

A LARGE DEFORMATION ANALYSIS OF CRYSTALLINE ELASTIC-VISCOPLASTIC MATERIALS

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SUMMARY

The thermodynamics of crystalline elastic-viscoplastic materials developed earlier by the authors (*Nuclear Engineering and Design*, to appear) is extended to account for finite-strains. The present theory utilizes the basic physical concepts derived from the theory of dislocations in crystals and the thermodynamics of continua with internal state variables. A crystalline simple solid is considered to be a homogeneous elastic-plastic continuum containing dislocations which constitute the intrinsic, internal mechanism of plasticity phenomena. The appropriate internal state variables and the basic constitutive relations for the description of the elastic-viscoplastic behavior are deduced from the consideration of dislocation dynamics.

The theory proposed in the present paper is based on the assumption that both elastic and inelastic deformations take place at every stage of loading and unloading. This assumption has a definite physical basis and is the underlying consideration in the field of dislocation dynamics. Unlike other theories, the present one does not require the specification of a yield criterion or the prior determination of whether the material is loading or unloading. It can be shown that under appropriate assumptions on the constitutive laws the present theory reduces to the case of classical thermoelasticity or thermoplasticity.

The general finite-element formulation of an initial-boundary value problem is briefly presented. A specific example is carried out in detail which involves the solution of equations governing the coupled thermomechanical response of titanium. To demonstrate the effectiveness of the present formulation, a scheme for calculating the deformations, the stresses and temperature distribution is developed and applied to a three-dimensional structure subjected to high temperature, surface heat flux, volume heat supply as well as mechanical loading. The theory and the analysis should be beneficial in the study of the behavior of reactor materials at high temperatures.

1. Introduction

Recent developments in theoretical plasticity have moved far afield from the classical notions of the subject. Now it is possible to approach plasticity in a fairly deductive way so as to simultaneously blend it with accepted ideas in continuum mechanics, show how these ideas may be consistent with dislocation theory, and to extract out of the general theory everything essential to classical plasticity. Several versions of such general continuum theories of plasticity, and the relation of one theory to another, have been discussed in recent work by Oden and Bhandari [1] and Bhandari and Oden [2,3]. Moreover, the theory has already proved to be effective in finite-element analysis of certain thermoplastic phenomena (see Oden, et.al.[4]). It is our aim in the present paper to expand certain technical aspects of the theory described by the authors so as to accommodate certain recently reported experimental results, to extend the formulation given by Oden, et.al. [4] to finite deformations, to develop corresponding finite-element models, and to cite some representative numerical results obtained in specific applications.

The theory described in the present investigation utilizes the basic physical concepts derived from the theory of dislocations in crystals and the thermodynamics of continua with internal state variables. A crystalline simple solid is considered to be a homogeneous elastic-plastic continuum containing dislocations which constitute the intrinsic, internal mechanism of plasticity phenomena. The appropriate internal state variables and the basic constitutive relations for the description of the elastic-viscoplastic behavior are deduced from considerations of dislocation dynamics. The theory proposed in the present paper is based on the assumption that both elastic and inelastic deformations take place at every stage of loading and unloading. This assumption has a definite physical basis and is the underlying consideration in the field of dislocation dynamics. Unlike classical theories, the present one does not require the specification of a yield criterion or the prior determination of whether the material is loading or unloading. The approach taken in this paper is quite general and the techniques described here can be expanded to include virtually any type of constitutive law that falls within the framework of our theory. A discussion of most of the pertinent ideas, together with complete references to the related work is given by Bhandari and Oden [3].

Basic thermodynamic preliminaries and the proposed constitutive equations for our thermodynamic theory of viscoplastic materials are briefly presented in sections 2 thru 4. In section 5, we briefly review the essential features in which the finite-element models of our generalized constitutive laws are formulated to obtain the heat conduction equations and the equations of equilibrium. Finally, in sections 6 and 7, we present the application of our theory to solve a representative example problem in transient, nonlinear, coupled, thermo-viscoplasticity of a three-dimensional body.

2. Thermomechanical Preliminaries

2.1 Kinematics

Most of the usual kinematical relations are assumed to hold. As is customary in continuum physics, we identify each material point X of a continuous body \mathcal{B} with its position vector \underline{X} in a fixed reference configuration C_0 at some definite time $t = t_0$ (or $\tau = t - t_0 = 0$). The motion of the body \mathcal{B} relative to C_0 is given by the relation

$$\underline{x} = \underline{\chi}(\underline{X}, t) \quad (1)$$

in which $\underline{\chi}$ describes the mapping that carries \underline{X} in the reference configuration C_0 onto a place \underline{x} at time t . Effectively, $\underline{\chi}(\underline{X}, t)$ is a one-parameter family of mappings of C_0 onto current configurations C_t . In addition to eq. (1), we introduce the deformation gradient \underline{F} of the motion $\underline{\chi}$ relative to C_0 , as the second order tensor

$$\underline{F} = \underline{F}(\underline{X}, t) = \nabla_{\underline{X}} \underline{\chi}(\underline{X}, t) \quad (2)$$

where $\nabla_{\underline{X}}$ is the material gradient, and we assume that $\det \underline{F} > 0$ for every \underline{X} and t . The Green Saint-Venant strain tensor $\underline{\gamma}$ is defined by

$$\underline{\gamma} = \frac{1}{2}(\underline{F}^T \underline{F} - \underline{I}) \quad (3)$$

where \underline{I} is the unit tensor and \underline{F}^T denotes the transpose of \underline{F} .

