A CONTINUUM MODEL FOR A METAL THAT RECRYSTALLIZES DURING THE DEFORMATION HISTORY

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Unusual response characteristics have been observed in materials due to recrystallization. This could be important for structures exposed to elevated temperatures and subjected to stresses beyond the yield point. In the research reported herein, a phenomenological theory is developed for a material that strain-hardens and recrystallizes during the deformation history. Specifically, the objective is to develop an understanding of the kinematics, energy balance, dissipation and constitutive equations for a material that experiences significant microstructural changes. An internal state variable approach to constitutive modeling is used to account for these changes. Of particular interest is the development of the evolution equations for the internal state variables.

An analysis of the kinematics of recrystallization leads to a multiplicative decomposition of the deformation gradient $F$, into three parts corresponding to a perfectly plastic deformation, $F^p$, into a fully annealed configuration; a strain-hardening deformation, $F^e$, into the actual plastic configuration; and an elastic deformation, $F^e$, into the current configuration. As a consequence, the total work can be written as a mechanically reversible or elastic work; the work associated with perfectly plastic deformation which is dissipated as heat; and, the work of strain-hardening which is partially stored in the material microstructure and partially dissipated as heat. The stored energy (of cold work) is subsequently released as heat during recrystallization.

An analysis of the thermodynamics of the process, together with the above representation of the deformation and work, leads to a decomposition of the Helmholtz free energy and the internal energy into reversible and irreversible components. It is shown that only the irreversible parts depend on the internal state variables. The energy balance equation leads to a relationship between the stored energy of cold work and the heat released during recrystallization.
1. Introduction

The response of metals at elevated temperatures has been a subject of investigation for quite some time because of its application to structures like nuclear reactors, jet engines and MHD generators. Among the most commonly studied phenomena have been creep, fatigue and fracture [1,2]. However, another extremely important phenomenon that has escaped attention of many in Continuum Mechanics is recrystallization which occurs in deformed metals at high temperatures [3]. This phenomenon has been found to produce unusual responses in materials. For example, Morrow and Halford [4] observed an oscillatory stress-strain response for chemically pure lead in tests run at constant strain-rate. This response was attributed to cyclic action of strain-hardening and recrystallization. That is, as the specimen is loaded, strain-hardening occurs and a small fraction of the work done during deformation remains in the metal as stored energy of cold work. When a minimum energy state is obtained, the stored energy is released by recrystallization and softening occurs reducing the stress. In the above experiment the material was loaded at constant strain-rate, it strain-hardens and the cycle is repeated. Similar observation has been made by Sellers [5] for 99.9% pure nickel deformed in constant shear-strain rate at 934°C. It is therefore expected that other metals will exhibit similar response characteristics under suitable strain-temperature conditions. It is apparent from experimental observations that softening produced by recrystallization could lead to extremely large strains that may at times assume catastrophic proportions.

The purpose of this research is to develop a constitutive representation for a material that experiences the simultaneous effects of strain-hardening and recrystallization. The theory is phenomenologically formulated within the framework of continuum mechanics and thermodynamics. State variables [6] are used to model the complex microstructural changes that accompany strain-hardening and recrystallization. These microstructural changes include the generation of numerous point defects such as vacancies, interstitial atoms and dislocations of various types [7] that are essentially eliminated as a result of recrystallization. Because of the numerous microscopic changes, the constitutive modeling is considered extremely difficult, and hopefully this research will provide some insight into the problem area.

The internal state variables are intended to represent the overall effect of the microstructure variables on the response of the metal and are not specifically identified. They also include the effect of the deformation and temperature histories. The kinematics and energy balance for the process is analyzed with respect to a reference configuration that is assumed stress-free, at a reference temperature and fully annealed. The state variables are initialized in the reference configuration. During isothermal temperature histories, these variables are assumed to undergo changes only during inelastic (irreversible or plastic) deformation. Using thermodynamics, the stored energy of cold work is identified as the increase in internal energy during plastic deformation. A representation for the stored energy is developed.

