitious cylindrical grain with transversely isotropic elastic properties. The stress increment in the actual cylinder due to the strain increment

$$\Delta \sigma_{ij} = D_{ijkl}^c \{ S_{klmn} \Delta \beta_{mn} + \langle \Delta \epsilon_{kl} \rangle - \Delta \epsilon_{kl} \}. \quad (26)$$

If the stress increments in equations (25) and (26) are equal, the actual cylindrical grain which has the elasticity tensor D^c appropriate to cubic symmetry and which undergoes an increment of transformation strain $\Delta \beta$, may be replaced with the fictitious cylindrical grain with elasticity tensor D^m equal to that of the matrix without upsetting continuity of displacements and tractions across the cylinder-matrix interface. Equating (25) and (26) shows that

$$\Delta \beta_{ij} = [(D_{ijkl}^c - D_{ijkl}^m) S_{klmn} + D_{ijmn}^m]^{-1} D_{mnpq}^c \{ \Delta \epsilon_{pq} - \langle \Delta \epsilon_{pq} \rangle \}. \quad (27)$$

If this transformation strain increment occurs in a cylinder with elasticity tensor D^m , the stress increment in the cylinder is equal to that which actually occurs in the single crystal cylinder with elasticity tensor D^c undergoing a transformation strain increment $\Delta \epsilon - \langle \Delta \epsilon \rangle$. Substitution of the expression for $\Delta \beta$ into equation (25) [or (26)] gives the stress increment in the cylindrical single crystal grain at the end of the creep re-

sponse in the form

$$\Delta\sigma_{ij} = D_{ijkl}^m (S_{klmn} - I_{klmn}) \left[(D_{mnpq}^c - D_{mnpq}^m) S_{pqrs} + D_{mnr}^m \right]^{-1} \times D_{rstu}^c \{ \Delta c_{tu} - \langle \Delta c_{tu} \rangle \}. \quad (28)$$

According to the Euler forward difference integration method the crystal grain and matrix are now to be instantaneously loaded with the elastic strain increment $\langle \Delta \underline{\underline{\epsilon}} \rangle - \langle \Delta \underline{\underline{c}} \rangle$. To this end we first consider the single crystal to be replaced by a fictitious cylinder having the same transversely isotropic properties as the surrounding matrix. If the fictitious cylinder undergoes a stress increment free uniform strain increment $\Delta \underline{\underline{\epsilon}}^T$, the final strain increment inside the cylinder is $(S_{ijkl} - I_{ijkl}) \Delta \underline{\underline{\epsilon}}_{kl}^T$. A uniform strain increment $\langle \Delta \underline{\underline{\epsilon}} \rangle - \langle \Delta \underline{\underline{c}} \rangle$ may now be applied to the matrix and fictitious cylinder to produce the final strain increment of $(S_{ijkl} - I_{ijkl}) \Delta \underline{\underline{\epsilon}}_{kl}^T + \langle \Delta \underline{\underline{\epsilon}}_{ij} \rangle - \langle \Delta c_{ij} \rangle$. The resulting stress increment in the fictitious cylinder is

$$\Delta\sigma_{ij} = D_{ijkl}^m \left\{ (S_{klmn} - I_{klmn}) \Delta \underline{\underline{\epsilon}}_{mn}^T + \langle \Delta \underline{\underline{\epsilon}}_{kl} \rangle - \langle \Delta c_{kl} \rangle \right\}. \quad (29)$$

Only the strain increment $\underline{\underline{\epsilon}} = \Delta \underline{\underline{\epsilon}}^T + \langle \Delta \underline{\underline{\epsilon}} \rangle - \langle \Delta \underline{\underline{c}} \rangle$ is responsible for changing the size of the cylindrical volume, since the strain increment $-\Delta \underline{\underline{\epsilon}}^T$ is used to force the cylindrical volume back to its original size after removal from the matrix. If the actual cylindrical grain with elasticity tensor D^c is now subjected to the strain increment $\underline{\underline{\epsilon}} = \Delta \underline{\underline{\epsilon}}^T + \langle \Delta \underline{\underline{\epsilon}} \rangle - \langle \Delta \underline{\underline{c}} \rangle$ it will acquire the same shape and size as the fictitious cylinder which has elastic properties identical to the matrix. The stress increment in the actual single crystal is then given by

$$\Delta\sigma_{ij} = D_{ijkl}^c \left\{ S_{klmn} \Delta \underline{\underline{\epsilon}}_{mn}^T + \langle \Delta \underline{\underline{\epsilon}}_{kl} \rangle - \langle \Delta c_{kl} \rangle \right\}. \quad (30)$$