Consider a configuration $C_{\hat{t}}$, $t_0 \leq \hat{t} \leq t$, intermediate between C_0 and C_t , and define the place of \underline{X} at time \hat{t} by

$$\underline{y} = \underline{\chi}(\underline{X}, \hat{t}) \quad (4)$$

Formally, $\underline{y} = \underline{\chi}(\hat{\mathcal{R}}^{-1}(\underline{X}), \hat{t})$ where $\hat{\mathcal{R}}(\underline{X}) = \underline{X}$ defines the place of particle \underline{X} in $C_{\hat{t}}$; thus $C_{\hat{t}}$ (or, for that matter, C_0 and C_t) need not be a configuration actually occupied by \mathcal{B} during its motion. The deformation gradient is then

$$\hat{\underline{F}} = \nabla_{\underline{X}} \underline{\chi}(\underline{X}, \hat{t}) \quad (5)$$

For fixed \hat{t} , it is assumed that (4) is invertible so that it can be written $\underline{X} = \underline{\chi}^{-1}(\underline{y}) \Big|_{t=\hat{t}}$. Then

$$\underline{x} = \underline{\chi}(\underline{\chi}^{-1}(\underline{y}), \hat{t}) = \underline{\chi}(\underline{y}, \hat{t}) \quad (6)$$

and by chain rule of differentiation

$$\underline{F} = \tilde{\underline{F}} \hat{\underline{F}} \quad (7)$$

where $\hat{\underline{F}}$ is given by eq. (5) and $\tilde{\underline{F}} = \nabla_{\underline{y}} \underline{\chi}$. Substitution of eq. (7) into eq. (3) yields

$$\underline{\gamma} = \frac{1}{2}(\hat{\underline{F}}^T \tilde{\underline{F}}^T \tilde{\underline{F}} \hat{\underline{F}} - \underline{I}) \quad (8)$$

which can be written in the form

$$\underline{\gamma} = \underline{\eta} + \underline{\xi} \quad (9)$$

wherein

$$2\underline{\eta} = \hat{\underline{F}}^T \hat{\underline{F}} - \underline{I}, \quad 2\underline{\xi} = \hat{\underline{F}}^T (\tilde{\underline{F}}^T \tilde{\underline{F}} - \underline{I}) \hat{\underline{F}} \quad (10a, b)$$

In most crystalline solids, plastic deformation (i.e., yielding in the sense of permanent deformation) is attributed to a flow process of crystalline lattice defects normally described in terms of development and propagation of dislocations. In such situations it is possible to interpret the homogeneous deformation $\underline{\chi}(t)$ of eq. (1) of the body \mathcal{B} as consisting of homogeneous lattice distortion and homogeneous shape distortion produced by homogeneous motion of dislocations. The lattice distortion is restorable, and on restoration the lattice distortion disappears completely (except locally at dislocation lines) and the body \mathcal{B} occupies a different configuration $C_{\hat{t}}$. Then in view of eq. (7) it follows that

$$\underline{\chi} = \tilde{\underline{\chi}} \hat{\underline{\chi}} \quad (11)$$

That is, the total deformation $\underline{\chi}$ is the composition of two deformations $\tilde{\underline{\chi}}$ and $\hat{\underline{\chi}}$, where $\hat{\underline{\chi}}$ is that part of the deformation associated with homogeneous shape distortions rather than homogeneous lattice distortions and, therefore, not recoverable according to the hypothesis. It is then possible to associate with this part of the deformation a strain

$$\underline{\eta} = \frac{1}{2}(\hat{\underline{F}}^T \hat{\underline{F}} - \underline{I}) \quad (12)$$

which we refer to as the inelastic strain tensor. In eq. (9) the tensor $\underline{\xi} = \underline{\gamma} - \underline{\eta}$ shall be referred to as the difference strain tensor and $\underline{\gamma}$ as the total strain tensor.

2.2 Thermodynamic Process

A thermodynamic process for a body \mathfrak{B} is described by nine functions of \underline{X} and t , whose values have the following interpretations: The function $\underline{\chi}(\underline{X}, t)$ which describes the motion of the body \mathfrak{B} , the symmetric second Piola-Kirchhoff stress tensor $\underline{\sigma} = \underline{\sigma}(\underline{X}, t)$, the specific body force $\underline{F} = \underline{F}(\underline{X}, t)$ per unit mass, the specific internal energy $\epsilon = \epsilon(\underline{X}, t)$ per unit mass, the heat flux vector $\underline{q} = \underline{q}(\underline{X}, t)$ on the boundary $\partial\mathfrak{B}$ of \mathfrak{B} , the absolute temperature $\theta = \theta(\underline{X}, t) > 0$, the specific heat supply $h = h(\underline{X}, t)$ per unit mass and per unit time, the specific entropy $S = S(\underline{X}, t)$ per unit mass, and the set of N functions $\underline{\alpha}^{(i)} = \underline{\alpha}^{(i)}(\underline{X}, t)$, $i = 1, 2, \dots, N$, called the 'internal state variables' which may be scalar, vector or tensor functions of \underline{X} and time t .

