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Deborah Brandon
Carnegie Mellon University

Robert C. Rogers

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Deborah Brandon
Carnegie Mellon University
Robert C. Rogers
Virginia Polytechnic Institute
and State University

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Constitutive Laws for Pseudo-Elastic Materials

Deborah Brandon
Department of Mathematics, Carnegie Mellon University
Pittsburgh, Pennsylvania 15213

Robert C. Rogers
Department of Mathematics and ICAM
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061-0123

Abstract
In this paper a new model of pseudo-elastic materials based on experimental observations of one-dimensional motions of SMA materials is introduced. The model incorporates phase fractions as an internal variable and allows for both reversible (elastic) and irreversible (plastic) modes inside the hysteresis loop. As such, the model accounts for a wider range of physical phenomena than the traditional plasticity theories. The constitutive equations predict transitions between elastic and plastic modes through a dependence on the time history of strain and phase fractions. These history effects are included in a way that allows for easy computation.

1 Introduction
At a certain range of temperatures, one-dimensional motions of shape memory alloys display pseudo-elastic behavior; i.e., under large strain cycles, specimens go through a hysteresis loop of the form exhibited schematically in Figure 1. Recently Müller and Xu [7] have conducted experiments on single crystals of CuZnAl which display interesting behavior under partial loading and unloading cycles (i.e., inside the hysteresis loop). Briefly, their experiments indicate the following sequence of events depicted in Figure 2.

1. Initially, a material body is in its undeformed state, point (a). As a tensile load is applied, the body deforms elastically up to the critical point (b). (In this elastic phase the deformation is reversible.)

2. As the tensile load increases beyond point (b), the body deforms plastically. This deformation is irreversible.

3. If the load is increased to the point (c) and the load is then reduced to zero, the usual full hysteresis loop (cf. Figure 1) is traced.
4. However, if the load is only increased from point (b) to (c'), and then reduced, a "subloop" is formed. This subloop differs in character from those described by traditional plasticity theory.

(a) As the load is decreased from (c') to (d'), the body undergoes a reversible elastic deformation.

(b) In contrast to the traditional theory of elasto-plastic materials (where the body would unload elastically all the way down to (d)), Müller and Xu's experiments indicate that at the point (d'), the body switches to irreversible plastic unloading.
By varying the maximum deformation at which one begins unloading (i.e., the position of (c')), one obtains a family of partial loading subloops (cf. Figure 3a). A similar series of experiments in which the body is fully loaded and then partially unloaded leads to a family of curves depicted in Figure 3b. Note that in Figure 3, the locus of the points within the outermost loop at which the material switches from elastic to plastic behavior (both in loading and unloading) forms a curve (a straight line in these sketches), which will be referred to as the switching curve. In [7] the observation of elasto-plastic switching within the hysteresis loop is justified by the use of an interfacial energy term.

**Note:** In this paper we use the term plastic strain to refer to deformations that are locally irreversible. Despite the term's association with "permanent" deformations, we prefer it to such terms as pseudo-elastic strain which describes global rather than local behavior.

A number of mathematical models have been proposed for shape memory alloys. While many of these models have been successful in other contexts, none of them seem to predict the behavior inside the hysteresis loop described above. In particular, several models restrict their attention to behavior on the outermost loop (cf., e.g., the work of Tanaka [11] and Liang and C. Rogers [6]). Traditional plasticity models behavior inside the hysteresis loop, but as we indicated above (cf. Figure 2), the traditional theory does not allow for plastic modes within the loop (cf. e.g., Antman and Szymczak [1]). On the other hand, many other well-known constitutive laws based on hysteresis functions (i.e., the Preisach and Ishlinskii operators) do not allow for reversible (elastic) modes (cf. e.g., Krasnosel'skii and Pokrovskii [5], Brokate and Visintine [2]). Finally, models based on a nonconvex Gibbs-Landau energy functional (cf. e.g. Hoffman and Songmu [4], Niezgódka and Sprekels [8], etc.) have been difficult to analyze, and it is unclear what type of local behavior is exhibited by their solutions.

In this paper we introduce a macroscopic model which incorporates the types of behaviors observed by Müller and Xu. This model generalizes traditional plasticity theory by allowing for a greater number of possibilities for switching between plastic and elastic modes. In Section 2 we give a general three-dimensional formulation of our constitutive equations and
discuss thermodynamic restrictions. In Section 3 we study more specific one-dimensional models designed to reflect the empirical results of [7]. These models are essentially phenomenological. In particular, we do not incorporate interfacial energy, and we make no attempt to derive our model from a more primitive (microscopic or microstructural) theory. Our aim is to pose a theory that is amenable to analysis and easy to approach from a computational point of view.