The actual and fictitious cylinders now have the same final shape and size and if the stress increments in equations (29) and (30) are equal, the actual crystal cylinder can replace the transversely isotropic cylinder and still preserve continuity of displacements and tractions across the cylinder-matrix interface. Equating (29) and (30) gives

$$\Delta \underline{\underline{\epsilon}}_{ij}^T = - \left[(D_{ijkl}^c - D_{ijkl}^m) S_{klmn} + D_{ijmn}^m \right]^{-1} (D_{mnpq}^c - D_{mnpq}^m) \left\{ \langle \Delta \underline{\underline{\epsilon}}_{pq} \rangle - \langle \Delta c_{pq} \rangle \right\}. \quad (31)$$

Substitution of this result into equation (29) [or (30)] produces the stress increment in the cylinder due to the instantaneous application of the strain increment $\langle \Delta \underline{\underline{\epsilon}} \rangle - \langle \Delta \underline{\underline{c}} \rangle$ in the matrix in the form

$$\Delta\sigma_{ij} = D_{ijkl}^m \left(\langle \Delta \underline{\underline{\epsilon}}_{kl} \rangle - \langle \Delta c_{kl} \rangle \right) - D_{ijkl}^m (S_{klmn} - I_{klmn}) \left[(D_{mnpq}^c - D_{mnpq}^m) S_{pqrs} + D_{mnr}^m \right]^{-1} \times (D_{rstu}^c - D_{rstu}^m) \left\{ \langle \Delta \underline{\underline{\epsilon}}_{tu} \rangle - \langle \Delta c_{tu} \rangle \right\}. \quad (31)$$

At the end of the creep response during the time interval Δt the stress increment in the single crystal cylindrical grain is given by equation (28). When the matrix is further elastically strained by the instantaneous application of the strain increment $\langle \Delta \underline{\underline{\epsilon}} \rangle - \langle \Delta \underline{\underline{c}} \rangle$ the additional stress

increment in the single crystal grain is given by equation (31). Accordingly, the total stress increment in the single crystal due to the application of the strain increment $\langle \Delta \underline{\epsilon} \rangle$ in the time interval Δt is given by the Euler forward difference method as the sum of the stress increments in equations (28) and (31), viz.

$$\Delta \sigma_{ij} = \langle \Delta \sigma_{ij} \rangle + D_{ijkl}^m (S_{klmn} - I_{klmn}) \left[(D_{mnpq}^c - D_{mnpq}^m) S_{pqrs} + D_{mnpq}^m \right]^{-1} \\ \times \left\{ D_{rstu}^c (\Delta c_{tu} - \langle \Delta c_{tu} \rangle) - (D_{rstu}^c - D_{rstu}^m) (\langle \Delta \epsilon_{tu} \rangle - \langle \Delta c_{tu} \rangle) \right\}, \quad (32)$$

where the first term in equation (31) is the definition of the matrix stress increment given in equation (17):

Provided the stress level $\underline{\sigma}$ is known in the single crystal at the beginning of the increment, the single crystal analysis in the preceding section furnishes the value of the inelastic strain increment $\Delta \underline{\epsilon}$. Averaging $\Delta \underline{\epsilon}$ over the basal plane for crystals of different orientation by means of equation (18) then furnishes the value of $\langle \Delta \underline{\epsilon} \rangle$. Assuming that the strain increment in the matrix is given, equation (17) furnishes the required stress increment in the matrix. The stress increment in the single crystal constrained by the transversely isotropic matrix is given by equation (32). All pertinent quantities can now be updated according to the Euler forward difference procedure and the process repeated for the next time increment. A procedure for evaluating the Eshelby tensor $\underline{\underline{S}}$ is given in the appendix.

WORK IN PROGRESS

The single crystal analysis has been coded into a FORTRAN subroutine and is currently undergoing numerical test experiments. Coding of the directionally solidified analysis is due to commence shortly. Single crystal tubular specimens of PWA 1480 are being machined and will be tested at 1600°F under biaxial tension-torsion loading conditions.