The set of nine functions $\{\underline{\chi}, \underline{\sigma}, \underline{F}, \epsilon, \underline{q}, \theta, h, S, \underline{\alpha}^{(i)}\}$ defined for all \underline{X} in \mathfrak{B} and all t is called a thermodynamic process in \mathfrak{B} , if and only if, it is compatible with the laws of balance of linear momentum, angular momentum, and energy. Under sufficient smoothness assumptions, the local forms of these laws are:

balance of linear momentum

$$(\sigma^{ij} x_{n,j})_{,i} + \rho F_n = \rho \dot{u}_n \quad (13)$$

balance of angular momentum

$$\sigma^{ij} = \sigma^{ji} \quad (14)$$

balance of energy

$$\rho \dot{\epsilon} = \sigma^{ij} \dot{\gamma}_{i,j} + q^i_{,i} + \rho h \quad (15)$$

where ρ is the mass density and the super-imposed dots indicate time rates. We require also that for each point \underline{X} and at every instant of time t , the thermodynamic process in \mathfrak{B} satisfies the entropy production inequality (i.e. Clausius-Duhem inequality) given in the form

$$\rho \theta \dot{S} - \rho \dot{\epsilon} + \sigma^{ij} \dot{\gamma}_{i,j} + \frac{1}{\theta} q^i \theta_{,i} \geq 0 \quad (16)$$

It is often convenient to introduce the specific free energy φ (Helmholtz free energy per unit mass) by the relation

$$\varphi = \epsilon - S\theta \quad (17)$$

Then, with the aid of eq. (17), the balance of energy (eq. (15)) can be recast into alternate forms:

$$\rho \dot{\varphi} = \sigma^{ij} \dot{\gamma}_{i,j} - \rho S \dot{\theta} - \sigma^* \quad (18)$$

$$\rho \theta \dot{S} = q^i_{,i} + \rho h + \sigma^* \quad (19)$$

where σ^* is the internal dissipation.

In order to define the thermodynamic process in \mathfrak{B} it suffices to specify only seven functions $\{\underline{\chi}, \underline{\sigma}, \varphi, \underline{q}, S, \theta, \underline{\alpha}^{(i)}\}$; for the remaining two functions, \underline{F} and h can uniquely be determined from eqs. (13) and (15). A thermodynamic process in \mathfrak{B} , compatible with the constitutive equations at each point \underline{X} of \mathfrak{B} and all time t is called an admissible process.

3. Thermoelastic-Viscoplastic Materials with Internal State Variables

The general constitutive relations for an elasticviscoplastic crystalline simple solid can be represented by the general forms (see e.g. the work of Oden and Bhandari [1-4] and also Kratochvil and Dillon [5])

$$\varphi = \hat{\varphi}(\underline{\xi}, \theta, \underline{g}, \underline{\eta}, \underline{A}^{(i)}) \quad (20)$$

$$\underline{\sigma} = \underline{\hat{\sigma}}(\underline{\xi}, \theta, \underline{g}, \underline{\eta}, \underline{A}^{(i)}) \quad (21)$$

$$s = \mathfrak{S}(\underline{\xi}, \theta, \underline{g}, \underline{\eta}, \underline{A}^{(1)}) \quad (22)$$

$$\underline{q} = \underline{\mathfrak{Q}}(\underline{\xi}, \theta, \underline{g}, \underline{\eta}, \underline{A}^{(1)}) \quad (23)$$

and the internal state variables are assumed to be given by the functional relationships,

$$\underline{\eta} = \underline{\mathfrak{M}}(\underline{\xi}, \theta, \underline{\eta}, \underline{A}^{(1)}) \quad (24)$$

$$\underline{\dot{A}}^{(1)} = \underline{\mathfrak{Q}}^{(1)}(\underline{\xi}, \theta, \underline{\eta}, \underline{A}^{(1)}) \quad (25)$$

wherein eqs. (20) - (23) $\underline{g} = \text{grad } \theta$. It should be noted that in the present formulation one of the independent variables appearing above is $\underline{\xi}$ instead of $\underline{\gamma}$. It was, however, pointed out by Green and Naghdi [6,7] that the use of the tensor $\underline{\xi}$ instead of $\underline{\gamma}$ implies no loss of generality in the general theory.

We now require that for every admissible thermodynamic process in \mathfrak{B} , the response functions appearing in the above constitutive equations must be such that postulate (16), of positive entropy production is satisfied at each point \underline{x} of \mathfrak{B} and for all time t . Then, with the aid of eqs. (9), (17) and (20), the Clausius-Duhem inequality eq. (16) can be rewritten in the form

$$\text{tr}[(\underline{\sigma} - \rho \frac{\partial \bar{\Phi}}{\partial \underline{\xi}}) \underline{\dot{\xi}}^T] - \rho (s + \frac{\partial \bar{\Phi}}{\partial \theta}) \dot{\theta} - \rho \frac{\partial \bar{\Phi}}{\partial \underline{g}} \cdot \underline{\dot{g}} + \text{tr}[(\underline{\sigma} - \rho \frac{\partial \bar{\Phi}}{\partial \underline{\eta}}) \underline{\dot{\eta}}^T] - \text{tr}[\rho \frac{\partial \bar{\Phi}}{\partial \underline{A}^{(1)}} \underline{\dot{A}}^{T(1)}] + \frac{1}{\theta} \underline{q} \cdot \underline{g} \geq 0 \quad (26)$$

We observe that by fixing $\underline{\xi}, \theta, \underline{\eta}$ and $\underline{A}^{(1)}$ at time t we also fix $\underline{\eta}$ and $\underline{\dot{A}}^{(1)}$ (as a result of eqs. (24) and (25)) but $\underline{\xi}, \dot{\theta}$ and $\underline{\dot{g}}$ are left arbitrary. Thus, for the inequality eq. (26) to hold independent of the signs $\underline{\xi}, \dot{\theta}$ and $\underline{\dot{g}}$, their coefficient must vanish. Consequently, we conclude that the free energy is independent of \underline{g} and the stress and entropy are derivable from the free energy, i.e.

