CONTINUUM MODELING OF MATERIALS THAT CAN UNDERGO MARTENSITIC PHASE TRANSFORMATIONS

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ABSTRACT

A continuum model for materials that can undergo martensitic phase transformations is developed and applied to the study of several problems that involve such transformations. One of the several advantages of using this continuum model is that the corresponding boundary value problem is in a form that permits direct linearization, while retaining finite shape deformations for the martensite phases. The continuum model is used to study several problems dealing with which variant of martensite is preferred during the application of a loading. Among these problems is the case of a uniaxial tensile traction applied to a two-phase cylindrical body, and the case of a hydrostatic pressure applied to a two-phase body that has a finite shape deformation with an infinitesimal dilatation. The results that are obtained correspond with those that have been observed from experiments and with those that might be expected from physical considerations. The next problem that is considered involves the temperature at the interface and quasi-static motions of a two-phase thermoelastic bar. The bar is subject to different temperatures at each boundary and to a mechanical end-loading. The last problem that is considered involves the longitudinal free vibrations of a fixed-free, two-phase bar. The main focus in this problem is the damping behavior of the two-phase bar that is due to the motions of the interface during the free vibrations. A finite-difference numerical routine is used to approximate the displacement solutions for this problem. The damping of the bar is studied as the material coefficients are varied, and the values of the material coefficients that produce the maximum damping are investigated.

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CHAPTER 1

INTRODUCTION

In this thesis, a continuum model for materials that can undergo martensitic phase transformations is developed and applied to the study of several problems that involve such transformations. In comparison to some of the other continuum models, the continuum model that is developed here provides a more accurate representation of certain aspects of martensitic phase transformations and simplifies the construction of the constitutive equations and the forms of the boundary value problems that are considered. Several of the problems that this continuum model is applied to deal with the issue of which phase or which variant of martensite is preferred during the growth process when a boundary traction is applied. Among these problems are the case of a uniaxial tensile traction applied to a cylindrical body, and the case of a hydrostatic pressure applied to a material that has a finite shape deformation with an infinitesimal dilatation. The next problem that is considered involves a finite, twophase, thermoelastic bar. The bar is subject to different temperatures at each boundary and to a mechanical end-loading. The temperature at the interface is calculated, and the motion of the interface is determined during a quasi-static process. The last problem that is considered involves the longitudinal free vibrations of a fixed-free, two-phase bar. The main focus of this study is the damping behavior of the twophase bar that is due to the motion of the interface during the free vibrations. A finite-difference numerical routine is used to obtain the vibration solutions for this problem.

1.1 Allotropy

Materials that can exist in more than one type of crystal structure are said to exhibit *allotropy* if the transformation from one crystal structure to another is reversible, and *polymorphism* if this transformation is not reversible. Each of the different crystal structures of an allotropic (or polymorphic) material is considered to represent a different phase of the material. The particular crystal structure(s) that a given allotropic material will exist in depends, in part, on the relative values of the Gibbs free energies of the different phases of the material. The quantities that the Gibbs free energy of a phase depends on are determined by the type of constitutive behavior the phase exhibits. However, for most types of constitutive behavior, the Gibbs free energy of a phase can usually be considered to depend, at least in some way, on the temperature and the deformation of the phase. The phase that is preferred is the phase with the lowest Gibbs free energy, although there are other considerations for this issue, which will be discussed at later points in this thesis.

1.2 Martensitic Phase Transformations

The term *martensitic phase transformation* was originally given to the diffusion-less phase transformation that occurs when the high-temperature austenite phase of a steel is quenched, and the term *martensite* was originally given to the phase that is created from this solid-solid phase transformation.² The term martensitic phase transformation has since been given to almost all solid-solid phase transformations that proceed by a diffusionless cooperative movement of atoms at the phase boundary, involve a change in crystal structure, have a distinct orientation relation between the

¹ Here, the term reversible means that if, e.g., crystal structure A can be transformed into crystal structure B, then crystal structure B can be transformed into crystal structure A, and not that the transformation is necessarily conservative with respect to energy dissipation.

