Journal of Elasticity **44:** 145–160, 1996.

Modeling of Macroscopic Response of Phase Transforming Materials under Quasi-Static Loading

XIAOGUANG ZHONG* and R.C. BATRA
Department of Engineering Science and Mechanics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0219, USA

Received 16 May 1996

Abstract. Based on a continuum model of solid-solid phase transformations, the macroscopic response of a bar of a thermoelastic phase transforming material loaded quasistatically is investigated. A critical loading rate is identified for the evolution of a single phase boundary in the bar during an isothermal process. It is shown that, when the loading rate is larger than this critical loading rate, nucleation occurs either continuously or at multiple sites; when the loading rate is lower than this critical loading rate, the size of the hysteresis loop increases with increasing loading rate, and decreases with an increase in the mobility of the phase boundary. The heat conduction due to the heat generated by the latent heat of the phase transformation is considered for a special case.

Key words: Continuum mechanics, phase transformation, mathematical modeling

1. Introduction

Martensitic transformation can be induced by mechanical loading when the temperature is within a certain range. This is the so-called stress-induced martensitic transformation. One of the main features of the stress-induced martensitic transformation is that the load-deformation curve in a uniaxial test is hysteretic during the loading and unloading process. This phenomenon is called pseudo-elasticity. The stress-induced martensitic transformation is thermomechanical because there is latent heat generated during the phase transformation (Grujici et al., 1985; Shaw and Kyriakides, 1994). However, when the loading rate is very low, the transformation process can be treated as isothermal (Shaw and Kyriakides, 1994). Efforts have been made towards understanding and modeling of pseudo-elasticity, see for example the work of Abeyaratne and Knowles (1993), Falk (1980), Jiang (1993), Kim and Abeyaratne (1995), Leo et al. (1993), and Müller and Xu (1991). Here we investigate the macroscopic response of the stress-induced phase transformation by using the model proposed by Abeyaratne and Knowles (1993), though our view point is different.

---

* Current address: Graduate Aeronautical Laboratories, Mail code 105-50, The California Institute of Technology, Pasadena, CA 91125, USA.

Borrowing from an idea widely used in materials science, Abeyaratne and Knowles (1988) proposed a nucleation criterion and a kinetic relation to describe solid-solid phase transformations at the continuum level. With these two constitutive relations added to the conventional constitutive relation, Abeyaratne and Knowles (1988, 1993) predicted hysteresis, and Abeyaratne et al. (1994) predicted shape-memory effects in martensitic transformations. However, the nucleation criterion does not determine uniquely the nucleation site in a uniform bar. One way to ascertain this is to assume a geometrical inhomogeneity in the bar, as Abeyaratne and Knowles (1988) did; another way is to select a favorable nucleation site, as was done by Abeyaratne and Knowles (1993), and Kim and Abeyaratne (1995). For the latter case, it is implied that once nucleation begins, the kinetic relation takes over.

Here we build upon the model of Abeyaratne and co-workers, and do not assume a priori a nucleation site in the form of a geometrical inhomogeneity or a defect. Instead we consider the effect of gravitational force and presume that the nucleation criterion holds at all times. The specimen's weight provides a natural inhomogeneity in the specimen, and models more closely test configurations in which a specimen is held vertically in a testing machine. We analyse both a displacement controlled test and a load controlled test. In each case, deformations are assumed to be isothermal and a critical loading rate is identified. When the loading rate is smaller than this critical value, a single phase boundary separating two distinct phases propagates slowly. When the loading rate is larger than this critical loading rate, the nucleation takes place either continuously or at multiple sites. Furthermore, if the loading rate is smaller than the critical loading rate, the size of the hysteresis loop increases with an increase in the loading rate, but decreases with an increase in the speed of the phase boundary. Also, the analysis reveals that the transformation process should be treated as dynamic for loading rates exceeding the critical loading rate even though it may be small in the usual sense. If the latent heat is taken into consideration, we have a coupled nonlinear thermo-mechanical problem. We consider a special case for which an analytical solution is formally obtained. We observe that the phase boundary speed decreases due to the latent heat generated at the phase boundary, and the reverse transformation can occur even under a monotonically increasing load; this was speculated by Kim and Abeyaratne (1995). Also serrations in the load-displacement curve can be caused by local heating.

Many conclusions drawn from this work agree qualitatively with test findings. In Section 2, the model used is summarized briefly. We analyze analytically the hysteresis of the stress-induced phase transformation in an isothermal process under various loading conditions in Section 3. A thermomechanical problem is considered in Section 4.