$$\partial_{\underline{g}} \bar{\Phi}(\cdot) = \underline{0} \quad (27)$$

$$\underline{\sigma} = \rho \partial_{\underline{\xi}} \bar{\Phi}(\underline{\xi}, \theta, \underline{\eta}, \underline{A}^{(1)}) \quad (28)$$

$$s = -\partial_{\theta} \bar{\Phi}(\underline{\xi}, \theta, \underline{\eta}, \underline{A}^{(1)}) \quad (29)$$

where $\partial_{\underline{g}} \bar{\Phi}(\cdot)$, $\partial_{\underline{\xi}} \bar{\Phi}(\cdot)$ and $\partial_{\theta} \bar{\Phi}(\cdot)$ denote the partial differentiation of $\bar{\Phi}$ with respect to \underline{g} , $\underline{\xi}$ and θ , respectively.

In view of eq. (18), the internal dissipation inequality is

$$\sigma^* = \{ \text{tr}[(\underline{\sigma} - \rho \frac{\partial \bar{\Phi}}{\partial \underline{\eta}}) \underline{\dot{\eta}}^T] - \text{tr}[\rho \frac{\partial \bar{\Phi}}{\partial \underline{A}^{(1)}} \underline{\dot{A}}^{T(1)}] \} \geq 0 \quad (30)$$

and the heat conduction inequality

$$\underline{q} \cdot \underline{g} \geq 0 \quad (31)$$

As a consequence of eqs. (30) and (31), the general dissipation inequality takes the form

$$\sigma^* + \frac{1}{\theta} \underline{q} \cdot \underline{g} \geq 0 \quad (32)$$

The frame-work of the theory presented thusfar aims at a general description of the fundamental features of the elastic-viscoplastic behavior of crystalline simple solids. Before this mathematical model can be applied to a given boundary value problem, it is necessary to deduce the explicit forms of the constitutive equations (eqs. (20) - (25)) for a particular material. In what follows, we shall employ a specific model of the theory to deduce the specific forms of the constitutive equations for titanium and then present a solution to the initial-boundary value problem in transient, nonlinear, coupled thermoelasticviscoplasticity of a three-dimensional crystalline solid.

4. Constitutive Equations for Titanium

In this section we shall primarily use the results and theory of Conrad et.al. [8-16] to develop the constitutive equations which are suitable to characterize the elastic-viscoplastic behavior of titanium. In constructing these constitutive relations for general deformation processes, such as those discussed in section 3, one main difficulty arises due to the fact that the information available in the literature on the mechanical properties of titanium is still incomplete. This lack of information naturally restricts the applications suggested by the theoretical development. It is, however, sufficient in this study to introduce simplified forms of the constitutive relations obtained by imposing certain heuristic assumptions.

We assume that the material under study is an isotropic elastic-viscoplastic crystalline simple solid for which the thermoelastic properties are specified by a free energy function $\bar{\Phi}$ and viscoplastic behavior described by Conrad's [9] exponential law. We then postulate that the free energy function $\bar{\Phi}$ is expressed in the form

$$\rho \bar{\Phi} \equiv \frac{1}{2} E^{ijkl} \xi_{ij} \xi_{kl} - B^{ij} T \xi_{ij} - \frac{C}{2T_0} T^2 + \nu \alpha \quad (33)$$

Where E^{ijkl} and B^{ij} denote the elastic and thermoelastic moduli; C is the specific heat; T_0 and T denote the reference temperature and the temperature changes related by $\theta = T_0 + T$; ν is the energy of dislocation per unit length and α denotes the dislocation density. The first term in eq. (33) describes the elastic energy of the system, the second term represents the energy connected with the thermal expansion, the third is a thermal energy term, and the last term is the energy of all dislocations stored in a unit volume. In writing eq. (33), we have assumed that the dislocation (defect) arrangements $\underline{A}^{(i)}$ are characterized by a scalar quantity α , called the dislocation density, which may be considered as an average quantity of all defects and is assumed to be given by the relation

$$\alpha = \sqrt{\text{tr}(\underline{A}^{(i)} \underline{A}^{(i)})} \quad (34)$$

Since the body in its reference state is assumed to be unstrained, the linear terms appearing in the free energy expansion eq. (33) are neglected. Then, with the aid of eqs. (9), (28) and (29), we obtain stress and entropy:

$$\sigma^{ij} = E^{ijkl} (\gamma_{kl} - \eta_{kl}) - B^{ij} T \quad (35)$$

$$S = B^{ij} (\gamma_{ij} - \eta_{ij}) + \frac{C}{T_0} \quad (36)$$

The internal dissipation σ^* is then obtained by using eq. (30); i.e.

$$\sigma^* = \sigma^{ij} \dot{\eta}_{ij} - \nu \dot{\alpha} \quad (37)$$

Further, the heat flux is assumed to be given by a simple Fourier law, i.e.

$$q^i = \kappa^{ij} T_{,j} \quad (38)$$

where κ^{ij} is the thermal conductivity tensor.