APPENDIX

The Eshelby tensor $\underline{\underline{S}}$ is defined by the relation

$$S_{ijklm} = -\frac{1}{2} D_{kijlm}^m \left\{ \frac{\partial^2}{\partial x_i \partial x_k} \iiint_V G_{pj}(\underline{r}-\underline{r}') dV(\underline{r}') + \frac{\partial^2}{\partial x_p \partial x_k} \iiint_V G_{ij}(\underline{r}-\underline{r}') dV(\underline{r}') \right\}, \quad (1)$$

where $G_{ij}(\underline{r}-\underline{r}')$ is the elastic Green's function for the transversely isotropic matrix material. Although the Green's function for transversely isotropic materials is known [18], it is more convenient to work with the Fourier representation of the Green's function. The Fourier transform of $G_{ij}(\underline{r}-\underline{r}')$ is known [19,20] and it can be shown, by taking the Fourier transform of the defining equation, viz.

$$D_{jkmn}^m \frac{\partial^2 G_{im}(\underline{r}-\underline{r}')}{\partial x_k \partial x_n} + \delta_{ij} \delta(\underline{r}-\underline{r}') = 0, \quad (2)$$

and inverting the result, that

$$G_{ij}(\underline{r}-\underline{r}') = \frac{1}{8\pi^3} \iiint_{-\infty}^{\infty} d^3\kappa \frac{M_{ij}^{-1}(\underline{\underline{\xi}})}{\kappa^2} e^{-i\underline{\kappa} \cdot (\underline{r}-\underline{r}')}. \quad (3)$$

In this equation the real part of the Fourier integral corresponds to the Green's function, and the Christoffel tensor $\underline{\underline{M}}$ is defined by

$$M_{ij}(\underline{\underline{\xi}}) = \xi_p D_{pijq}^m \xi_q \quad (4)$$

with

$$\underline{\underline{\xi}} = \underline{\kappa} / \sqrt{\kappa_i \kappa_i} = \underline{\kappa} / \kappa \quad (5)$$

being a unit wave vector in the direction of the Fourier wave vector $\underline{\kappa}$. Introduction of this result into one of the integral terms in the definition of $\underline{\underline{S}}$ gives, on reversing the order of the volume and wave vector integrations,

$$\begin{aligned} L_{kgij} &= \frac{\partial^2}{\partial x_k \partial x_g} \iiint_V G_{ij}(\underline{r}-\underline{r}') dV(\underline{r}') \\ &= \frac{1}{8\pi^3} \frac{\partial^2}{\partial x_k \partial x_g} \iiint_{-\infty}^{\infty} d^3\kappa \frac{M_{ij}^{-1}(\underline{\underline{\xi}})}{\kappa^2} e^{-i\underline{\kappa} \cdot \underline{r}} \iiint_V e^{i\underline{\kappa} \cdot \underline{r}'} dV(\underline{r}'). \end{aligned} \quad (6)$$

The volume integration extends over the cylindrical volume of the fictitious cylindrical grain and can be written as

$$I = \iiint_V e^{i\underline{\kappa} \cdot \underline{r}'} dV(\underline{r}') = \iiint_V e^{i(\kappa_1 x_1 + \kappa_2 x_2 + \kappa_3 x_3)} dx_1 dx_2 dx_3. \quad (7)$$

Let $x_1 = \rho \cos \theta$, $x_2 = \rho \sin \theta$. Then in cylindrical coordinates

$$I = \int_{\theta=0}^{2\pi} \int_{\rho=0}^a \int_{x_3=-\infty}^{\infty} e^{i\kappa_3 x_3} e^{i(\kappa_1 \rho \cos \theta + \kappa_2 \rho \sin \theta)} dx_3 \rho d\rho d\theta, \quad (8)$$

where a is the cylindrical radius. Since

$$\int_{-\infty}^{\infty} e^{i\kappa_3 x_3} dx_3 = 2\pi \delta(\kappa_3), \quad (9)$$

where $\delta(K_3)$ is the Dirac delta function, the integral takes the form

$$I = 2\pi \delta(K_3) \int_{\theta=0}^{2\pi} \int_{\rho=0}^a e^{i(K_1 \rho \cos \theta + K_2 \rho \sin \theta)} \rho d\rho d\theta. \quad (10)$$