2. A Model of Phase-Transforming Material

Consider a one-dimensional bar with uniform cross section A that occupies the interval [0, L] in an unstressed reference configuration, see Figure 1. A thermomechanical process in the bar is characterized by the longitudinal displacement field $u(x, t)$ and the temperature field $\theta(x, t)$. We assume that u and θ are continuous with piecewise continuous first and second derivatives in $(0, L)$ for $t > 0$. Let $\gamma(x, t) = u_x(x, t) \equiv \partial u(x, t)/\partial x$ denote the axial strain in the bar. The material of the bar is assumed to be thermoelastic and is characterized by a two-well Helmholtz free energy potential $\psi(\gamma, \theta)$ in a certain range of temperature. Such kinds of materials can undergo solid–solid phase transformations. In fact, the material has two stable or metastable phases; one can be dentified as austenite which is stable at high temperatures, and the other as martensite which is stable at low temperatures. The axial stress σ and the entropy per unit mass η in the bar at a particle can be expressed as

$$\sigma = \hat{\sigma}(\gamma, \theta) = \rho\psi_\gamma(\gamma, \theta), \tag{2.1}$$

$$\eta = \hat{\eta}(\gamma, \theta) = -\psi_\theta(\gamma, \theta), \tag{2.2}$$

where ρ is the referential mass density of the bar. On neglecting the effects of inertia forces, the principle of linear momentum and the first and second laws of thermodynamics give the following governing equations in a smooth region:

$$\sigma_x + \rho g = 0, \tag{2.3}$$

$$q_x = \rho\theta\eta_t, \tag{2.4}$$

and

$$q\theta_x \geqslant 0, \tag{2.5}$$

where g is the gravitational constant, and q is the heat flux.

At a discontinuity $x = s(t)$ where a phase boundary, if there is one, is situated, the following jump conditions must hold:

$$[\sigma] = 0, \tag{2.6}$$

$$[q] + f\dot{s} + \rho\theta[\eta]\dot{s} = 0, \tag{2.7}$$

where f defined by

$$f \equiv \rho[\psi] - \sigma[\gamma] \tag{2.8}$$

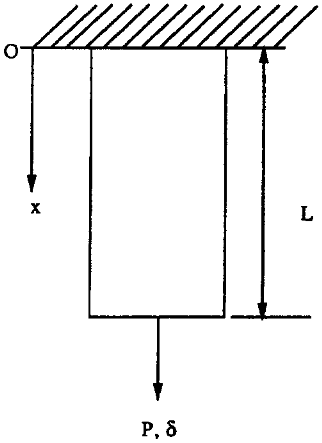


Fig. 1. A schematic sketch of the problem studied.

is the driving traction on the phase boundary, a superimposed dot denotes the material time derivative, and $[\sigma]$ indicates the jump in σ across the phase boundary.

In addition to constitutive relations (2.1) and (2.2), we also have the following constitutive relations for the phase transformation process: one is the nucleation criterion which determines when and where a new phase will initiate, and the other is the kinetic relation which determines the rate of phase transformation. The nucleation criterion can be stated as

$$\text{austenite} \rightarrow \text{martensite} : \sigma(x,t) \geqslant \sigma_{\text{cr}}(\theta), \tag{2.9}$$

$$\text{martensite} \rightarrow \text{austenite} : \sigma(x,t) \leqslant \sigma^*_{\text{cr}}(\theta), \tag{2.10}$$

where $\sigma_{\text{cr}}(\theta)$ and $\sigma^*_{\text{cr}}(\theta)$ are the appropriate critical stresses. The kinetic relation can be stated as

$$f = \phi(\dot{s}, \theta), \tag{2.11}$$

where $\phi(\dot{s}, \theta)$ is a monotonically increasing function of $\dot{s}$ and *may* be discontinuous at $\dot{s} = 0$, but is continuous elsewhere. Alternatively, we can express the kinetic relation as

$$\dot{s} = V(f, \theta). \tag{2.12}$$

We use the model proposed by Abeyaratne and Knowles (1993). For $0 < \theta < \theta_c$, the Helmholtz free energy function is given by

$$\psi(\gamma,\theta) = \begin{cases} \frac{\mu}{2\rho}\gamma^2 - \alpha\frac{\mu}{\rho}\gamma(\theta-\theta_T) - c\theta\log\frac{\theta}{\theta_T}, & -1 < \gamma < \gamma_m(\theta), \\ -\frac{\mu}{2\rho}\frac{\gamma_T(\gamma-\gamma_m)^2-(\gamma_M(\theta)-\nu_m(\theta))\gamma^2}{\gamma_M(\theta)-\gamma_m(\theta)} & \\ \quad -\alpha\mu/\rho\gamma(\theta-\theta_T) - c\theta\log\frac{\theta}{\theta_T}, & \gamma_m(\theta) < \gamma < \gamma_M(\theta), \\ \frac{\mu}{2\rho}((\gamma-\gamma_T)^2 + \gamma_T(\gamma_M(\theta)+\nu_m(\theta)-\gamma_T)) & \\ \quad -\mu/\rho\alpha\gamma(\theta-\theta_T) - c\theta\log\frac{\theta}{\theta_T}, & \gamma_M(\theta) < \gamma. \end{cases} \tag{2.13}$$