2. Kinematics

Kinematics of the process of strain-hardening and recrystallization is analyzed with the use of mappings shown in Figure 1. The material under consideration is assumed to be a continuum. Assume at time t = 0 the material is fully annealed and in the reference config-
uration, \( k \). Apply to it a homogeneous time-dependent deformation
\[
\hat{\mathbf{F}}(\hat{\mathbf{x}}, t) = \nabla \hat{\psi}_k(\hat{\mathbf{x}}, t).
\] (1)

The variable \( \hat{\mathbf{x}} \) is the position of a material particle in the reference configuration and \( \hat{\psi}_k \) describes the motion of the body with respect to \( k \) at any time \( t \geq 0 \) such that \( \hat{\mathbf{x}}_1 = \hat{\psi}_k(\hat{\mathbf{x}}, t) \). Since \( \hat{\psi}_k \) is a homogeneous deformation we assume that it is always possible to unload from configuration I to a stress-free configuration II using an elastic mapping \( \hat{\psi}_e(\cdot, t) \) such that \( \hat{\mathbf{x}}_2 = \hat{\psi}_e(\hat{\mathbf{x}}, t) \). Assuming that all mappings are continuous and differentiable as many times as needed, then
\[
\hat{\mathbf{F}}_e(\cdot, t) = \nabla \hat{\psi}_e(\cdot, t)
\]
and
\[
\hat{\mathbf{F}}_p(\cdot, t) = \nabla \hat{\psi}_p(\cdot, t)
\] (2)

wherein the arguments have been suppressed. This multiplicative decomposition of the total deformation into elastic and plastic parts is unique if the elastic deformation gradient, \( \hat{\mathbf{F}}_e \), is symmetric [8]. Equation (3) can be rewritten using the Polar Decomposition Theorem \( \hat{\mathbf{F}}_e = \hat{\mathbf{V}}_e \hat{\mathbf{R}}_e \) as
\[
\hat{\mathbf{F}} = \hat{\mathbf{V}}_e \hat{\mathbf{R}}_e \hat{\mathbf{F}}_p
\] (4)
where \( \hat{\mathbf{R}}_e \) is a symmetric \( \hat{\mathbf{F}}_p \).

Let us now assume that the stress-free configuration is heated to a temperature high enough to produce the recrystallized configuration III. Introducing the mappings \( \hat{\mathbf{x}}_3 = \hat{\psi}_a(\hat{\mathbf{x}}, t) \) and \( \hat{\mathbf{x}}_2 = \hat{\psi}_a(\hat{\mathbf{x}}, t) \) which relate configuration III to the reference and second configurations respectively, then
\[
\hat{\mathbf{F}}_a(\cdot, t) = \nabla \hat{\psi}_a(\cdot, t)
\] (5)
and
\[
\hat{\mathbf{F}}_p = \hat{\mathbf{R}}_a \hat{\mathbf{F}}_a
\] (6)

Substituting this decomposition in (3) we obtain
\[
\hat{\mathbf{F}} = \hat{\mathbf{V}}_e \hat{\mathbf{R}}_e \hat{\mathbf{R}}_a \hat{\mathbf{F}}_a
\] (7)

which on simplification gives
\[
\hat{\mathbf{F}} = \hat{\mathbf{V}}_e \hat{\mathbf{R}}_a \hat{\mathbf{F}}_a = \hat{\mathbf{V}}_e \hat{\mathbf{V}}_a \hat{\mathbf{F}}_a
\] (8)

where \( \hat{\mathbf{R}}_a = \hat{\mathbf{V}}_e \hat{\mathbf{R}}_a \hat{\mathbf{V}}_a \) and \( \hat{\mathbf{R}}_a = \hat{\mathbf{R}}_a \hat{\mathbf{V}}_a \).