Let $\rho = q/\sqrt{K_1^2 + K_2^2}$, $d\rho = dq/\sqrt{K_1^2 + K_2^2}$. Then

$$I = 2\pi \delta(K_3) \int_{\theta=0}^{2\pi} \int_{q=0}^{a\sqrt{K_1^2 + K_2^2}} e^{i \left\{ q \frac{K_1}{\sqrt{K_1^2 + K_2^2}} \cos \theta + q \frac{K_2}{\sqrt{K_1^2 + K_2^2}} \sin \theta \right\}} \frac{q dq d\theta}{\sqrt{K_1^2 + K_2^2}}. \quad (11)$$

If we now set $K_1/\sqrt{K_1^2 + K_2^2} = \cos \theta'$, then $K_2/\sqrt{K_1^2 + K_2^2} = \sin \theta'$, so that

$$I = \frac{2\pi \delta(K_3)}{K_1^2 + K_2^2} \int_{q=0}^{a\sqrt{K_1^2 + K_2^2}} \int_{\theta=0}^{2\pi} e^{iq \cos(\theta - \theta')} q dq d\theta. \quad (12)$$

Since the integration extends over a whole circumference, it is immaterial where the origin of θ is placed. The integral may therefore be written as

$$\begin{aligned} I &= \frac{2\pi \delta(K_3)}{K_1^2 + K_2^2} \int_{q=0}^{a\sqrt{K_1^2 + K_2^2}} q dq \int_{\theta=0}^{2\pi} e^{iq \cos \theta} d\theta \\ &= \frac{2\pi \delta(K_3)}{K_1^2 + K_2^2} \int_{q=0}^{a\sqrt{K_1^2 + K_2^2}} q dq \cdot 2\pi J_0(q) \end{aligned}$$

or

$$I = \frac{4\pi^2 \delta(K_3)}{K_1^2 + K_2^2} a\sqrt{K_1^2 + K_2^2} J_1(a\sqrt{K_1^2 + K_2^2}), \quad (13)$$

where J_0 and J_1 denote the usual Bessel functions.

Equation (6) can now be written as

$$L_{kgij} = \frac{1}{8\pi^3} \iiint_{-\infty}^{\infty} d^3K \frac{M_{ij}^{-1}(\xi)}{K^2} \cdot \frac{\partial^2 e^{-iK \cdot r}}{\partial x_k \partial x_g} \cdot \frac{4\pi^2 \delta(K_3)}{K_1^2 + K_2^2} \cdot a\sqrt{K_1^2 + K_2^2} J_1(a\sqrt{K_1^2 + K_2^2}) \quad (14)$$

Now $\frac{\partial^2 e^{-iK \cdot r}}{\partial x_k \partial x_g} = -K_k K_g e^{-iK \cdot r}$, so that

$$L_{kgij} = -\frac{1}{2\pi} \iiint_{-\infty}^{\infty} \frac{dK_1 dK_2 dK_3}{K_1^2 + K_2^2 + K_3^2} M_{ij}^{-1}(\xi) K_k K_g e^{-iK_3 z_3 - i(K_1 z_1 + K_2 z_2)} \frac{\delta(K_3)}{K_1^2 + K_2^2} a\sqrt{K_1^2 + K_2^2} J_1(a\sqrt{K_1^2 + K_2^2}). \quad (15)$$

If $k=3$ or $g=3$, the Dirac delta function $\delta(K_3)$ gives zero values for the integral. Hence, the non-zero values of the Eshelby tensor $\underline{\underline{S}}$ are given by $k=1,2$ and $g=1,2$. This arises because there are no components of the body force layer of surface tractions in the x_3 direction at the cylindrical interface between the grain and the matrix. Invoking the properties of the Dirac delta function gives

$$L_{k_{gij}} = -\frac{1}{2\pi} \int_{-\infty}^{\infty} dK_1 dK_2 M_{ij}^{-1}(\xi_1, \xi_2, \xi_3=0) \xi_k \xi_g e^{-i(K_1 x_1 + K_2 x_2)} \frac{a}{\sqrt{K_1^2 + K_2^2}} J_1(a\sqrt{K_1^2 + K_2^2}). \quad (16)$$

