A LARGE DEFORMATION ANALYSIS OF CRYSTALLINE ELASTIC–VICCOPLASTIC MATERIALS*

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The thermodynamics of crystalline elastic–viscoplastic materials developed earlier by the authors 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 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 notations 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 ref. [4]). It is our aim in this 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 in ref. [4] to finite deformations, to develop corresponding finite-element models, and to cite some representative numerical results obtained in specific applications.

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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 this 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 in ref. [3].

Basic thermodynamic preliminaries and the proposed constitutive equations for our thermodynamic theory of viscoplastic materials are briefly presented in sections 2—4. In section 5 we review briefly 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, thermoviscoplasticity 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 \( X \) 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

\[
x = \chi(X, t).
\]

in which \( \chi \) describes the mapping that carries \( X \) in the reference configuration \( C_0 \) onto a place \( x \) at time \( t \).

Effectively, \( \chi(X, t) \) 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 \( F \) of the motion \( \chi \) relative to \( C_0 \), as the second order tensor

\[
F = F(X, t) = \nabla_X \chi(X, t).
\]

where \( \nabla_X \) is the material gradient, and we assume that \( \det F > 0 \) for every \( X \) and \( t \). The Green—Saint Venant strain tensor \( \gamma \) is defined by

\[
\gamma = \frac{1}{2}(F^T F - I)
\]

where \( I \) is the unit tensor and \( F^T \) denotes the transpose of \( F \).

Consider a configuration \( C_i, t_0 < i \leq t \), intermediate between \( C_0 \) and \( C_t \), and define the place of \( X \) at time \( i \) by

\[
y = \chi(X, i).
\]

Formally, \( y = \chi(k^{-1}(X), i) \) where \( k(X) = X \) defines the place of particle \( X \) in \( C_i \); thus \( C_i \) (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

\[
\bar{F} = \nabla_y \chi(X, i)
\]

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

\[
x = \chi(X(y), i) = \chi(y, i)
\]

and by chain rule of differentiation,

\[
F = \tilde{F} \bar{F},
\]

where \( \tilde{F} \) is given by eq. (5) and \( \bar{F} = \nabla_y \chi \). Substitution of eq. (7) into eq. (3) yields

\[
\gamma = \frac{1}{2}(\tilde{F}^T \bar{F} \tilde{F} - I)
\]

which can be written in the form

\[
\gamma = \eta + \xi,
\]

wherein

\[
2\eta = \tilde{F}^T \tilde{F} - I, \quad 2\xi = \tilde{F}^T (\tilde{F} \bar{F} - I) \tilde{F}.
\]

In most crystalline solids, plastic deformation (i.e. yielding in the sense of permanent deformation) is attri-
buted to a flow process of crystalline lattice defects
normally described in terms of development and propa-
gation of dislocations. In such situations it is possible
to interpret the homogeneous deformation \( \chi(t) \) of eq.
(1) of the body \( \mathcal{J} \) 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 dis-
location lines) and the body \( \mathcal{J} \) occupies a different
configuration \( C_i \): Then in view of eq. (7) it follows that
\[
\chi = \dot{\chi} \ddot{\chi}. \tag{11}
\]
That is, the total deformation \( \chi \) is the composition of
two deformations \( \dot{\chi} \) and \( \ddot{\chi} \), where \( \dot{\chi} \) is that part of
the deformation associated with homogeneous shape dis-
tortions rather than homogeneous lattice distortions
and therefore not recoverable according to the hypo-
thesis. It is then possible to associate with this part of
the deformation a strain
\[
\eta = \frac{1}{2}(F^T \dot{F} - I) \tag{12}
\]
which we refer to as the \emph{inelastic strain tensor}. In eq.
(9) the tensor \( \xi = \gamma - \eta \) shall be referred to as the
\emph{difference strain tensor} and \( \gamma \) as the \emph{total strain tensor}.