2 Equations for three-dimensional motions

In this section we develop a theory for three-dimensional material bodies that display both elastic and plastic behavior inside the hysteresis loop. Our approach owes much to the work of Antman and Szymczak [1] on classical plasticity.

2.1 Balance laws

Let \( \Omega \subset \mathbb{R}^3 \) be (the reference configuration of) a body. Let

\[
\Omega \ni x \mapsto \rho_0(x)
\]

be the density per unit reference volume of \( \Omega \). Our goal is to develop a continuum theory that predicts the trajectory

\[
\Omega \times \mathbb{R} \ni (x,t) \mapsto p(x,t) \in \mathbb{R}^3
\]

and the (absolute) temperature distribution

\[
\Omega \times \mathbb{R} \ni (x,t) \mapsto \theta(x,t) \in (0, \infty)
\]

of the body. We require that the deformation preserves orientation locally; i.e.,

\[
det F > 0,
\]

where \( F \) is the deformation gradient defined by

\[
F(x,t) := p_x(x,t).
\]

As the first step in the development of our model we state the following balance laws.

1. The balance of linear momentum:

\[
div T + f = \rho_0 \ddot{p}.
\]

Here \( T \) is the first Piola-Kirchhoff stress tensor or stress per unit reference area, \( f \) is the external body force per unit reference volume, \( div \) is the divergence with respect to Lagrangian coordinates, and the superposed dot indicates a material time derivative.

2. The balance of angular momentum:

\[
F^*T = T^*F.
\]
Here $A^*$ indicates the transpose of a tensor $A$.

3. The balance of energy:

$$\rho_0 \dot{E} = -\text{div} \, q + T : \dot{\mathbf{F}} + \rho_0 r.$$  \hfill (2.8)

Here $E$ is the internal energy per unit mass, $q$ is the heat flux per unit reference area, $A : B$ indicates the scalar product of two tensors $A$ and $B$, and $r$ is the external heat supply per unit mass.

### 2.2 Rate-independent constitutive laws

The balance laws stated above are assumed to hold for all types of material bodies. In order to distinguish one material from another we must specify constitutive equations that characterize the material response. We follow the common practice of describing our constitutive laws in terms of the strain tensor

$$E := \frac{1}{2} (F^* F - I)$$ \hfill (2.9)

and the second Piola-Kirchhoff stress tensor

$$S := F^{-1} T.$$ \hfill (2.10)

Here $I$ is the identity tensor. We also define the temperature gradient

$$g(x,t) := \nabla_x (x,t),$$ \hfill (2.11)

and write the internal energy as

$$E := \psi + \theta \eta,$$ \hfill (2.12)

where $\psi$ is the Helmholtz free energy and $\eta$ is the entropy per unit reference volume.

In order to describe the yielding of our material we introduce a new internal variable $\Omega \times \mathbb{R} \ni (x,t) \mapsto \Pi(x,t) \in \mathbb{R}^m$, for some $m$. At this time we do not restrict the physical interpretation of $\Pi$. In Section 3 below, $\Pi$ is the scalar-valued phase fraction of austenite-martensite variants in a wire of pseudo-elastic material. However, other versions of plasticity theory include internal variables such as a plastic strain, a hardening parameter, and a back stress. Any or all of these could be incorporated into the variable $\Pi$.

We now define the state variable

$$U(x,t) := (E(x,t), \theta(x,t), g(x,t)),$$ \hfill (2.13)

and assume that $S$, $q$, $\psi$, and $\eta$ depend on the present values of $U$ and $\Pi$,

$$S(x,t) = \hat{S}(U(x,t), \Pi(x,t), x) \hfill (2.14)$$
$$q(x,t) = \hat{q}(U(x,t), \Pi(x,t), x) \hfill (2.15)$$
$$\psi(x,t) = \hat{\psi}(U(x,t), \Pi(x,t), x) \hfill (2.16)$$
$$\eta(x,t) = \hat{\eta}(U(x,t), \Pi(x,t), x) \hfill (2.17)$$
The internal variable II is used to incorporate the past history of the independent variables into our constitutive laws in a very simple way. We will use the notation

$$\mathbb{R}^+ := [0, \infty) \ni \zeta \mapsto A^i(x, \zeta) := A(x, t - \zeta)$$ (2.18)

for the past history of the function $A(x, \cdot)$ up to time $t$. In this paper we assume that $U$ and $II$ are smooth, more precisely they lie in the space

$$\mathcal{H} := C^1(\mathbb{R}^+, C_b^1(\Omega)).$$ (2.19)