The generalized constitutive equation for plastic strain-rate $\dot{\eta}_{ij}$ is developed from the experimental results and theory presented by Conrad [9]. It is based on the concept that a single thermally-activated dislocation mechanism may be rate-controlling over a given range of temperature and strain-rate and that the plastic shear strain-rate $\dot{\eta}_{(s)}$ is then given by

$$\dot{\eta}_{(s)} = \alpha b^2 v_0 \exp \left[- \frac{H_0}{k\theta} \left(1 - \frac{\tau^*}{\tau_0^*} \right)^2 \right] \quad (39)$$

where α is the mobile dislocation density; b is the length of Burger's vector; ν_D is Debye frequency; H_0 is the thermal activation energy; k is Boltzmann's constant; θ the absolute temperature; and τ^* is the effective shear stress (thermal component of stress) which is given by the difference between the applied shear stress τ and the internal back stress τ_μ (athermal component of stress, which is proportional to shear modulus μ). The so called 'athermal stress' is of a type known in many work-hardening theories and is taken to be of the form $\tau_\mu = \lambda\mu b\alpha^{\frac{1}{2}}$, λ being the work-hardening factor.

In a recent paper, Kratochvil and Angelis [17] have suggested that eq. (39) is not satisfactory for small values of τ^* (for $\tau^*=0, \dot{\eta}_{(\theta)}=0$) and therefore they have employed a slightly modified form of eq. (39) in their analysis of a simple one-dimensional problem of torsion of a circular titanium shaft. This form of the equation has been suggested by Alefeld [19] and is given by

$$\dot{\eta}_{(\theta)} = 2\alpha b^2 \nu_D \exp\left(-\frac{H_0}{k\theta}\right) \sinh\left\{\frac{2H_0}{k\theta}\left(\frac{\tau-\tau_\mu}{\tau_0^*}\right) - \frac{H_0}{k\theta}\left(\frac{\tau-\tau^*}{\tau_0^*}\right)^2\right\} \quad (40)$$

In writing eq. (40) Kratochvil and Angelis [17] have assumed that the plastic flow will occur when $\tau \geq \tau_\mu$ i.e. the rate of inelastic strain is controlled by a special form of the yield function

$$f = \tau - \lambda\mu b\alpha^{\frac{1}{2}} \quad (41)$$

In their approach eq. (40) holds when $\tau \geq \lambda\mu b\alpha^{\frac{1}{2}}$, and $\dot{\eta}_{(\theta)} = 0$ if $\tau \leq \lambda\mu b\alpha^{\frac{1}{2}}$. However, in our approach it is assumed that the inelastic strain-rate is always non-zero and that both elastic and inelastic deformations take place at every stage of loading and unloading. We, then postulate here that for a general case, the constitutive equation for the plastic strain-rate is taken to be of the form

$$\dot{\eta}_{ij} = \alpha b^2 \nu_D \exp\left\{-\frac{H_0}{k\theta}\left[1 - \frac{\sigma^*(\theta)}{\sigma_0^*}\right]^2\right\} \frac{S_{ij}}{|S_{\Pi}|^{\frac{1}{2}}} \quad (42)$$

where $\sigma^*(\theta)$ is the thermal stress; σ_0^* is the athermal stress component; S_{Π} is the second principal invariant of the deviatoric stress tensor \underline{S} defined by the relations

$$\underline{S} = \underline{\sigma} - \frac{1}{3} \text{tr}(\underline{S}) \underline{1} \quad (43)$$

and

$$S_{\Pi} = \frac{1}{2} \text{tr}(\underline{S}^2) \quad (44)$$

in which tr stands for trace and $\underline{1}$ a unit tensor.

Finally, the rate-of-change of dislocation density α is taken in a simple form

$$\dot{\alpha} = \beta [\text{tr}(\dot{\eta}^2)]^{\frac{1}{2}} \quad (45)$$

wherein β is a material constant.

The constants H_0 , τ_0^* or σ_0^* , λ , and β appearing in the constitutive equations (40) - (45) depend on the temperature, the grain size, strain rate and the impurity contents. Some of these dependences for $\alpha - T_1$ "A-70" have been studied by Conrad et.al [9,14,15].

In the following sections, we shall make use of the constitutive equations (35) - (38) together with eqs. (42) and (45) in the finite-element formulation to solve our boundary value problem.

5. Finite Element Formulation - Heat Conduction and Equilibrium Equations

5.1 Heat Conduction Equation

The governing heat conduction equation is derived by introducing eqs. (35) - (37) into eq. (19). We obtain

$$\theta [B^{1j} (\dot{\gamma}_{1j} - \dot{\eta}_{1j}) + \frac{C}{T_0} \dot{T}] - q_{,1}^1 - \rho h - \sigma^{1j} \dot{\eta}_{1j} + \nu \dot{\alpha} = 0 \quad (46)$$

Multiplying eq. (46) by the temperature variation δT and integrating throughout the volume, we obtain

$$\int_V \delta T [\theta [B^{1j} (\dot{\gamma}_{1j} - \dot{\eta}_{1j}) + \frac{C}{T_0} \dot{T}] - q_{,1}^1 - \rho h - \sigma^{1j} \dot{\eta}_{1j} + \nu \dot{\alpha}] dv = 0 \quad (47)$$

Noting that

$$\int_V \delta T q_{,1}^1 dv = - \int_V \delta T_{,1} q^1 dv + \int_A \delta T q^1 n_1 dA \quad (48)$$

eq. (46) can assume the form

$$\int_V \delta T [\theta [B^{1j} (\dot{\gamma}_{1j} - \dot{\eta}_{1j}) + \frac{C}{T_0} \dot{T}] - \rho h - \sigma^{1j} \dot{\eta}_{1j} + \nu \dot{\alpha}] dv + \int_V \delta T_{,1} q^1 dv - \int_A \delta T q^1 n_1 dA = 0 \quad (49)$$

where $\int_A dA$ represents the integration over the surface and n_1 is the unit normal to the surface.