² These terms are in honor of the metallurgist A. Martens, who studied these phase transformations in the late nineteenth century.

crystal lattice of the parent phase and the crystal lattice of the product phase, and have a shape deformation associated with the product phase [13, 17].³ Similarly, the phase created by a transformation considered to be martensitic is sometimes referred to as the martensite phase of the given material. In this thesis, when a martensitic phase transformation between a high-temperature phase and a low-temperature phase is being considered, the high-temperature phase will be referred to as the *austenite phase* or the *parent phase*, and the low-temperature phase will be referred to as the *martensite phase* or the *product phase*, regardless of which phase is being created by the martensitic phase transformation. Additionally, the martensitic phase transformation that creates the austenite phase may sometimes be referred to as the *austenite phase transformation*, and the martensitic phase transformation that creates the martensite phase may sometimes be referred to as the *martensite phase transformation*.

1.2.1 The Transformation Temperatures

As indicated earlier, one of the quantities that determines what phase or phases the material exists in is the temperature of the material, since the Gibbs free energies of the different phases of the material depend on this quantity. In the absence of any external mechanical loading, the temperature at which the martensite phase transformation first occurs as the temperature is lowered is called the *martensitic start temperature* (M_s) , and the temperature at which the austenite phase transformation first occurs as the temperature is raised is called the *austenite start temperature* (A_s) . These temperatures are material-dependent. At the temperature M_s , the Gibbs free energy of the unstressed austenite phase, and at the temperature A_s , the Gibbs free energy of the unstressed austenite phase, and at the temperature A_s , the Gibbs free energy of the unstressed

³ There are other properties of martensitic phase transformations; however, these are the primary defining ones.

austenite phase is less than the Gibbs free energy of the unstressed martensite phase. The temperature at which the Gibbs free energies of the unstressed martensite phase and the unstressed austenite phase are equal will be denoted by T_0 . For most materials, the temperatures M_s , A_s , and T_0 do not coincide, and for most of these materials, $M_s < T_0 < A_s$. For these latter materials, because $M_s < T_0$, it is said that supercooling is necessary to induce the martensite phase transformation, and because $A_s > T_0$, it is said that superheating is necessary to induce the austenite phase transformation. The difference in Gibbs free energies of the martensite and austenite phases is considered by materials scientists to represent a "driving force" for the phase transformation. Thus, e.g., $M_s \neq T_0$ is equivalent to a positive driving force being necessary for the martensite phase transformation to take place.

The temperature at which a martensitic phase transformation first occurs can be affected by the application of a boundary traction.⁴ Whether the transformation temperatures are lowered or are raised by the boundary traction depends on the particular type of material considered and the type of boundary traction involved. In this thesis, when the martensite is produced at a constant temperature by applying a boundary traction, the martensite is considered to be *stress-induced*, and when the martensite is produced at a constant boundary traction (which may be zero) by lowering the temperature, the martensite is considered to be *thermally-induced*.

1.2.2 The Shape Deformation and Growth of the Martensite

Once nucleation takes place and a phase boundary emerges, growth of the martensite phase proceeds by the phase boundary passing over particles of austenite and transforming them into particles of martensite, or vice-versa if the austenite phase

⁴ This, of course, includes a boundary traction that is produced by applying a boundary displacement or some other type of mechanical boundary condition.

transformation is taking place. As this occurs, a cooperative movement of atoms takes place at the phase boundary which, in effect, "deforms" the crystal structure of the austenite phase into the crystal structure of the martensite phase. Partly as a consequence of this, the martensite phase has a macroscopic deformation relative to the undeformed austenite phase. This deformation is, in general, a *finite* deformation. No long-range diffusion of atoms takes place at the phase boundary, and the phase transformation takes place only at the phase boundary. Additionally, there is usually a discontinuity of strain and continuity of displacements at the phase boundary.

The total deformation corresponding to the martensite phase consists mostly of the deformation that occurs solely from the mechanisms of the martensitic phase transformation that occur at the phase boundary. This portion of the total deformation corresponds to an unstressed state of the martensite and will henceforth be referred to as the shape deformation of the martensite.⁵ Additionally, the strain corresponding to the shape deformation will sometimes be referred to as the transformation strain. The shape deformation is in general a finite deformation, and consists primarily of the deformation that would be necessary to deform the austenite crystal lattice into the martensite crystal lattice, and for some materials the deformation that is necessary to maintain continuity of displacements at the phase boundary. The remaining portion of the total deformation corresponding to the martensite is due to the surrounding matrix material constraining the formation of the shape deformation and/or by any applied boundary tractions. These deformations are usually infinitesimal deformations, even though they may be greater than the yield strain of the martensite, and in this thesis they will be considered to be superimposed upon the finite shape deformation. If the martensite is stressed, it is due solely to these superimposed deformations.