We assume that the evolution of $II$ is governed by an ordinary differential equation of the form

$$\dot{II}(x, t) = s(U^i(x, \cdot), II^i(x, \cdot))M(U(x, t), II(x, t))U(x, t).$$ (2.20)

Here the constitutive function $M$ is a linear transformation such that

$$M(U(x, t), II(x, t))U(x, t) = M^E(U(x, t), II(x, t))\dot{E}(x, t) + M^E(U(x, t), II(x, t))\dot{\theta}(x, t) + M^E(U(x, t), II(x, t))\dot{\phi}(x, t).$$ (2.21)

This assumption follows from the treatment of classical plasticity by Antman and Szymczak [1]. The more interesting part of this theory is the specification of the plastic switching function

$$s(U^i(x, \cdot), II^i(x, \cdot)) \mapsto s(U^i(x, \cdot), II^i(x, \cdot)) \in \{0, 1\}.$$ (2.22)

We will assume that the switching function is rate-independent; i.e., for any smooth function $\sigma : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ satisfying

$$\sigma' > 0, \quad \sigma(0) = 0, \quad \text{and} \quad \lim_{\zeta \to \infty} \sigma(\zeta) = \infty,$$ (2.23)

we have

$$s(U^i(x, \sigma(-)), II^i(x, \sigma(-))) = s(U^i(x, \cdot), II^i(x, \cdot))$$ (2.24)

We say that at time $t$, the material particle $x$, with state history $U^i(x, \cdot)$ and $II^i(x, \cdot)$, is in the

- **plastic mode** if $s(U^i(x, \cdot), II^i(x, \cdot)) = 1$, and in the
- **elastic mode** if $s(U^i(x, \cdot), II^i(x, \cdot)) = 0$.

Note that this terminology does not agree with many of the traditional notions of plasticity. For instance, the types of behavior described in [1] as plastic neutral loading, plastic unloading, and elastic are all contained in what we call the elastic mode.

In Section 3, we give more detailed descriptions of switching functions for one-dimensional, isothermal pseudo-elastic materials. We make a few preliminary comments at this time.

1. Our hypotheses are more general than the constitutive hypotheses for hypoelastic materials (cf. [12]), which are a special case of the theory addressed in this section.
2. The elasto-plasticity theory described in [1] is also a special case of the theory described here. However, the materials considered in [1] can only be in plastic mode on a surface in the \((U, \Pi)\) state space described by a level surface of a yield function. In a one-dimensional analysis of such a model, the most natural assumption (and the one explored in [1]) is that plastic yielding can take place only on the upper and lower branches of the hysteresis loop. This is a good model for many types of materials; and in fact, similar assumptions are sometimes made in modeling shape memory alloys. However, as we have indicated in the introduction, the experimental evidence strongly indicates that pseudo-elastic materials can have yield curves at all points within the hysteresis loop, and this is the behavior that we attempt to model below.

2.3 Constitutive restrictions

We assume that the following two restrictions on our constitutive equations hold. We first assume that the constitutive relations are such that the balance of angular momentum is satisfied automatically. This is accomplished by assuming that the constitutive function \(\hat{S}\) always yields a symmetric tensor.

Second, we adopt the view of Coleman and Noll [3] that our constitutive laws must satisfy the Clausius-Duhem inequality

\[-\psi_t - \eta \theta_t + S : E_t + \frac{1}{\theta} q \cdot g \geq 0\]  \hspace{1cm} (2.25)

for all admissible past histories of the state variables.

Substituting our constitutive equations into (2.25) yields

\[
0 \leq [+[-\hat{\psi}_E - \hat{\psi}_\Pi s M^E + \hat{S}] : E_t + [-\hat{\psi}_\theta - \hat{\psi}_\Pi s M^\theta - \eta] \theta_t \\
+ [-\hat{\psi}_g - \hat{\psi}_\Pi s M^g] \cdot g_t - \frac{1}{\theta} \hat{q} \cdot g
\]

(2.26)

Note that because the switching function \(s\) depends on the histories of the state variables, we cannot assume that one can construct histories such that \(E_t, \theta_t\) and \(g_t\) are independent of the value of the quantities in the brackets. Thus, we cannot deduce that the quantities in the brackets are zero. The specific constitutive equations below are constructed so that the plastic mode is locally irreversible and the elastic mode locally reversible. Local reversibility will allow us to use the Clausius-Duhem inequality to derive some restrictions on our constitutive equations.