When $\theta > \theta_c$, the material can have only the austenite phase. For the Helmholtz free energy function given by (2.13), we have

$$\hat{\sigma}(\gamma,\theta) = \begin{cases} \mu\gamma - \mu\alpha(\theta-\theta_T), & -1 < \gamma < \gamma_m(\theta), \\ \mu(\gamma - \gamma_T(\gamma-\gamma_M(\theta))/(\gamma_m(\theta) & \\ \quad -\gamma_M(\theta))) - \mu\alpha(\theta-\theta_T), & \gamma_m(\theta) < \gamma < \gamma_M(\theta), \\ \mu(\gamma-\gamma_T) - \mu\alpha(\theta-\theta_T), & \gamma_M(\theta) < \gamma < \infty. \end{cases} \tag{2.14}$$

Furthermore, from (2.8), we have

$$f = \gamma_T(\sigma - \sigma_T), \tag{2.15}$$

$$\lambda_T = \frac{\mu}{\rho}\gamma_T\theta_T\left(\frac{M+m}{2} - \alpha\right), \tag{2.16}$$

and

$$\sigma_T = \frac{\rho\lambda_T}{\theta_T\gamma_T}(\theta-\theta_T), \tag{2.17}$$

where $\gamma_m(\theta) = \gamma_c + m(\theta-\theta_c)$, and $\gamma_M(\theta) = \gamma_c + M(\theta-\theta_c)$. Here α is the coefficient of thermal expansion, γ_T the transformation strain, θ_T the transformation temperature, c the specific heat, λ_T the latent heat, and σ_T the Maxwell stress at temperature θ.

We call strain interval $-1 < \gamma < \gamma_m(\theta)$ 'the low-strain phase' or 'austenite', the interval $\gamma_m(\theta) < \gamma < \gamma_M(\theta)$ 'the unstable phase', and $\gamma_M(\theta) < \gamma$ 'the high-strain phase' or 'martensite'. The low-strain and the high-strain phases are metastable phases.

We further assume that heat conduction is governed by Fourier's law,

$$q = k\theta_x, \tag{2.18}$$

where the thermal conductivity k is taken to be a positive constant.

3. An Isothermal Process

For an isothermal process, the temperature and entropy in the bar are necessarily constants (see Abeyaratne and Knowles, 1993), and are denoted by θ_0 and η_0 respectively. Thus there is no heat conduction. In this section, we omit θ and η in all expressions and reformulate the mathematical problem as a mechanical one. It is also assumed that there is at most one phase boundary in the bar at $x = s(t)$. The corresponding governing equation is, when $x \neq s(t)$,

$$\sigma_x + \rho g = 0, \tag{3.1}$$

and at $x = s(t)$, the jump condition

$$[\sigma] = 0 \tag{3.2}$$

must hold. The stress–strain relation (2.14) can be expressed as

$$\sigma(\gamma) = \begin{cases} \mu\gamma, & -1 < \gamma < \gamma_m, \\ (\sigma_m - \sigma_M)(\gamma - \gamma_M)/(\gamma_m - \gamma_M) + \sigma_M, & \gamma_m < \gamma < \gamma_M, \\ \mu(\gamma - \gamma_T), & \gamma_M < \gamma < \infty, \end{cases} \tag{3.3}$$

where $\sigma_m = \mu\gamma_m, \sigma_M = \mu(\gamma_M - \gamma_T)$. The driving traction is given by

$$f = \gamma_T(\sigma - \sigma_0), \tag{3.4}$$

where σ_0 is the Maxwell stress at temperature θ_0.

3.1. DISPLACEMENT-CONTROLLED TEST

The displacement $\Delta(t)$ is imposed at $x = L$ with $\Delta(0) = 0$. Let $\tilde{\delta}(t) = \Delta(t)/L$. If we denote the stress at $x = L$ by $p(t)$, then $\sigma(x,t) = p(t) + \rho g(L - x)$, so we have for $-1 < \sigma/\mu < \gamma_m$

$$\tilde{\delta}(t) = \frac{1}{L}\int_0^L \frac{\sigma(x,t)}{\mu}\,\mathrm{d}x = \frac{p(t)}{\mu} + \frac{\rho g L}{2\mu}. \tag{3.5}$$