2.2. Thermodynamic process

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

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

\begin{align*}
\text{balance of linear momentum:} & \quad (\alpha^{(i)}X_m^m)_i + \rho F^m = \rho \ddot{u}^m, \quad (13) \\
\text{balance of angular momentum:} & \quad \sigma^{ij} = \sigma^{ij}, \quad (14) \\
\text{balance of energy:} & \quad \rho \dot{\epsilon} = \sigma^{ij} \dot{\gamma}^{ij} + q_i^l + \dot{p} h, \quad (15)
\end{align*}

where \( \rho \) is the mass density and the superimposed dots
indicate time rates. We require also that for each point
\( X \) and at every instant of time \( t \), the thermodynamic
process in \( \mathcal{J} \) satisfies the entropy production inequality
(i.e. Clausius-Duhem inequality) given in the form
\[
\rho \theta \dot{S} - \rho \dot{\epsilon} + \sigma^{ij} \dot{\gamma}^{ij} + (1/\theta) q_i^l \geq 0. \tag{16}
\]

It is often convenient to introduce the specific free
energy \( \varphi \) (Helmholtz free energy per unit mass) by the
relation
\[
\varphi = \epsilon - S \theta. \tag{17}
\]

Then, with the aid of eq. (17), the balance of energy
(eq. (15)) can be recast into alternate forms:
\[
\rho \dot{\varphi} = \sigma^{ij} \dot{\gamma}^{ij} - \rho \theta \dot{S} - \sigma^*, \tag{18}
\]
and
\[
\rho \theta \dot{S} = q_i^l + \dot{p} h + \sigma^*. \tag{19}
\]

where \( \sigma^* \) is the internal dissipation.

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

3. Thermoelastic—viscoelastic materials with internal
state variables

The general constitutive relations for an elastic—visco-
elastic crystalline simple solid can be represented by
the general forms (see e.g. refs [1]—[5])
\begin{align*}
\varphi &= \Phi(\xi, \theta, g, \eta, \alpha^{(i)}), \quad (20) \\
\sigma &= \Sigma(\xi, \theta, g, \eta, \alpha^{(i)}), \quad (21) \\
S &= S(\xi, \theta, g, \eta, \alpha^{(i)}), \quad (22)
\end{align*}
where \( g \), \( \theta \) and \( \eta \) denote the partial differentiation of \( \Phi \) with respect to \( g \), \( \xi \) and \( \theta \), respectively.

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

\[
\sigma^* = \left( \text{tr} \left[ \left( \sigma - \rho \frac{\partial \Phi}{\partial \eta} \right) \right] \right) \cdot \eta - \text{tr} \left[ \rho \frac{\partial \Phi}{\partial A^{(i)}} A^{(i)} \right] \geq 0.
\]

and the heat conduction inequality

\[
\mathcal{Q} \cdot g \geq 0.
\]

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

\[
\sigma^* + \frac{1}{\theta} \cdot g \cdot g \geq 0.
\]

The framework of the theory presented thus far 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 (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 thermoelastic-viscoplasticity of a three-dimensional crystalline solid.

4. Constitutive equations for titanium

In this section we shall use primarily 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 \( \Phi \) and viscoplastic behavior described by Conrad's [9] exponential law. We then pos-
tulate that the free energy function $\Phi$ is expressed in the form
\[
\rho \Phi = \frac{1}{2} E^{ijkl} \xi_{ij} \xi_{kl} - B^{ij} T \xi_{ij} - \frac{C}{2T_0} T^2 + \nu \alpha,
\]
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 $\theta = T_0 + T$; $\nu$ is the modulus of elasticity per unit length and $\alpha$ 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 $A^{(i)}$ are characterized by a scalar quantity $\alpha$, called the dislocation density, which may be considered as an average quantity of all defects and is assumed to be given by the relation
\[
\alpha = \{\text{tr}(A^{(i)} A^{(i)})\}^{1/2}.
\]

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:
\[
\sigma^{ij} = E^{ijkl} (\gamma_{kl} - \eta_{kl}) - B^{ij} T, \quad S = B^{ij} (\gamma_{ij} - \eta_{ij}) + C/T_0.
\]

The internal dissipation $\sigma^*$ is then obtained by using eq. (30), i.e.
\[
\sigma^* = \sigma^{ij} \eta_{ij} - \nu \alpha.
\]