A comparison of eqs. (8) and (4) indicates that
\[
\hat{\mathbf{F}} = \hat{\mathbf{V}}_e \hat{\mathbf{R}}_a \hat{\mathbf{F}}_a
\]

For convenience of notation assume configuration III is the unique configuration obtained after elastic unloading so that \( \hat{\mathbf{R}}_e = \hat{\mathbf{I}} \) and drop the bars in eqs. (8) and (4) so that
\[
\hat{\mathbf{F}} = \hat{\mathbf{V}}_e \hat{\mathbf{F}}_a
\] (9)

is the decomposition of total deformation into elastic, recrystallized and annealed deformation gradients.

Notice that configuration I in Figure I is arbitrary for any time \( t \) and need not be unloaded and recrystallized at each time to obtain configurations II and III. However, any
deformation can be viewed as the successive mapping onto configurations II and III so that eq. (9) always holds. The microstructure and density of the material in configuration III and the reference configuration are assumed to be identical implying that \( \det \frac{a}{v} = 1 \), where 'det' stands for determinant. Thus

\[
\det \frac{a}{v} = (\det \frac{a}{v})(\det \frac{a}{v}) = (\det \frac{a}{v})(\det \frac{a}{v})
\]

and it follows that \( \det \frac{a}{v} \neq 1 \); that is, in general the plastic deformation cannot be considered isochoric. This is consistent with experimental observations [9] where some volumetric changes have been observed during plastic deformation for real materials.

3. Work of Deformation

As discussed in the first section, an essential assumption in the development of this model is that the internal state variables remain invariant under a deformation process that does not cause energy to be stored irreversibly in the deformed material. For example, elastic deformation is considered reversible, and during perfectly plastic deformation all the work done is dissipated as heat. Therefore, both these deformation processes are assumed to leave the internal state variables unchanged. Next we shall evaluate the work done during deformation.

The instantaneous rate of work, \( \dot{W} \), consumed in deforming the body as it passes through configuration I is given by

\[
\dot{W} = \int_{\Omega_1} \dot{w} = \int_{\Omega_1} \text{tr}(T \dot{L})
\]

(11)

where \( T \) is the Cauchy stress tensor, \( \dot{L} = \frac{a}{v} \frac{a}{v}^{-1} \) is the velocity gradient and \( \Omega_1 = \Omega_2 (\det \frac{a}{v}) \) where \( \Omega_1 \) and \( \Omega_2 \) are the volumes of the body in the current and reference configurations, respectively. Differentiating eq. (9) and using it in eq. (11) the work-rate in the reference configuration can be written as

\[
\dot{W} = \int_{\Omega_2} \left[ \text{tr}(T \dot{L}^E) + \text{tr}(T' \dot{L}^R) + \text{tr}(T^{\text{th}} \dot{L}^A) \right] (\det \frac{a}{v})
\]

(12)

where \( L^E = \dot{v}^E \dot{v}^E^{-1} \), \( L^R = \dot{v}^R \dot{v}^R^{-1} \), \( L^A = \dot{v}^A \dot{v}^A^{-1} \) and \( T' = \dot{v}^E \dot{v}^E^{-1} \). Thus, the total work rate can be decomposed into three components, \( \dot{W} = \dot{W}^E + \dot{W}^R + \dot{W}^A \) and the total work done, \( W \), can be written as

\[
W = \int_0^t \int_{\Omega_2} \left( \dot{w}^E + \dot{w}^R + \dot{w}^A \right) (\det \frac{a}{v}) dt.
\]

(13)

In equation (13) \( \dot{w}^E \) is obviously the elastic work rate. This is reversible since energy is stored during elastic loading and is released during unloading. For a perfectly plastic material all plastic work of deformation is dissipated as heat. Thus, no hardening or recrystallization occurs during the deformation history so that configurations II and III coincide. Therefore, \( \dot{w}^A \) represents a hypothetical perfectly plastic deformation and the associated work, \( w^A \), is dissipated as heat. Finally, \( \dot{w}^R \) is the "deformation" that carries the fully recrystallized body into the strain-hardened body. Thus, part of the associated work, \( w^R \), must represent the stored energy of cold work and the remaining work is dissipated as heat. Thus, we have established a theoretical upper bound for the stored energy of cold
work, $e_s$, that is
\[ w^r = e_s \]  
(14)