Let $\delta(t) = \tilde{\delta}(t) - (\rho g L/2\mu)$, then

$$\delta(t) = \frac{p(t)}{\mu}. \tag{3.6}$$

When $\sigma(0,t) = p(t) + \rho g L = \sigma_{\text{cr}}$, martensite will initiate at $x = 0$. As the axial stress is monotonically decreasing along x, the point $x = 0$ is the only place in the bar where nucleation occurs. The phase transition initiates at time $t = t^*$ given by

$$\delta(t^*) = \frac{\sigma_{\text{cr}} - \rho g L}{\mu}. \tag{3.7}$$

Reset the time scale by taking $t = t^*$ as a new starting time. Then we have $s(0) = 0$, where $s(t)$ is the position of the phase boundary at time $t, \delta(0) = (\sigma_{\text{cr}} - \rho g L)/\mu$ and $p(0) = \sigma_{\text{cr}} - \rho g L$. Recalling (3.3)$_3$ and (3.5), we have

$$\delta(t) = \frac{p(t)}{\mu} + \frac{\gamma_T}{L} s(t). \tag{3.8}$$

The phase boundary position $s(t)$ is determined from equation (3.8) and the following kinetic relation at the phase boundary:

$$\gamma_T(\sigma(s,t) - \sigma_0) = \phi(\dot{s}). \tag{3.9}$$

As

$$\sigma(s,t) = p(t) + \rho g(L - s(t)) = \mu\delta(t) + \rho g L - \frac{\mu\gamma_T + \rho g L}{L} s(t),$$

from (3.9), for *constant loading rate*, we have

$$\phi'(\dot{s})\ddot{s} + \frac{\mu\gamma_T^2}{L}(1 + a)\dot{s} = \mu\gamma_T\dot{\delta}, \tag{3.10}$$

where $\dot{s}(0) = \phi^{-1}(\gamma_T(\sigma_{\text{cr}} - \sigma_0)), a = (\rho g L)/(\mu\gamma_T^2)$.

It is easy to show that equation (3.10) has a single stable equilibrium point

$$\dot{s}_{\text{eq}} = \frac{L}{(1 + a)\gamma_T}\dot{\delta}. \tag{3.11}$$

On the other hand, from (3.9), we also have

$$\phi'(\dot{s})\ddot{s} = -\frac{\mu\gamma_T^2}{L}\left(\dot{s}(0) - \frac{L\dot{\delta}}{(1 + a)\gamma_T}\right). \tag{3.12}$$

Thus we have

- if $\dot{\delta} < (1 + a)\dot{s}(0)(\gamma_T/L)$, then $\ddot{s}(t) < 0, \dot{s}(t) < \dot{s}(0)$ and $\dot{s}(t) \to (L\dot{\delta})/((1 + a)\gamma_T)$.
- if $\dot{\delta} > (1 + a)\dot{s}(0)(\gamma_T/L)$, then $\ddot{s}(0) > 0$, which means $\dot{s}(0+) > \dot{s}(0)$. Thus the stress at $x = s(0+)+$ will be greater than σ_{cr}, which indicates that nucleation occurs in front of the phase boundary. This means that when the single phase boundary assumption is removed, the nucleation of new phase occurs either continuously or at multiple sites.

So we have identified a critical loading rate,

$$\dot{\delta}_{\mathrm{cr}} = (1+a)\phi^{-1}(\gamma_T(\sigma_{\mathrm{cr}} - \sigma_0))\frac{\gamma_T}{L}. \tag{3.13}$$

When $\dot{\delta} < \dot{\delta}_{\mathrm{cr}}$, we check the macroscopic response of the bar, i.e., the relation between $p(t)$ and $\delta(t)$.

Using equation (3.8), we can rewrite equation (3.9) as

$$\phi\left(\frac{L}{\gamma_T}\left(\dot{\delta} - \frac{\dot{p}}{\mu}\right)\right) - \gamma_T(1+a)p + \mu\gamma_T a\delta + \hat{\sigma}_0\gamma_T = 0, \tag{3.14}$$

where $\hat{\sigma}_0 = \sigma_0 - \rho g L$, and

$$\dot{p}(0) = \mu\left(\dot{\delta} - \frac{\gamma_T}{L}\dot{s}(0)\right). \tag{3.15}$$

Therefore,

- If $\dot{\delta} < (\gamma_T/L)\dot{s}(0)$, then $\dot{p}(0) < 0$, and the load will drop due to the nucleation of the new phase.
- If $(\gamma_T/L)\dot{s}(0) < \dot{\delta} < \dot{\delta}_{\mathrm{cr}}$, then $\dot{p}(0) > 0$, and the force at $x = L$ will increase due to the nucleation of the new phase.

With

$$p_r(t) = p(t) - \left(\phi\left(\frac{L\dot{\delta}}{\gamma_T}\right) + \mu\gamma_T a\delta + \sigma_0\gamma_T\right)\Big/(\gamma_T(1+a)), \tag{3.16}$$

equation (3.14) can be written as

$$\phi\left(\frac{L}{\gamma_T}\left(\dot{\delta}\frac{1+2a}{1+a} - \frac{\dot{p}_r}{\mu}\right)\right) - \phi\left(\frac{L}{\gamma_T}\dot{\delta}\right) = \gamma_T(1+a)p_r. \tag{3.17}$$

We can show that equation (3.17) has a stable equilibrium point,

$$p_r^{\mathrm{eq}} = \left(\phi\left(\frac{L}{\gamma_T}\frac{\dot{\delta}}{1+a}\right) - \phi\left(\frac{L}{\gamma_T}\dot{\delta}\right)\right)\Big/(\gamma_T(1+a)). \tag{3.18}$$