Further, the heat flux is assumed to be given by a simple Fourier law, i.e.
\[
\begin{align*}
q_t &= \kappa^{ij} \theta_{ij},
\end{align*}
\]
where $\kappa^{ij}$ 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
\[
\dot{\eta}_{(s)} = ab^2 \nu \exp \left( -\frac{H_0}{kT} \left( 1 - \frac{\tau^*}{\tau_0^*} \right)^2 \right),
\]
where $a$ is the mobile dislocation density; $b$ is the length of Burger's vector; $\nu_D$ is Debye frequency; $H_0$ is the thermal activation energy; $k$ is Boltzmann's constant; $\theta$ is the absolute temperature; and $\tau^*$ is the effective shear stress (thermal component of stress) which is given by the difference between the applied shear stress $\tau$ and the internal back stress $\tau_\mu$ (athermal component of stress, which is proportional to shear modulus $\mu$). The so-called 'athermal stress' is of a type known in many work-hardening theories and is taken to be of the form $\tau_\mu = \lambda \mu b a^{1/2}$, $\lambda$ 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 $\tau^*$ (for $\tau^* = 0$, $\dot{\eta}_{(s)} = 0$) 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 [18] and is given by
\[
\dot{\eta}_{(s)} = 2ab^2 \nu_D \exp \left( -\frac{H_0}{kT} \left( 1 - \frac{\tau^*}{\tau_0^*} \right)^2 \right).
\]

In writing eq. (40) Kratochvil and Angelis [17] have assumed that the plastic flow will occur when $\tau \gg \tau_\mu$, i.e. the rate of inelastic strain is controlled by a special form of the yield function
\[
f = \tau - \lambda \mu b a^{1/2}.
\]
In their approach eq. (40) holds when $\tau \gg \lambda \mu b a^{1/2}$, and $\dot{\eta}_{(s)} = 0$ if $\tau \leq \lambda \mu b a^{1/2}$. 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
\[
\dot{\eta}_{ij} = ab^2 \nu_D \exp \left( -\frac{H_0}{kT} \left[ 1 - \frac{\sigma^*(\theta)}{\sigma_0^*} \right]^2 \right) \frac{S_{ij}}{|S|^2/2},
\]
where $\sigma^*(\theta)$ is the thermal stress; $\sigma_0^*$ is the athermal
5.1. Heat conduction equation

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

\[ \frac{\partial}{\partial t} \left( B^{ij}(\gamma_{ij} - \eta_{ij}) + \frac{C}{T_0} \tilde{T} \right) - q_{ij}' - \rho h = 0. \]  

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

\[ \int V \left[ \frac{\partial}{\partial t} \left( B^{ij}(\gamma_{ij} - \eta_{ij}) + \frac{C}{T_0} \tilde{T} \right) \right] - q_{ij}' - \rho h - \sigma^{ij} \eta_{ij} + \nu \dot{\alpha} \right] \, dv = 0. \]  

Noting that

\[ \int V \left( \delta T q_{ij}' \right) \, dv = - \int V \left( \delta T, q_{ij}' \right) \, dv + \int \delta T q_{ij}' n_i \, dA \]  

eq. (46) can assume the form

\[ \int V \left[ \frac{\partial}{\partial t} \left( B^{ij}(\gamma_{ij} - \eta_{ij}) + \frac{C}{T_0} \tilde{T} \right) \right] - \rho h - \sigma^{ij} \eta_{ij} + \nu \dot{\alpha} \right] \, dv 
+ \int V \left( \delta T, q_{ij}' \right) \, dv - \int A \delta T q_{ij}' n_i \, dA = 0. \]

where \( f_A \, dA \) represents the integration over the surface and \( n_i \) 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

\[ u_i = \psi_N(X)u_i^N. \]  

\[ T = \varphi_N(X)T^N. \]

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

The strain–displacement relationship is given by

\[ \gamma_{ij} = \frac{1}{2}(u_{ij} + u_{ji} + u_{k,i}u_{k,j}). \]  

Substituting eq. (50) into eq. (52) yields

\[ \gamma_{ij} = A_N^{ij}u_i^N + C_{NMij}u_k^N u_k^M. \]

wherein

\[ A_N^{ij} = \frac{1}{2}(\psi_{N,i}\delta^k_j + \psi_{N,j}\delta^k_i) \]

\[ C_{NMij} = \frac{1}{2}\psi_{M,i}\psi_{M,j} \]