In order to apply the finite element method to eq. (49), we follow a procedure similar to that of Oden et.al. [4] and introduce the local approximations for displacement and temperature fields in the form

$$u_1 = \psi_N(\underline{X}) u_1^N \quad (50)$$

$$T = \varphi_N(\underline{X}) T^N \quad (51)$$

where u_1^N and T^N are the displacement components and temperature change at node N of the element, and the dependence of u_1^N and T^N on t is understood; $\psi_N(\underline{X})$ and $\varphi_N(\underline{X})$ are the normalized local interpolation functions for displacements and temperatures respectively.

The strain-displacement relationship is given by

$$\gamma_{1j} = \frac{1}{2} (u_{1,j} + u_{j,1} + u_{k,1} u_{k,j}) \quad (52)$$

Substitution of eq. (50) into eq. (52) yields

$$\gamma_{1j} = A_{N1j}^k u_k^N + C_{NM1j} u_k^M u_k^N \quad (53)$$

wherein

$$A_{N1j}^k = \frac{1}{2} (\psi_{N,j} \delta_1^k + \psi_{N,1} \delta_j^k) \quad (54)$$

$$C_{NM1j} = \frac{1}{2} \psi_{M,j} \psi_{N,1} \quad (55)$$

Finally, introducing eqs. (38), (51) and (53) into eq. (49) we arrive at the heat conduction equation for the finite element Ω_e :

$$\int_V [\varphi_N (T_0 + \varphi_N T^M) \{ B^{1j} (A_{N1j}^k \dot{u}_k^N + 2C_{NM1j} u_k^M \dot{u}_k^N) - B^{1j} \dot{\eta}_{1j} + \frac{C}{T_0} \varphi_{R,1} \dot{T}^R \} + \varphi_{N,j} \varphi_{M,1} \sigma^{1j} T^M - \varphi_N \rho h - \varphi_N \sigma^{1j} \dot{\eta}_{1j} + \varphi_N \nu \dot{\alpha}] dv - \int_A \varphi_N q^1 n_1 dA = 0 \quad (56)$$

After some simple algebraic manipulations, eq. (56) can be rewritten in an alternate form

$$D_{NM} \dot{T}^M + E_{NM} T^M = G_N (u_N^k, \dot{u}_N^k, T^R, \dot{T}^R) + H_N + q_N \quad (57)$$

where

$$D_{NM} = \int_V C \varphi_N \varphi_M dv \quad (58)$$

$$E_{NM} = \int_V \kappa^{i,j} \varphi_{N,i} \varphi_{M,j} dv \quad (59)$$

$$G_N = \int_V \left[\varphi_N \sigma^{i,j} \dot{\eta}_{i,j} - \varphi_N \nu \dot{\alpha} - \frac{C}{T_0} \varphi_N \varphi_M \varphi_R T^M \dot{T}^R - \varphi_N (T_0 + \varphi_M T^M) B^{i,j} (A_{R1,j}^k \dot{u}_k^R + 2C_{R1,j} u_k^R \dot{u}_k^R - \dot{\eta}_{i,j}) \right] dv \quad (60)$$

$$H_N = \int_V \varphi_N \rho h dv \quad (61)$$

and

$$q_N = \int_A \varphi_N q^i n_i dA \quad (62)$$

5.2 Equilibrium Equations

We now write the finite element equilibrium equations in the form (see e.g. [4]),

$$\int_V \sigma^{i,j} \frac{\partial \gamma_{i,j}}{\partial u_k^N} dv = \frac{(a)}{F_N^k} \quad (63)$$

where $\frac{(a)}{F_N^k}$ is the applied nodal load vector. Then taking the variation of eq. (63), we obtain the incremental forms

$$\int_V d\sigma^{i,j} \frac{\partial \gamma_{i,j}}{\partial u_k^N} dv + \int_V \sigma^{i,j} d\left(\frac{\partial \gamma_{i,j}}{\partial u_k^N}\right) dv = d\frac{(a)}{F_N^k} \quad (64)$$

Now, introducing eqs. (35) and (53) into eq. (64) yields

$$\int_V \left[\{E^{i,jmn} (A_{p,nn}^r du_r^p + 2C_{p,rmn} u_r^m du_p^r - d\eta_{mn}) - B^{i,j} dT\} \{A_{N1,j}^k + 2C_{NM1,j} u_k^M\} \right] dv + \int_V 2\sigma^{i,j} C_{NM1,j} du_k^M dv = d\frac{(a)}{F_N^k} \quad (65)$$

Equation (65) can be rewritten in a compact form,

$$(K_{NP}^{(a)} + K_{NP}^{(g)}) du_k^p = dF_N^k + dF_N^k + dF_N^k + dF_N^k \quad (66)$$

where $K_{NP}^{(a)}$ and $K_{NP}^{(g)}$ are, respectively, the elastic and geometric stiffness matrices, given by

$$K_{NP}^{(a)} = \int_V E^{i,jmn} A_{N1,j}^r A_{p,nn}^r dv \quad (67)$$

$$K_{NP}^{(g)} = \int_V 2\sigma^{i,j} C_{NP1,j} dv \quad (68)$$

and dF_N^k , dF_N^k and dF_N^k are defined by

$$dF_N^k = \int_V \{B^{i,j} (A_{N1,j}^k + 2C_{NM1,j} u_k^M) \varphi_R dT^R\} dv \quad (69)$$

$$dF_N^k = \int_V \{E^{i,jmn} (A_{N1,j}^k + 2C_{NM1,j} u_k^M) d\eta_{mn}\} dv \quad (70)$$

$$dF_N^k = - \int_V \{4E^{i,jmn} (A_{N1,j}^k + C_{NM1,j} u_k^M) C_{p,rmn} u_r^m du_p^r\} dv \quad (71)$$