Thus, for large t,

$$p(t) \to \frac{\phi\left(\frac{L}{\gamma_T}\frac{\dot{\delta}}{1+a}\right)}{\gamma_T(1+a)} + \frac{\mu a\delta}{1+a} + \frac{\hat{\sigma}_0}{1+a}. \tag{3.19}$$

For an unloading process we obtain similar results, and omit the analysis. As $\phi(x)$ is a monotonically increasing function of x, from (3.19), we can see that the larger the loading rate, the larger the size of hysteresis loop which equals

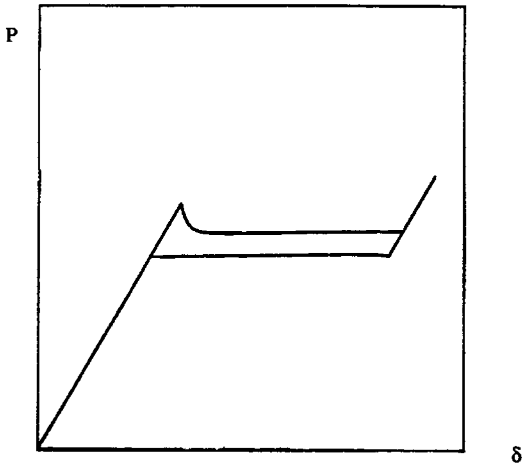


Fig. 2. A typical macroscopic response of the bar in an isothermal process.

the difference between the load during the forward transformation and the load during the reverse transformation. If we take the kinetic relation as linear, such as $\phi(\dot{s}) = \omega\dot{s}$, then we see that the size of the hysteresis loop will decrease as the mobility $(1/\omega)$ of the phase boundary increases.

Heretofore, we have assumed that the kinetic function $\phi(\dot{s})$ is continuous. For a kinetic function discontinuous at $\dot{s} = 0$, but continuous and monotonic elsewhere, we can obtain similar results.

A typical $p - \delta$ curve predicted by this model is given in Figure 2. It should be noted that the load drop due to the nucleation of the new phase depends on the critical stress, loading rate, and the mobility of the phase boundary.

3.2. FORCE-CONTROLLED TEST

The analysis here is similar to that in Section 3.1, except that $p(t)$ is known instead of $\delta(t)$. The elastic loading part is exactly the same as before; once a new phase initiates at $x = 0$, equation (3.8) holds, but the equation obtained from the kinetic relation is quite different now. For *constant loading rate*, it is

$$\phi(\dot{s}) + a\frac{\mu\gamma_T^2}{L}s = \gamma_T p(t) - \gamma_T\hat{\sigma}_0 \tag{3.20}$$

with $s(0) = 0$, or alternatively,

$$\phi'(\dot{s})\ddot{s} = \gamma_T\left(\dot{p} - a\frac{\mu\gamma_T}{L}\dot{s}\right). \tag{3.21}$$

Therefore,

1. If $\dot{p} < a(\mu\gamma_T/L)\dot{s}(0)$, then $\dot{s}(t) < \dot{s}(0)$, and the axial stress at the phase boundary drops. The phase boundary propagation speed will approach a constant,

$$\dot{s} \to \frac{L}{\mu\gamma_T}\frac{\dot{p}}{a}. \tag{3.22}$$

In other words, if we have a long enough specimen, then the eventual transformation rate will be in equilibrium with the loading rate.

2. If $\dot{p} > a(\mu\gamma_T/L)\dot{s}(0)$, then $\dot{s}(t) > \dot{s}(0)$, and the axial stress at the phase boundary is greater than the critical stress. Due to the continuity of the stress in the bar, the axial stress in front of the phase boundary is larger than the critical stress. Thus rather than the evolution of a single phase boundary according to the kinetic relation, we have either a continuous nucleation of new phase or nucleation of new phase at multiple sites. Hence the critical loading rate is

$$\dot{p}_{\text{cr}} = a\frac{\mu\gamma_T}{L}\phi^{-1}(\gamma_T(\sigma_{\text{cr}} - \sigma_0)). \tag{3.23}$$

3.3. REMARKS

The foregoing results illustrate that, the evolution of the phase transformation at one location in a quasistatically loaded bar can happen only in a limited, and practically very small loading rate range. When the loading rate is larger than the critical loading rate, the single phase boundary assumption is not valid.