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

\[ \int V \left[ \frac{\partial}{\partial t} \left( B^{ij}(A_N^{ij}u_i^N + 2C_{NMij}u_k^N u_k^M) \right) - B^{ij}\tilde{\eta}_{ij} + \frac{C}{T_0} \tilde{T} \right] + \varphi_{N,i}\varphi_{M,k}\delta^{ij}T^M 
- \varphi_{N,ij}\varphi_{M,k}\delta^{ij}T^M \right] \, dv - \int A \varphi_{N,ij} \, dA = 0. \]
After some simple algebraic manipulations, eq. (56) can be rewritten in an alternative form:

\[ D_{NM} T^M + E_{NM} T^M = G_N(u_N^k, \dot{u}_N^k, T^R, \dot{T}^R) + H_N + q_N. \]  

(57)

where

\[ D_{NM} = \int_\nu C_{\varphi M}\varphi_M dv. \]  

(58)

\[ E_{NM} = \int_\nu K_{ij}\varphi_N,\varphi_M, dv. \]  

(59)

\[ G_N = \int_\nu \left( \varphi_N \partial_{ij} \dot{u}_i - \varphi_N \partial_{ij} \frac{C}{T_0} \varphi_N \varphi_M \varphi_R T^M T^R \right. \]

\[ \left. - \varphi_N (T_0 + \varphi_M T^M) \partial_{ij} \right) \]

\[ \times \left( A_{R ij}^k \partial_{ij}^R + 2C_{R ij}^k \partial_{ij}^R \dot{u}_k^R - \dot{u}_k^R \right) dv. \]  

(60)

\[ H_N = \int_\nu \varphi_N \rho h dv. \]  

(61)

and

\[ q_N = \int_\nu \varphi_N q \dot{u}_i dA. \]  

(62)

5.2. Equilibrium equations

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

\[ \int_\nu \sigma_{ij} \partial_{ij}^N \frac{d\nu}{du_k^N} d\nu = [F^a_N], \]  

(63)

where \( F^a_N \) is the applied nodal load vector. Then taking the variation of eq. (63), we obtain the incremental forms

\[ \int_\nu d\sigma_{ij} \partial_{ij}^N \frac{d\nu}{du_k^N} d\nu + \int_\nu \sigma_{ij} \frac{d\gamma_{ij}^N}{du_k^N} d\nu = [F^{(a)}_N]. \]  

(64)

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

\[ \int_\nu \left[ \{E_{ij}^{mn} (A_{mn}^R du_i^R + 2C_{PR mn} U^R du_i^R - d\eta_{mn}) - B^i dT \right] \]

\[ \times \{A_N^k + 2C_{N mn} U^M_k \} \]  

\[ + \int_\nu 2\sigma_{ij} C_{N mn} du_k^R \]  

\[ \frac{dF_N^a}{dv} = dF_N^{(a)}. \]  

(65)

Eq. (65) can be rewritten in a compact form:

\[ (K^{(a)}_N + K^{(p)}_N) du_k^R = dF_N^{(a)} + dF_N^{(p)} + dF_N^{(n)} \]  

(66)

where \( K^{(a)}_N \) and \( K^{(p)}_N \) are, respectively, the elastic and geometric stiffness matrices, given by \[ K^{(a)}_N = \int_\nu E_{ij}^{mn} A_{ij}^R A_{mn}^R dv. \]  

(67)

\[ K^{(p)}_N = \int_\nu 2\sigma_{ij} C_{N mn} du_k^R dv, \]  

(68)

and \( dF_N^{(a)}, dF_N^{(p)} \) and \( dF_N^{(n)} \) are defined by

\[ \int_\nu \left\{ \partial_{ij} dF_N^{(a)} \right\} \]  

\[ = \int_\nu \left\{ E_{ij}^{mn} (A_{ij}^R + 2C_{N mn} U^M_k) \right\} d\eta_{mn} \]  

(69)

\[ \int_\nu \left\{ 4E_{ij}^{mn} (A_{ij}^R + C_{N mn} U^M_k) \right\} \]  

\[ \times C_{PR mn} U^R \]  

\[ du_i^R \]  

(70)

\[ dF_N^{(p)} = \int_\nu \{ E_{ij}^{mn} (A_{ij}^R + 2C_{N mn} U^M_k) \} d\eta_{mn} \]  

(71)