The contribution of the load vector dF_N^k of eq. (71) to the over-all solution of the problem is negligible (see e.g. Chung and Yagawa [19]) and therefore it may be dropped, from the computational point of view. It should also be noted that $\sigma^{i,j}$ in eq. (68) represents the initial stress or the residual stress in the structure just prior to a new change in geometry.

6. Solution Procedure

The approach employed here is essentially that used in the previous calculations of this type (see Oden et.al. [4]). The high nonlinearity is handled by solving the heat conduction equation (57) and the equations of equilibrium (66) iteratively within a small time increment. As shown by Oden et.al [4], a difference operator for a linear variation of temperature within a time increment is combined with the iterative solution of equilibrium equation.

The incremental nodal temperature at any time step k in eq. (57) is solved according to Wilson and Nickel [20]:

$$T_{(K)}^M = \left[\frac{D_{NM}}{\Delta t} + \frac{E_{NM}}{2} \right]^{-1} \left\{ G_{N_2, (K-\frac{1}{2})} + \left[\frac{D_{NH}}{\Delta t} - \frac{E_{NM}}{2} \right] T_{(K-1)}^M \right\} \quad (72)$$

where Δt is the small time increment; (K), $(K - \frac{1}{2})$ and (K - 1) represent the value at time step (K), $(K - \frac{1}{2})$ and (K - 1), respectively. The reference temperature and the initial thermal input can easily be incorporated into eq. (72), and the temperature change at the end of the first time increment calculated. The results of this solution are then used in the assembled incremental equations of equilibrium to determine the displacements and stresses. The constitutive equation for plastic strain-rate eq. (42) at each time of loading is incorporated into the equilibrium equations (66) and the iterative procedures within a time increment are repeated until convergence is achieved. With the final values of the displacements so determined, it is possible to calculate the displacement rates by means of the approximation

$$\dot{u}_{(K)} = (u_{(K)} - u_{(K-1)}) / \Delta t \quad (73)$$

for the use in the heat conduction calculations. Returning to the heat conduction equations for the next time increment, the process is repeated, as before, until the desired length of time has been reached.

In the present investigation, a three-dimensional linear isoparametric function for both temperature and displacement is used, and the integration is performed by an eight point Gaussian quadrature (see Oden [21]).

7. Results and Discussion

Based on the concepts of dislocation dynamics that the rate-controlling mechanism during yielding and flow of α -titanium at temperatures below $0.4 T_M$ (where T_M is the melting temperature) is thermally activated, a specific solution to the heat conduction problem has been carried out. Values for the mechanical and thermal characteristics of commercially pure titanium A-70 used in the computations are given in Table I. A three-dimensional titanium solid for which the displacement and thermal boundary conditions are given is shown in Fig. 1. Here only one quarter of the symmetrical three-dimensional solid is shown. A temperature change of $360^\circ C$ is applied at the nodes BCDE of the center-left end element. Effects of elasto-plastic couplings are studied and the transient temperature distribution in X-direction with $Y=Z=0$ is shown in Fig. 2. The displacement W in Z-direction at $Y=Z=100$ mm for various time levels is shown in Fig. 3. In Fig. 4, the stress component σ_z is plotted for typical elements (a) and (b). As expected the magnitude of σ_z for element (a) is greater than (b) at all levels of ΔT .

One of the significant results obtained from these computations was the magnitude of the displacements and stresses increase predicted to occur. This has been shown in Figs. 3 and 4 which indicate the affect of increase of temperature on the mechanical response of titanium A-70.

It is important to note that the present results are partly based on the extrapolation of the conclusions reached by Conrad et al. The constitutive equations (42) - (45) and the material parameters H_0 , σ_0^* , λ and β used in the computations were deduced from the experimental results presented by Conrad et.al. In the present investigation, the rate of the dislocation energy stored in a unit volume has been neglected (the stored energy is usually at least one order of magnitude less than the dissipated energy of the plastic deformation).

The quantity α is identified as the average dislocation density as measured by Conrad et. al. Kratochvil and Angelis [17] in their investigation have pointed out that a better approximation would be to characterize an arrangement of dislocations by at least two scalar parameters. The first parameter would represent the density of dislocations which are unstable during reverse loading and the second parameter would describe the density of more complicated structures of dislocations which are stable in reverse loading process. Unfortunately, no such data exists concerning the stability of dislocation arrangements at different states of deformations.

It is observed that the constitutive equation (42) loses its physical meaning in the regions of high stresses. It is also pointed out by Conrad [9] that at temperatures beyond the critical temperatures T_c (i.e. $T > .4T_m$), eq. (42) cannot be applied in determining the plastic strain-rate. In such cases, the plastic strain rate is controlled by other mechanisms which are not incorporated in eq. (42). Other models for dislocation motion have been proposed which may be generalized in a manner similar to eq. (42) - (45). The thermally activation model is particularly useful because it describes the effect of both temperature and stress on dislocation motion in a relatively simple manner.