⁵ Because the shape deformation corresponds to an unstressed state of the martensite, it can be considered to represent the undeformed martensite.

The speed of the phase boundary, and hence the rate of the martensitic phase transformation, varies considerably with the type of material, although it can be affected, but to a much lesser degree, by an applied boundary traction. The speed is proportional to the amount of deformation that it would take to deform the austenite lattice into the martensite lattice, which is proportional to the shape deformation of the martensite. For materials with large shape deformations, the speed of the phase boundary can approach the speed of sound within the material, and for materials with smaller shape deformations, the speed of the phase boundary may be less than a millimeter per second. Additionally, growth of the martensite at a temperature less than the temperature M_s will proceed only partially and then stop. The transformation will not continue until the temperature is lowered further or a boundary traction is applied. Also, during the growth process, phase boundaries cannot, in general, cross grain boundaries. Therefore, one crystal of austenite will transform into one or more crystals of martensite.

1.2.3 The Morphologies and Other Properties of Martensite

The particular type of morphology that the martensite exists in depends on many factors. Some of these factors are the type of material, whether the martensite forms at or near a free surface or within the material, and how the martensite is formed (e.g., by quenching or stressing). Of all these factors, the type of material is the most dominant.

Many martensites have a shape deformation that appears to have the *macroscopic* form of an invariant plane strain,⁶ which in most cases is very close to a simple shear. When these martensites form at or near a free surface, there is negligible deformation superimposed upon their shape deformations. Consequently, these martensites are

⁶ See Section 2.7 for the mathematical definition of this type of deformation.

approximately unstressed. However, when such martensites form in the interior of a material, away from a free surface, their macroscopic shape deformations sometimes do have a slight superimposed, inhomogeneous deformation, which is primarily due to the constraint against the formation of their shape deformations imposed by the surrounding matrix material. These superimposed deformations occur mostly near the boundaries of the martensites and tend to alter their overall macroscopic shape from that of an invariant plane strain. Additionally, most of the martensites that have shape deformations with the macroscopic form of an invariant plane strain are internally twinned, internally slipped, or have some other structure on the "microscopic" level that tends to minimize the total energy of the martensite and helps preserve the continuity of displacements at the phase boundary.

There are materials, including some steels and other iron alloys, that have martensite phases with shape deformations that are always highly deformed. Many of these martensites have lens-like or nearly elliptical, overall macroscopic shapes and have shape deformations that are among the largest of all the known martensites. The deformations superimposed on the shape deformations of these martensites usually go beyond the elastic limit of the martensite and/or the surrounding austenite material, especially near the phase boundaries, and as a result, many dislocations appear at or near the phase boundaries in these materials.

Most materials that can undergo martensitic phase transformations have several variants of their martensite phase(s). These variants all have the same type of crystal lattice, but differ from each other in some other way. For example, they may be formed from the austenite lattice in a slightly different way, and as a result they may each have a different orientation with respect to the austenite lattice or their plane of slip may be different, if they have an internally slipped morphology. Several of these

variants may coexist in a material. When this is the case, the variants are sometimes twin-related. In fact, when the "microscopic" structure of the martensites that have a "homogeneous" invariant plane strain macroscopic shape deformation is an internally twinned structure, the structure is usually comprised of different twin-related variants of the same martensite.

The morphologies that have been briefly described above are only some of the different types of morphologies that have been observed in nature. Additionally, these morphologies may be induced thermally or by the application of a boundary traction. However, if they are induced by an applied boundary traction, the shape deformation of the martensite may be further deformed by the boundary traction, or the boundary traction may cause a particular morphology or variant of martensite to be preferred during the growth process.

1.2.4 Shape Memory Alloys

Some materials that can undergo martensitic phase transformations also exhibit a phenomenon known as the shape memory effect [14]. This phenomenon has the effect that if a material in its austenite phase is quenched to its martensite phase and then deformed, when it is heated to its austenite phase, it will return to the shape that it originally had in its austenite phase. Most of the materials that exhibit this phenomenon have relatively small shape deformations associated with their martensite phases. Also, the steels that martensitic phase transformations were first studied in are not shape memory materials. The interest in martensitic phase transformations in these materials stems from the fact that their martensite phase is a much harder material than the phase obtained by slowly cooling the austenite and allowing a diffusion-type phase transformation to occur.