The contribution of the load vector \( dF_N^{(a)} \) of eq. (71) to the overall solution of the problem is negligible (see e.g. ref. [19]) and therefore it may be dropped, from the computational point of view. It should also be noted that \( \sigma_{ij} \) 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 [4]. The high non-linearity is handled by solving the heat conduction equation (57) and the equations of equilibrium (66) iteratively within a small time increment. As shown in ref. [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]:

$$T^M_{(k)} = \left( \frac{D_{NM}}{\Delta t} + \frac{E_{NM}}{2} \right) \left\{ G_{N,(K-1/2)} + \left( \frac{D_{NM}}{\Delta t} - \frac{E_{NM}}{2} \right) T^M_{(K-1)} \right\},$$

where $\Delta t$ 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 incremen-
tal equations of equilibrium to determine the displace-
ments and stresses. The constitutive equation for plastic
strain rate eq. (42) at each time of loading is incorpor-
ated into the equilibrium equations (66) and the itera-
tive procedures within a time increment are repeated
until convergence is achieved. With the final values of
the displacements so determined, it is possible to calcu-
late the displacement rates by means of the approxima-
tion

$$\dot{u}(K) = \frac{u(K) - u(K-1)}{\Delta t}$$

(73)

for use in the heat conducton 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 this investigation, a three-dimensional linear iso-
parametric function for both temperature and dis-
placement 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
$\alpha$-titanium at temperatures below $0.4 T_M$ (where $T_M$
is the melting temperature) is thermally activated, a specif-
ic 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 1. 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
the $X$ direction with $Y = Z = 0$ is shown in fig. 2. The
displacement $W$ in the $Z$ direction at $Y = Z = 100$ mm

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>$E$</td>
<td>$11.5 \times 10^3$ kg/mm$^2$</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>$\mu$</td>
<td>$4.3 \times 10^3$ kg/mm$^2$</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>$4.5 \times 10^{-6}$ kg/mm$^3$</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu$</td>
<td>$0.3$</td>
</tr>
<tr>
<td>Debye frequency</td>
<td>$\nu_D$</td>
<td>$10^{13}$ sec$^{-1}$</td>
</tr>
<tr>
<td>Specific heat</td>
<td>$C$</td>
<td>$0.125$ cal°C g</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$\kappa$</td>
<td>$0.041$ cal/cm sec°C</td>
</tr>
<tr>
<td>Coefficient of thermal expansion</td>
<td>$\alpha_0$</td>
<td>$8.4 \times 10^{-6}$ °C</td>
</tr>
<tr>
<td>Reference temperature</td>
<td>$T_0$</td>
<td>$300^\circ$K</td>
</tr>
<tr>
<td>Activation energy</td>
<td>$\gamma_0$</td>
<td>$1.25$ ev</td>
</tr>
<tr>
<td>Athermal stress</td>
<td>$\sigma_0 = 2\gamma_0$</td>
<td>$147.0$ kg/mm$^2$</td>
</tr>
<tr>
<td>Boltzmann constant</td>
<td>$k$</td>
<td>$1.4 \times 10^{-21}$ kg/mm$^2$K</td>
</tr>
<tr>
<td>Burger’s vector</td>
<td>$b$</td>
<td>$2.95 \times 10^{-8}$ cm</td>
</tr>
<tr>
<td>Initial dislocation density</td>
<td>$\alpha$</td>
<td>$1.5 \times 10^{10}$ cm$^2$</td>
</tr>
<tr>
<td>Dislocation arrangement constant</td>
<td>$\beta$</td>
<td>$10^{11}$ cm$^2$</td>
</tr>
<tr>
<td>Work-hardening factor</td>
<td>$\lambda$</td>
<td>$0.97$</td>
</tr>
</tbody>
</table>
for various time levels is shown in fig. 3. In fig. 4, the stress component $\sigma_z$ is plotted for typical elements (a) and (b). As expected the magnitude of $\sigma_z$ for element (a) is greater than (b) at all levels of $\Delta T$.

One of the significant results obtained from these computations was that the magnitude of the displacements and stresses increase as predicted. This has been shown in figs 3 and 4 which indicate the effect 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 $H_0$, $\alpha_0$, $\lambda$ and $\beta$ 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 $\alpha$ is identified as the average dislocation density as measured by Conrad et al. Kratochvih 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. $T > 0.4T_M$), 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 eqs (42)–(45). The thermal activation model is particularly useful because it describes the effect of both temperature and stress on dislocation motion in a relatively simple manner.

Acknowledgement

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References