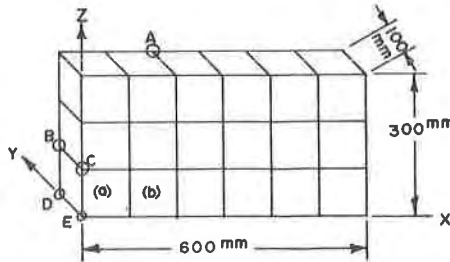
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Table I. Values of Characteristic Quantities for α -Titanium A-70

Characteristic	Symbol	Value
Young's modulus	E	$11.5 \times 10^3 \text{ kg/mm}^2$
Shear modulus	μ	$4.3 \times 10^3 \text{ kg/mm}^2$
Density	ρ	$4.5 \times 10^{-6} \text{ kg/mm}^3$
Poisson's ratio	ν	0.3
Debye frequency	ν_D	10^{13} sec^{-1}
Specific heat	C	$0.125 \text{ Cal/}^\circ\text{C g}$
Thermal conductivity	κ	$0.041 \text{ Cal/cm sec}^\circ\text{C}$
Coefficient of thermal expansion	α_0	$8.4 \times 10^{-6}/^\circ\text{C}$
Reference temperature	T_0	300°K
Activation energy	H_0	1.25 eV
Athermal stress	$\sigma_0^* = 2\tau_0^*$	147.0 kg/mm^2
Boltzmann constant	k	$1.4 \times 10^{-21} \text{ kg/mm}^\circ\text{K}$
Burger's vector	b	$2.95 \times 10^{-8} \text{ cm}$
Initial dislocation density	α	$1.5 \times 10^{10} \text{ cm}^2$
Dislocation arrangement constant	β	10^{11} cm^2
Work-hardening factor	λ	0.97



DISPLACEMENT BOUNDARY AND INITIAL CONDITIONS

$$\begin{aligned}
 U(t) = V(t) = W(t) = 0 & \quad \text{at } X=0 \text{ and } X=600 \text{ mm} \\
 V(t) = 0 & \quad \text{at } Y=0 \\
 W(t) = 0 & \quad \text{at } Z=0
 \end{aligned}$$

TEMPERATURE BOUNDARY AND INITIAL CONDITIONS

Insulated on all the surfaces and $T(t) = 0$ everywhere except at the points B, C, D, and E which are kept at $T(t) = 360^\circ\text{C}$.

Figure 1. Discretized geometry of three dimensional solid with boundary and initial conditions.

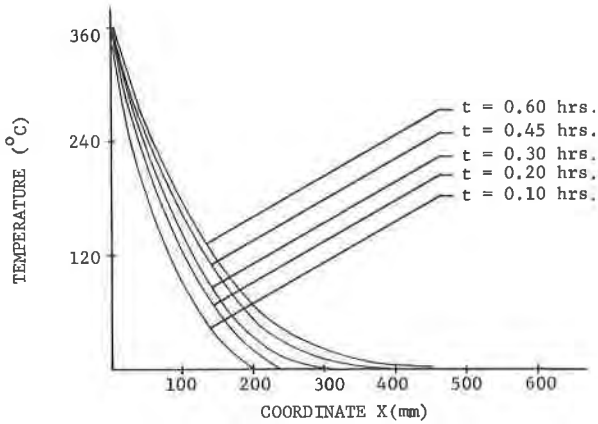


Figure 2. Temperature distribution.

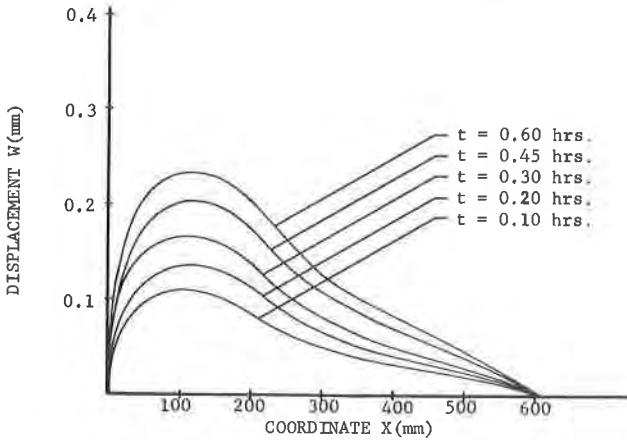


Figure 3. Displacement W in Z-direction at Y = 100 mm, Z = 300 mm

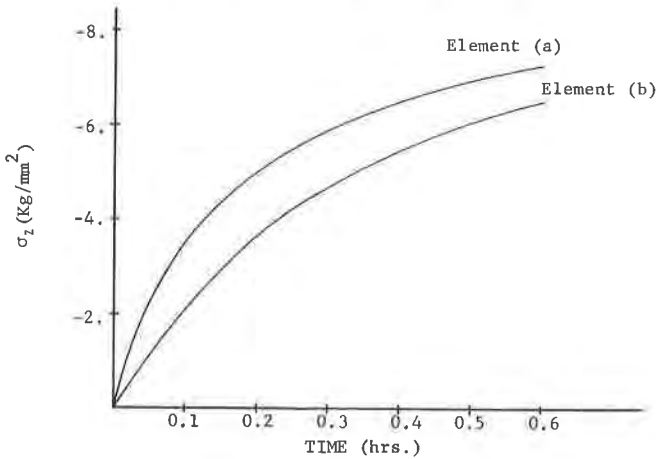


Figure 4. Variation of σ_z for elements (a) and (b).