Now put

$$\xi_1 = \frac{K_1}{\sqrt{K_1^2 + K_2^2}} = \cos \theta, \quad \xi_2 = \frac{K_2}{\sqrt{K_1^2 + K_2^2}} = \sin \theta,$$

so that the Fourier wave vector components K_1 and K_2 correspond to the x_1 and x_2 axes, respectively. Then in cylindrical coordinates,

or

$$L_{k_{gij}} = -\frac{1}{2\pi} \int_{\theta=0}^{2\pi} \int_{K=0}^{\infty} K dK d\theta M_{ij}^{-1}(\xi) \xi_k \xi_g e^{-iKr} \frac{a}{K} J_1(aK)$$

$$L_{k_{gij}} = -\frac{1}{2\pi} \int_{\theta=0}^{2\pi} M_{ij}^{-1}(\xi) \xi_k \xi_g d\theta \int_{K=0}^{\infty} a e^{-iKr} J_1(aK) dK. \quad (17)$$

Since ξ is real, the real part of the preceding integral is

$$J = \int_{K=0}^{\infty} a \cos(Kr) J_1(aK) dK.$$

But, (cf. Gradstyn and Ryzhik, p. 730, Eq. 6.671, No. 2)

$$J = [a \cos\{\sin^{-1}(r/a)\}] / \sqrt{a^2 - r^2} \text{ for } 0 \leq r \leq a.$$

If $\theta = \sin^{-1}(r/a)$, then $J = a \cos \theta / \sqrt{a^2 - r^2} = \cos \theta / [\sqrt{a^2 - r^2}/a] = \cos \theta / \cos \theta = 1$.

Thus

$$L_{k_{gij}} = -\frac{1}{2\pi} \int_0^{2\pi} M_{ij}^{-1}(\xi) \xi_k \xi_g d\theta,$$

independent of position \underline{r} in the cylinder as expected from Eshelby's result. In this integral we have $\xi_1 = \cos \theta$, $\xi_2 = \sin \theta$, $\xi_3 = 0$, $M_{ij}^{-1}(\xi) = (\xi_m D_{mijn}^{-1} \xi_n)^{-1}$ and k and g are restricted to the values 1 and 2. The Eshelby tensor may now be written as

$$S_{ijkl} = D_{kijlm}^m \left\{ \frac{1}{4\pi} \left(\int_0^{2\pi} M_{pj}^{-1}(\xi_1, \xi_2) \xi_i \xi_k d\theta + \int_0^{2\pi} M_{ij}^{-1}(\xi_1, \xi_2) \xi_p \xi_k d\theta \right) \right\}. \quad (19)$$

For a transversely isotropic material the Christoffel tensor \underline{M} has the component form

$$M_{ij}(\xi_1, \xi_2) = \begin{bmatrix} c_{11}\xi_1^2 + \frac{1}{2}(c_{11}-c_{12})\xi_2^2 & \frac{1}{2}(c_{11}+c_{12})\xi_1\xi_2 & 0 \\ \frac{1}{2}(c_{11}+c_{12})\xi_1\xi_2 & c_{11}\xi_2^2 + \frac{1}{2}(c_{11}-c_{12})\xi_1^2 & 0 \\ 0 & 0 & c_{44} \end{bmatrix}. \quad (20)$$

The Eshelby tensor can now be evaluated by inverting the matrix in equation (20) and integrating according to equation (19). Explicit results may be deduced, according to the calculations in Mura's book [21], for the resulting integrals. Checking of these integrals is currently in progress.