4. Thermodynamics of Recrystallization

To continue the development of a continuum mechanics framework for materials that strain-harden and recrystallize, it is necessary to include the Principles of Thermodynamics. To begin, let us assume the constitutive equations for the Helmholtz free energy, $\psi$, Cauchy stress, $T$, entropy, $\eta$, and heat flux, $q$, can be written in the form [6]
\[ \psi = \psi_k(F, \theta, \xi) \]
\[ T = T_k(F, \theta, \xi) = \rho \frac{\partial \psi_k}{\partial F} \]
\[ \eta = \eta_k(F, \theta, \xi) = -\frac{\partial \psi_k}{\partial \theta} \]
\[ q = q_k(F, \theta, \xi) \]
(15)

where $\rho$, $\theta$, $\xi$ and $F$ are current density, absolute temperature, temperature gradient and state variables, respectively. In addition, the evolution equations for the state variables are given by
\[ \dot{\xi}_i = f_i(F, \theta, \xi) \quad i=1,2,...N \]  
(16)

Next, we can show that the Helmholtz free energy can be decomposed into recoverable (elastic) and non-recoverable (inelastic) components. Consider the time derivative of the Helmholtz free energy,
\[ \frac{\partial \psi}{\partial t} = \rho \frac{\partial \psi_k}{\partial F} \cdot \dot{F} + \rho \frac{\partial \psi_k}{\partial \theta} \dot{\theta} + \rho \frac{\partial \psi_k}{\partial \xi} \cdot \dot{\xi} \]  
(17)

where $\cdot$ is the inner product of two tensors. Using eq. (15), the first term of eq. (17) is equal to $\text{tr}(T^{-1} \dot{T})$; however, noting eq. (9) we get
\[ \frac{\partial \psi}{\partial t} = (T^{-1} T^{\prime}) \cdot \dot{F} + (T^{-1} T^{\prime}) \cdot \dot{\theta} + \rho \frac{\partial \psi_k}{\partial \theta} \dot{\theta} + \rho \frac{\partial \psi_k}{\partial \xi} \cdot \dot{\xi} \]  
(18)

The elastic deformation from configuration II to I can be expressed by a second potential function that is independent of the state variables; i.e.
\[ \psi^e = \psi^e(\varphi^e, \theta) \]
Using Clausius-Duhem inequality it also follows that
\[ \rho \psi^e = (T^{-1} T^{\prime}) \cdot \varphi^e - \rho \eta^e \theta \]  
(19)

Subtracting eq. (19) from eq. (18) and defining the irreversible free energy, $\psi^p$, and entropy, $\eta^p$, as
\[ \psi^p = \psi - \psi^e \quad \text{and} \quad \eta^p = \eta - \eta^e \]  
(20)

we obtain
\[ \rho \psi^p = \rho(\psi - \psi^e) = (T^{-1} T^{\prime}) \cdot \varphi^e - \rho \eta^p \theta + \rho \frac{\partial \psi_k}{\partial \xi} \cdot \dot{\xi} \]  
(21)

Notice that the total time derivative, $\psi^p_t$, is expressed in terms of total time derivatives
of \( F^P \), \( \theta \) and \( \xi \). Therefore we have \( \psi^P = \psi^P_k(\xi, \theta, \xi) \).

Finally

\[
\psi_k(\xi, \theta, \xi) = \psi^e(\xi, \theta) + \psi^P(\xi, \theta, \xi)
\]  

(22)

is obtained as the decomposition of free energy into reversible and irreversible parts.