**Definition 2.1** We say that a state \((U(x,t), \Pi(x,t))\) is elastically reversible at \((x,t)\) if for every \(E_t(x,t), \theta_t(x,t), g_t(x,t)\) there exist histories \(U^i(x,\cdot)\) and \(\Pi^i(x,\cdot)\) such that

\[
s(U^i(x,\cdot), \Pi^i(x,\cdot)) = 0,
\]

(2.27)

\[
(U^i(x,0), \Pi^i(x,0)) = (U(x,t), \Pi(x,t)),
\]

(2.28)

\[
\dot{U}^i(x,0) = (E_t(x,t), \theta_t(x,t), g_t(x,t))
\]

(2.29)

Applying this definition to the Clausius-Duhem inequality leads to the following result.
Lemma 2.2 At any elastically reversible state \((U(x,t), \Pi(x,t))\) the following hold

\[
\begin{align*}
\dot{\psi}_e(U(x,t), \Pi(x,t), x) &= \dot{S}(U(x,t), \Pi(x,t), x), \\
-\dot{\psi}_\theta(U(x,t), \Pi(x,t), x) &= \dot{\eta}(U(x,t), \Pi(x,t), x), \\
\dot{\psi}_g(U(x,t), \Pi(x,t), x) &= 0,
\end{align*}
\]

and

\[
\dot{q} \cdot g \leq 0.
\]

3 One-dimensional isothermal motions

We now write some more specific constitutive relations for one-dimensional materials. Our equations are purely phenomenological and we make no attempt to justify them by referring to three-dimensional theories. The current literature on microstructure has influenced our hypotheses, but we cannot give a rigorous justification of our one-dimensional models in terms of more fundamental theories at this time.

3.1 General equations

We begin by describing some general stress-strain relations for an isothermal material.

We consider the following representation of longitudinal motions of a slender elastic body which we will refer to as a wire. The reference configuration is taken to be the interval \([0, L]\) and admissible deformations are represented by real-valued functions of the form

\[
[0, L] \times \mathbb{R}^+ \ni (x, t) \mapsto p(x, t) \in \mathbb{R}. 
\]

We write the deformation \(p\) in terms of the displacement \(u\) using

\[
p(x, t) =: x + u(x, t).
\]

We define the longitudinal strain

\[
\epsilon(x, t) := u_x(x, t). 
\]

(The function \(\epsilon\) is identified with \(E\) in the three-dimensional case.) The requirement of local invertibility translates to the constraint

\[
\epsilon(x, t) > -1.
\]

In this paper we consider only tensile motions \((\epsilon \geq 0)\) since these are the only type of motions that we can make any pretense of understanding.

We let

\[
T : [0, L] \times \mathbb{R}^+ \rightarrow \mathbb{R}
\]

be the longitudinal stress, and for an internal variable we use

\[
\beta : [0, L] \times \mathbb{R}^+ \rightarrow [0, 1]
\]
which we call the phase fraction. (The function \( \beta \) is identified with \( \Pi \) in the three-dimensional case.) We are motivated by the interpretation of \( \beta \) as the fraction of austenite and martensite phases of the crystal within the cross section of the wire.

If we let \( v(x, t) := p_t(x, t) \) be the velocity, then the balance of mass and momentum can be written as the first order system

\[
\begin{align*}
\epsilon_t &= v_x, \\
v_t &= T_x.
\end{align*}
\]  

The evolution of the phase fraction is governed by

\[
\beta_t = s(\epsilon^t, \beta^t) M(\epsilon, \beta) \epsilon_t
\]

where \( M : \mathbb{R}^+ \times [0, 1] \rightarrow \mathbb{R}^+ \) is a constitutive function which characterizes the plastic evolution of the phase fraction and \( s \) is a switching function (cf. (2.21) and (2.22)).

When the body is in elastic mode at a point, \( \beta \) is constant in time. When the body is in plastic mode \((s = 1)\) we see from (3.42) that \( \epsilon \) and \( \beta \) evolve along a family of curves in the \((\epsilon, \beta)\) plane described by the ordinary differential equation

\[
\frac{d\beta}{d\epsilon} = M(\epsilon, \beta).
\]

The solution of this equation with initial condition

\[
\beta(\epsilon_0) = 0
\]

will be denoted by \( \hat{\beta}(\epsilon; \epsilon_0) \). We will refer to this family as the phase-strain curves. We make the following assumption.

**Hypothesis 3.1** For every \( \epsilon_0 \in [\epsilon^-_0, \epsilon^+_0] \) there is solution of the equation

\[
\hat{\beta}(\epsilon; \epsilon_0) = 1.
\]

In other words, each of the phase-strain curves intersects both the line \( \beta = 0 \) and the line \( \beta = 1 \). Of course, we could give sufficient conditions on \( M \) to ensure that this hypothesis is satisfied (e.g., we might require \( M \) to be bounded below by a positive constant). We now define \( \epsilon^+_0 \) to be the solutions of

\[
\begin{align*}
\hat{\beta}(\epsilon^-_0 + \epsilon_0) &= 1, \\
\hat{\beta}(\epsilon^+_0; \epsilon_0) &= 1,
\end{align*}
\]

respectively. In Figure 4 we have depicted a typical family of phase-strain curves.