For the loading rate smaller than the critical loading rate, we make the following observations:

- Generally there is a load drop in the $p - \delta$ curve. However, the load rise is generally an indication of nucleation of the second phase at multiple sites. This conclusion is consistent with the experimental results (Grujicic et al., 1985).
- Though the propagation speed of the single phase boundary varies with time even when the loading rate is constant, it approaches a steady value very fast (see Equation (3.11)). So except at the time of initial nucleation of new phases, one can assume that the phase boundary propagation speed is nearly constant This has been assumed by Grujicic et al. (1985), Leo et al. (1993), and Shaw and Kyriakides (1994).
- The phase boundary propagation speed equals approximately $((1 + a)\gamma_T)^{-1}$ times the grip loading rate. For the NiTi specimens used by Leo et al. (1993) and Shaw and Kyriakides (1994), the single phase boundary propagation speed is predicted to be about an order of magnitude higher than the grip loading rate; this was observed by Shaw and Kyriakides (1994).
- If the body force is neglected, i.e., if we take $a \to 0$, for a displacement controlled experiment, we still have a finite magnitude of the critical loading rate, but for the force controlled experiment, the critical loading rate goes to

zero. So in the absence of body forces, even with the assumption that there exists a favorable nucleation site, the force controlled experiment on phase transitions can not be treated as quasi-static.

When the loading rate is larger than the critical loading rate, in displacement controlled or force controlled experiments, the phase transformation process should be treated as dynamic rather than quasi-static, even though the loading rate might be small in the usual sense. Thus, the comprehensive experimental results obtained by Shaw and Kyriakides (1994) and especially the multiple site nucleation shown in their $x - t$ plots, can be explained. We are currently working on the modeling of hysteresis in martensitic transformation by using a dynamical model.

We note that this model can not predict, in an isothermal process, the serrations commonly observed in the load-deformation curve. If we abandon the assumption that the kinetic function must be a monotonically increasing function of the propagation speed of the phase boundary, that is, if we consider an unstable kinetic function, then serrations can be accounted for by the model in an isothermal process (Rosakis and Knowles, 1996). However, it is more likely that serrations are either due to the thermal softening of the material caused by the latent heat generated at a phase boundary, or due to the nucleation at multiple sites in the specimen, or possibly due to the inertia effect in the phase transitions.

4. A Process with Heat Conduction

4.1. A SPECIAL CASE

The latent heat given off at the phase boundary (Grujicic et al., 1985) will serve as a source of heat and make the temperature in the bar nonuniform. In order to obtain an analytical solution, we assume that the coefficient of thermal expansion, α, is zero, and the bar is insulated from its surroundings. The latter assumption is reasonable for experiments conducted in air. Thus from equations (2.4), (2.2), (2.13) and (2.18), when $x \neq s(t)$,

$$\theta_t = \nu\theta_{xx}, \tag{4.1}$$

where $\nu = k/\rho c$ is the thermal diffusivity.

When $x = s(t)$, equations (2.7), (2.8), (2.2), (2.13), and (2.18) yield

$$[q] = [k\theta_x] = -\dot{s}(\gamma_T(p + \rho g(L - s)) + \rho\lambda_T). \tag{4.2}$$

So there is a moving heat source at $x = s(t)$.

The initial condition is

$$\theta(x, 0) = \theta_0, \tag{4.3}$$

and the boundary conditions are

$$\theta_x(0, t) = \theta_x(L, t) = 0. \tag{4.4}$$

We can rewrite the governing equations as

$$\theta_t = \nu\theta_{xx} + \zeta(x - s(t))\dot{s}(\gamma_T(p + \rho g(L - s)) + \rho\lambda_T)/(\rho c), \tag{4.5}$$

where ζ is the Dirac δ-function.

The phase boundary position $s(t)$ is determined by kinetic relation (2.12), i.e.,

$$\dot{s}(t) = V(f, \theta(s(t), t)), \tag{4.6}$$

where

$$f = \gamma_T \left(p(t) + \rho g(L - s(t)) - \rho\lambda_T\gamma_T \frac{\theta(s(t), t) - \theta_T}{\theta_T} \right). \tag{4.7}$$

We can solve equation (4.5) formally for θ and substitute the result into the kinetic relation (4.6). The formal solution of (4.5) is

$$\theta(x, t) = \theta_0 + \sum_{n=0}^{\infty} c_n(t) \cos\frac{n\pi x}{L}, \tag{4.8}$$

where, for $n \neq 0, c_n(t)$ is given by

$$\begin{aligned}
\rho c c_n(t) \;=\; & \frac{2}{n\pi} r(t) \sin\frac{n\pi s(t)}{L} - \frac{2\gamma_T(\mu\gamma_T + \rho g L)}{(n\pi)^2} \left(\cos\frac{n\pi s(t)}{L} - \mathrm{e}^{-\nu t(n\pi/L)^2} \right) \\
& - \frac{2\mu\gamma_T\dot{\delta}}{n\pi} \int_0^t \sin\frac{n\pi s(t)}{L}\, \mathrm{e}^{-\nu(t-\tau)(n\pi/L)^2}\, \mathrm{d}\tau \\
& - 2\nu\frac{n\pi}{L} \int_0^t \sin\frac{n\pi s(\tau)}{L}\, \mathrm{e}^{-\nu(t-\tau)(n\pi/L)^2}\, \mathrm{d}\tau \\
& + \frac{2\nu\gamma_T(\mu\gamma_T + \rho g L)}{L^2} \int_0^t \cos\frac{n\pi s(\tau)}{L}\, \mathrm{e}^{-\nu(t-\tau)(n\pi/L)^2}\, \mathrm{d}\tau;
\end{aligned} \tag{4.9}$$

and for $n = 0$, we have

$$\rho c c_0(t) = \frac{2}{L} s(t) r(t) - \frac{2}{L} \int_0^t \mu\gamma_T\dot{\delta} s(\tau)\, \mathrm{d}\tau + \frac{\gamma_T(\mu\gamma_T + \rho g L)}{L^2} s^2(t), \tag{4.10}$$

and $r(t) = p(t) + \rho g(L - s(t))$.