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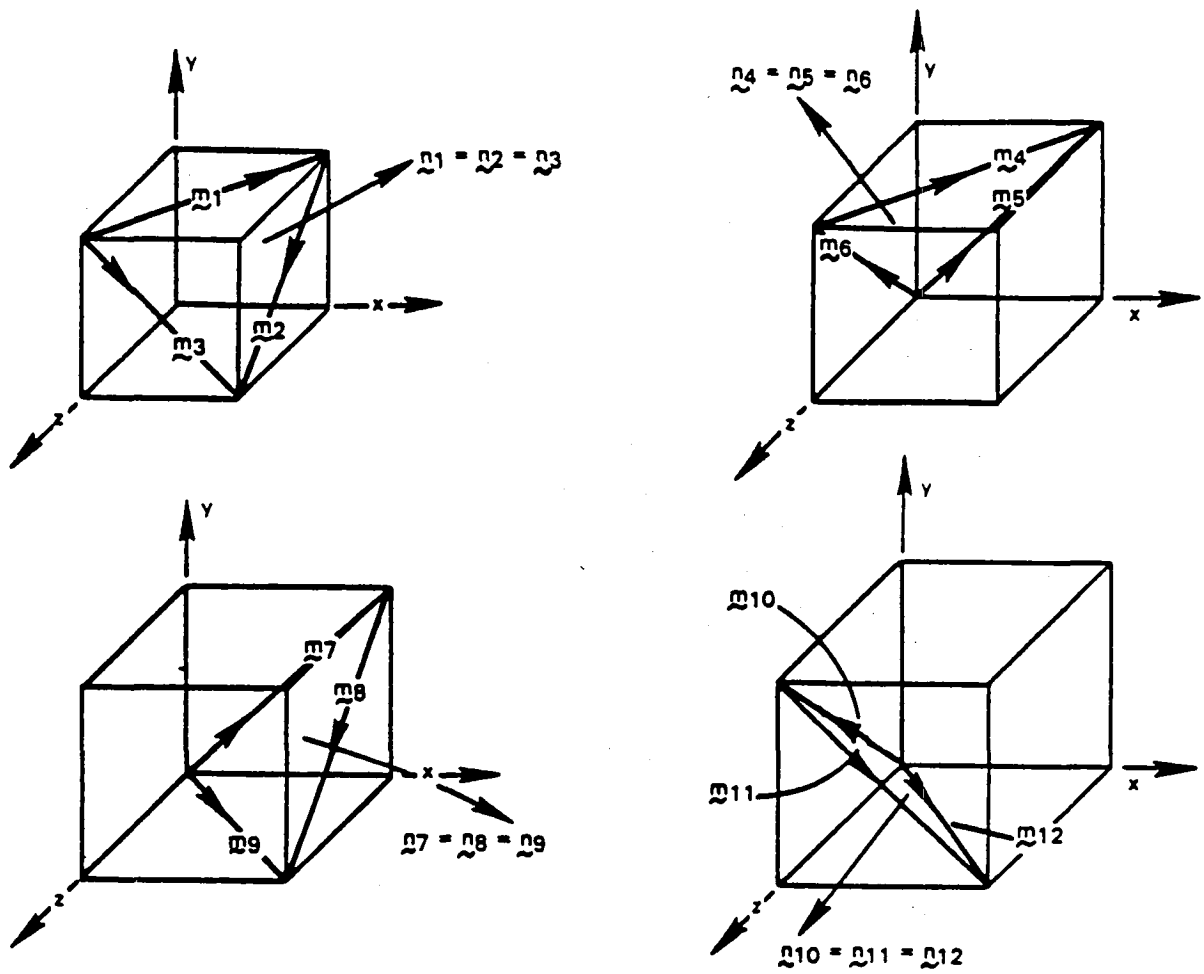


Fig. 1. The twelve $\langle 110 \rangle$ slip direction vectors on the four octahedral $\{111\}$ planes.

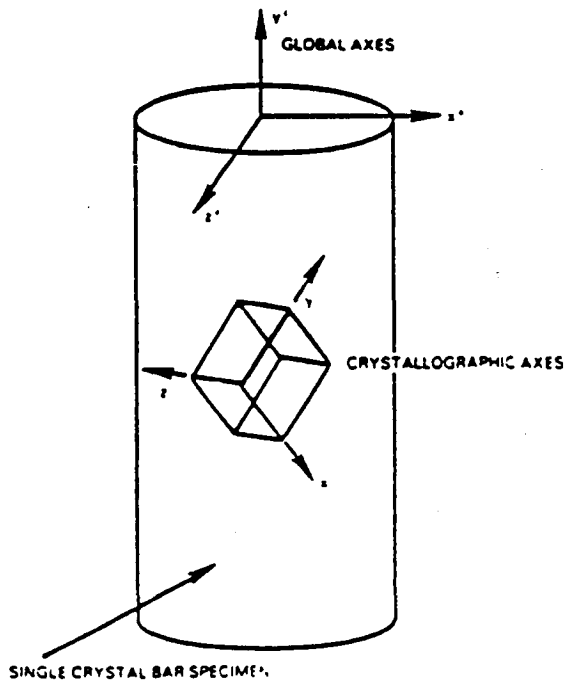


Fig. 2. Global and crystallographic axes of the specimen.