Notice that only the irreversible part depends on the internal state variables. Further, by definition, the internal energy, \( \varepsilon \), is given by \( \varepsilon = \psi + \theta \eta \), thus using decompositions for \( \psi \) and \( \eta \) as

\[
\varepsilon = (\psi^e + \psi^P) + \theta(\eta^e + \eta^P) = \varepsilon^e + \varepsilon^P
\]  

(23)

where \( \varepsilon^e = \psi^e + \theta \eta^e \) and \( \varepsilon^P = \psi^P + \theta \eta^P \)

Eq. (23), then, represents the decomposition of internal energy into reversible (\( \varepsilon^e \)) and irreversible (\( \varepsilon^P \)) components.

5. Stored Energy of Cold Work

Using the energy balance, the instantaneous rate of change of internal energy for a particle is given by

\[
\dot{\varepsilon} = \dot{\psi}^e + \dot{\psi}^P
\]

(25)

where \( \dot{\psi} \) is the heating rate (positive if absorbed) associated with the deformation process.

Substituting for \( \dot{\psi} \) from eq. (12) and eq. (13) we get

\[
\dot{\varepsilon} = \dot{\psi}^e + \dot{\psi}^P = \dot{\psi}^e + \dot{\psi}^S + \dot{\psi}^a + \dot{\psi}^r + \dot{\psi}^a
\]

(26)

where \( \dot{\psi}^a \) has been written as the sum of three rates of heating terms associated with elastic, strain-hardening and perfectly plastic deformations. By definition, all the work done during a perfectly plastic deformation is dissipated as heat. Therefore, \( \dot{\psi}^a \) and \( \dot{\psi}^a \) in eq. (26) cancel out. Moreover, for an elastic process

\[
\dot{\psi}^e = \dot{\psi}^e + \dot{\psi}^r
\]

Following this reasoning we finally obtain

\[
\dot{\psi}^P = \dot{\psi}^r + \dot{\psi}^r
\]

(27)

as the rate of change of inelastic internal energy during a deformation process that produces strain-hardening. We now identify \( \varepsilon^P \) as the rate of storage of energy of cold work, \( \varepsilon_s \), i.e.

\[
\varepsilon_s = \int_0^t \dot{\psi}^P dt
\]

(28)

Assuming \( \psi^P \) is equal to zero in the reference configuration, thus

\[
\varepsilon_s = \dot{\psi}^e + \psi^P \theta \eta^P
\]

(29)

Noting eq. (24) and \( \psi^P = -\frac{3\psi^P}{3\theta} \), eq. (29) can be expressed as

\[
\varepsilon_s = \psi^P + \frac{3\psi^P}{3\theta} \dot{\psi}^P
\]

(30)

In functional form, this could be written as

\[
\varepsilon_s = f(\psi^P, \theta, \xi)
\]

(31)

Since the energy stored during the process of deformation and its subsequent release during recrystallization are responsible for strain-hardening and softening, the internal state variables, \( \xi \), that have been chosen to represent this behavior must be closely related.
with \( e_s \). Using this motivation a more specific representation for eq. (16) is postulated as

\[
\dot{\xi} = f(e_s^*)
\]  

(32)

where \( e_s^* \) is given by eqs. (28), (30) or (31). Equations (15) and (32) now form a set of constitutive equations relevant for the processes of strain-hardening and recrystallization.

6. Conclusion

A general theory for homogeneous, isothermal plastic deformation for metals including the effect of recrystallization has been presented above. The role of stored energy of cold work has been emphasized and an evolution equation for the internal state variables postulated. For specializing this theory for a particular metal we need a strain-hardening constitutive equation involving internal variables and the appropriate evolution equation(s). This has been done for copper in a uniaxial isothermal deformation [10] using only one internal variable and a specific constitutive equation [11]. It is hoped that more complicated deformation processes at elevated temperatures can be modeled using more than one internal variable. It is also expected to provide an insight into modeling phase changes in metals.

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References


Figure 1. Kinematics of Recrystallization