Substitution from (4.8)–(4.10) into (4.7) results in

$$\dot{s}(t) = G(s(t), \delta(t)), \tag{4.11}$$

which is a highly nonlinear equation for $s(t)$. By solving this equation, we can find $s(t)$, and $\theta(x, t)$, the macroscopic response of the bar, i.e. the relation between $p(t)$ and $\delta(t)$. However, this equation can not be solved analytically.

4.2. CASE STUDY

We solve (4.11) approximately by the forward difference scheme,

$$s(t_{n+1}) = s(t_n) + \Delta t G(s(t_n), \delta(t_n)). \tag{4.12}$$

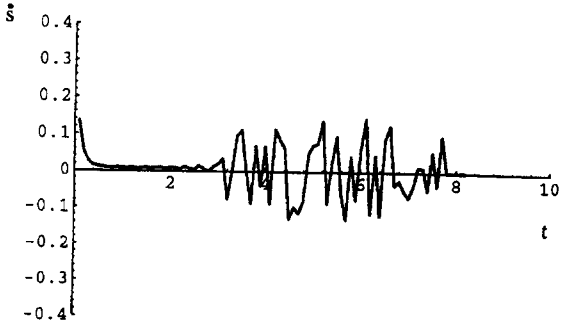
The parameters used in the calculations are of the right order of magnitude; it is hard to get a full set of parameters for a single material. We take $\mu = 10\,\text{GPa}, \rho = 10^3\,\text{kg/m}^3, \theta_T = 300°\text{K}, \theta_c = 400°\text{K}, \theta_0 = 325°\text{K}, \gamma_T = 1.25\%, M = 7.5 \times 10^{-5}, m = 10 \times 10^{-5}$, the thermal diffusivity $\nu = 10^{-4}\,\text{m}^2/\text{s}$, the thermal conductivity $k = 100\,\text{J/(ms°K)}$, the specific heat $c = 10^3\text{J/(kg°K)}$, and the length of the specimen $L = 1\,\text{cm}$.

The kinetic function used for calculations is $V(f, \theta) = f/\omega$ with $\omega = 10^6\,\text{Ns/m}^3$, and the loading rate $\dot{\delta}$ is taken to be 10^{-3}/s. The phase boundary propagation speed vs. time curve is given in Figure 3. Due to the latent heat given off at the phase boundary, it moves back and forth even though the bar is under monotonically increasing load; during the reverse phase transformation, the speed of the phase boundary decreases. The force-elongation curve is shown in Figure 4; we see the serrations in the $p - \delta$ curve due to the local heating. The temperature change at the center of the bar during the phase transition is given in Figure 5.

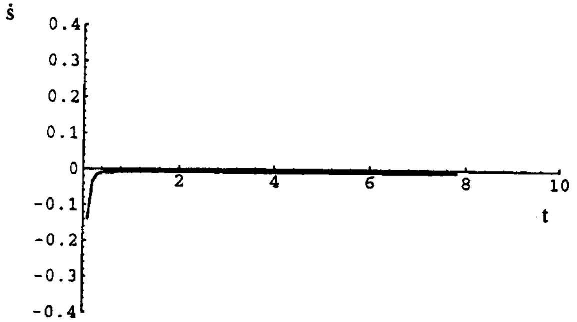
4.3. DISCUSSION

The analysis of the simplified thermomechanical process reveals some features of thermal effects on phase transitions. First, the latent heat given off at the phase boundary decreases its propagation speed. Secondly, when the loading rate is small enough, it can also induce reverse transformation even though the load is monotonically increasing. An analysis of the thermal effects on the phase transformation process in a more realistic setting was recently conducted by Kim and Abeyaratne (1995). However, no serrations in the load-displacement curve were observed by them. And thirdly, due to the elevation of the temperature near the phase boundary, load rise due to the nucleation of new phases is more likely than in an isothermal process.

From the present work and the experimental observations of Shaw and Kyriakides (1994), we conjecture that the thermal and interia effects play important roles in developing serrations in the load – deformation curve, and more generally in the solid-solid phase transitions.



a. The forward phase transformation



b. The reverse trsnsformation

Fig. 3. Variation with time of the phase boundary speed; (a) the forward phase transformation, (b) the reverse phase transformation.