The system of three evolution equations (3.40-3.42), is supplemented with a constitutive law

\[
T(x, t) = \hat{T}(\epsilon(x, t), \beta(x, t)).
\]

We call the family of curves

\[
\epsilon \mapsto \hat{T}(\epsilon, \beta)
\]
parameterized by $\beta \in [0,1]$ the \textbf{elastic stress-strain curves} (cf. Figure 5a). The \textbf{plastic yield curves} are the curves formed by composing the phase-strain function $\beta$ with $\hat{T}$:

$\epsilon \mapsto \hat{T}(\epsilon, \beta(\epsilon; \epsilon_0))$

where the parameter is $\epsilon_0 \in [\epsilon_0^-, \epsilon_0^+]$ (cf. Figure 5b). (We have yet to restrict the direction of plastic yielding.)

Note that the elastic stress-strain curves corresponding to $\beta = 0$ and $\beta = 1$ and the plastic yield curves corresponding to $\epsilon_0 = \epsilon_0^\pm$ determine the outermost hysteresis loop. Subloops are formed when we switch between elastic and plastic modes within the outermost loop. This switching is governed by the function $s$. We now give a more complete description of the dependence of $s$ on the histories of $\epsilon$ and $\beta$. To do this we first introduce a \textbf{switching curve} in the $(\epsilon, \beta)$ plane defined by the function

$$\dot{\epsilon} : [0,1] \to \mathbb{R}^+.$$ (3.48)
We assume

\[ \dot{\epsilon}(0) = \epsilon_0^+ \]  \hspace{1cm} (3.49)

\[ \dot{\epsilon}(1) = \epsilon_1^- . \]  \hspace{1cm} (3.50)

We also assume that at each point the switching curve intersects one (and only one) of the phase-strain curves (cf. Figure 6a). By composing \( \dot{\epsilon} \) with \( \hat{T} \) we obtain the corresponding curve in the stress-strain plane (cf Figure 6b).

![Diagram of switching curve superimposed on phase-strain curves and switching curve in stress-strain plane.]

Figure 6: (a) Switching curve superimposed on phase-strain curves. (b) Switching curve in stress-strain plane.

With the switching curve thus defined we can now describe the switching function \( s \). We give the definition in terms of a set of rules for switching between elastic and plastic modes.

**Definition 3.2**  
1. If the body is in the elastic mode at a point, it will remain in the elastic mode until \( (\epsilon(x,t), \beta(x,t)) \) intersects either

   (a) the switching curve \( \epsilon = \hat{\beta}(\beta) \),
   
   (b) \( \beta = \hat{\beta}(\epsilon; \epsilon_0^+ ) \), or
   
   (c) \( \beta = \hat{\beta}(\epsilon; \epsilon_0^- ) \).

2. If the body is in the plastic mode at a point, it will remain in the plastic mode until

   (a) \( \beta(x,t) = 0 \),
   
   (b) \( \beta(x,t) = 1 \),
   
   (c) \( \epsilon_t(x,t)[\epsilon(x,t) - \hat{\epsilon}(\beta(x,t))] < 0 \).

Note that the sign condition on \( \epsilon_t(\epsilon - \hat{\epsilon}) \) means that we stay in the plastic mode as long as we are "moving away" from the switching curve along the plastic yield curves. Hence the direction of irreversible motion is now determined.
4 Comments

1. If we assume that $M(\dot{e}(\beta), \beta) = 0$ we ensure that the transition from elastic to plastic mode at the switching curve is smooth. (The data in [7] seems to indicate that this should be the case.)

2. One can certainly question the validity of designing a local model based on macroscopic observations (especially when the microstructure is as complicated as it is in shape memory alloys). However, we take some comfort in the fact that the experiments in [7] were conducted using single crystals.

3. In this work we have restricted our attention to smooth processes. There is a vigorous ongoing debate on the proper way to extend physical systems that are not in conservation form to allow for the formation of discontinuities such as shocks. This discussion involves not only our model but numerous other theories such as plasticity, hypoelectricity, Cattaneo's model for heat flow, hysteresis models for ferromagnetic materials, etc. While some progress has been made in very specific cases (cf. Renardy [10], Plohr [9]) this remains a very difficult problem in general.

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