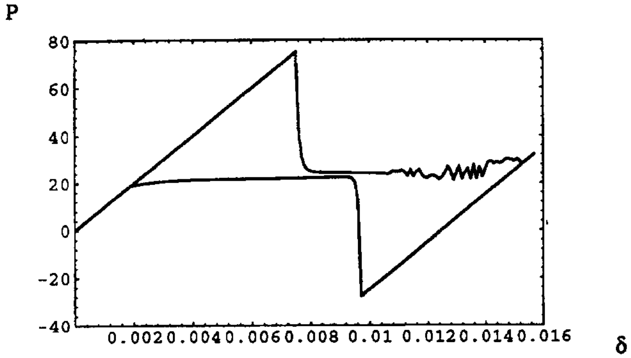
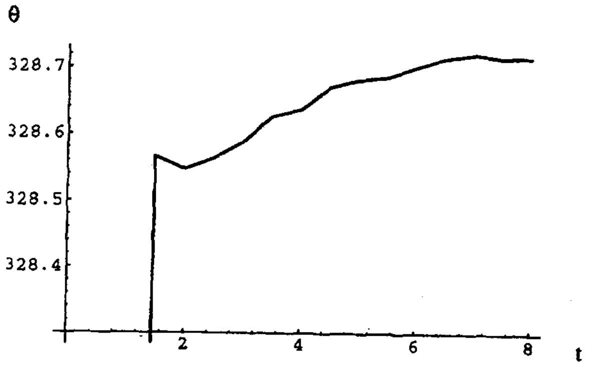
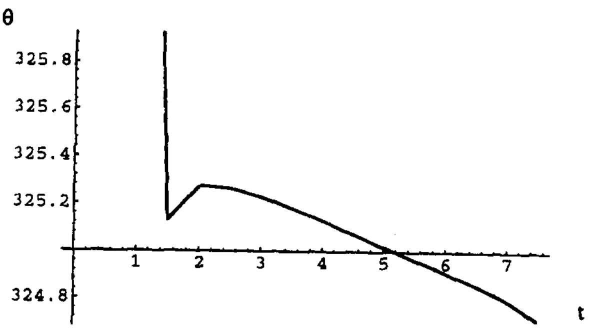


Fig. 4. The macroscopic response of the bar in a thermomechanical process.



a. The forward phase transformation



b. The reverse trsnsformation

Fig. 5. Temperature change at the center of the bar; (a) the forward phase transformation, (b) the reverse phase transformation.

Acknowledgement

This work was supported by the U.S. Army Research Office grant DAAH04-93-G-0214 to the University of Missouri-Rolla and a matching grant from the Missouri Research and Training Center. The Virginia Polytechnic Institute and State University acted as a subcontractor.

References

R. Abeyaratne and J.K. Knowles, On the dissipative response due to discontinuous strains in a bar of an unstable elastic material, *Int. J. Solids and Structures* **24** (1988) 1021–1044.

R. Abeyaratne and J.K. Knowles, On the driving traction acting on a surface of a discontinuity in a continuum, *J. Mechs. Physics Solids* **38** (1990) 345–360.

R. Abeyaratne and J.K. Knowles, A continuum model of a thermoelastic solid capable of undergoing phase transitions, *J. Mechs. Physics Solids* **41** (1993) 541–571.

R. Abeyaratne, S.-J. Kim and J.K. Knowles, A one-dimensional continuum model for shape memory alloys *Int. J. Solids Structures.* **31** (1994) 2229–2249.

Q. Jiang, On the modeling of thermoelastic phase transformations in solids, *J. Elasticity* **32** (1993) 61–91.

F. Falk, Model free energy, mechanics and thermodynamics of shape memory alloys, *Acta Metallurgica* **28** (1980) 1773–1783.

M. Grujicic, G.B. Olson and W.S. Owen, Mobility of the $\beta_1 - \gamma_1'$ martensitic interface in Cu-Al-Ni: Part I. Experimental measurements, *Metallurgical Transactions* **16A** (1985) 1723–1734.

S.-J. Kim and R. Abeyaratne, On the effect of the heat generated during a stress-induced thermoelastic phase transformation, *Continuum Mechanics and Thermodynamics* **8** (1995) 311–332.

P.H. Leo, T.W. Shield and O.P. Bruno, Transient heat transfer effects on the pseudoelastic behavior of shape memory wires, *Acta Metallurgica Mater.* **41** (1993) 2477–2485.

I. Müller and H. Xu, On the pseudo-elastic hysteresis, *Acta Metallurgica Mater.* **39** (1991) 263–271.

P. Rosakis and J.K. Knowles, On unstable kinetics (1996) (in preparation).

J.A. Shaw and S. Kyriakides, On the thermomechanical behavior of NiTi. EMRL Report No. 94/12, Department of Aerospace Engineering and Engineering Mechanics, The University of Texas at Austin, (1994).