1.3 The Continuum Model Developed in this Thesis and Some of the Other Continuum Models

One of the goals in this thesis is to develop a continuum model that provides an accurate representation of the change in crystal structure that takes place during a martensitic phase transformation and treats the shape deformation of the martensite as a finite deformation. Additionally, it is desired that this continuum model provide a feasible method of construction for the constitutive equations and a direct and relatively simple formulation of the boundary value problems that are considered.

The symmetry of a material's crystal lattice is reflected in the *material symmetry* group of the material. When a material is modeled as a continuum, the material's symmetry group restricts the functional form of the material's constitutive equations. Thus, when a particle of material in its austenite phase is transformed to its martensite phase, the material symmetry group of that particle of material should change accordingly, and this should be reflected in the constitutive equations of that particle of material both before and after the transformation. This change in material symmetry group should not only represent the change in the type of crystal lattice; it should also represent the orientation relation between the crystal lattices of the austenite and the martensite.

There are several other continuum models for materials that can undergo martensitic phase transformations. One of these continuum models assumes a "globally" elastic material with a single elastic potential that has relative minima at the deformation corresponding to the undeformed parent phase and the shape deformations associated with the different variants of martensite.⁷ This continuum model, however, does not provide the correct material symmetry groups for the martensite phases when

⁷ Technically speaking, this elastic potential may not be truly global; i.e., it may not be defined for *all* deformations. However, it is defined for a range of deformations that includes *all* of the deformations that correspond to *all* of the phases of the material.

the material symmetry group of the single "global" elastic potential is taken to be the crystallographic point group⁸ of the parent phase crystal.⁹ Therefore, as far as the constitutive equations are concerned, the change in crystal structure is not completely represented. Another difficulty of this continuum model is that a single "global" elastic potential with local minima corresponding to the different phases of the material has to be constructed. This may be relatively easy to do for a system with one or two components of strain to consider, as in the case of a one-dimensional bar with only one component of strain. However, this task would be very difficult for a general three-dimensional problem, where the elastic potential is a function of the six independent components of the right deformation tensor or the Lagrangian strain tensor.

Another continuum model for materials that can undergo martensitic phase transformations assumes that each phase has its own linear constitutive equations and treats the transformation strain of each martensite as an infinitesimal strain [5]. The fact that the transformation strain in this continuum model is treated as an infinitesimal strain and not as a finite strain has a very significant effect on the entire formulation and analysis of the problem. It should also significantly affect the solutions of most of these problems. There are also some who have used continuum models where each phase has its own elastic potential, and the shape deformation of each martensite is treated as a finite deformation (see [6])¹⁰. However, in [6] and in the references

⁸ Roughly speaking, the crystallographic point group of a crystal consists of the set of all *rotations* that rotate the crystal into a position that coincides with the crystal's position before it was rotated. For example, the crystallographic point group of a crystal with cubic symmetry consists of the twenty four rotations that map a cube into itself (see [15]).

⁹ This can be readily seen by considering the crystallographic point group of the parent phase with respect to the reference configuration coinciding with the shape deformation of one of the martensite phases. This is discussed further in Section 2.5, where the change of reference configuration formula for a material symmetry group is presented.

¹⁰ In [6], there is also a list of references (p.99) that use a single elastic potential, and a list of references that use a different elastic potential for each phase.

listed in [6] that also use a different elastic potential for each phase and treat the shape deformations of the martensites as finite deformations, specific equations representing the elastic potentials of the martensites, where the shape deformations are treated as finite deformations, are not constructed, and the manner in which the material symmetry groups for the martensites must be specified, so that they are correct, is not discussed.

The continuum model that is developed in this thesis provides the correct material symmetry group for each phase of the material and treats the shape deformation of each martensite as a finite deformation. Additionally, "global" constitutive equations do not have to be constructed, although they can be accommodated if required, and a feasible method of construction for the constitutive equations is provided. In fact, constitutive equations are constructed for most of the problems considered in Chapters 3–5 of this thesis.

CHAPTER 2

THE CONTINUUM MODEL

In this chapter, a continuum model for materials that can undergo martensitic phase transformations is developed, and the corresponding field equations for a purely mechanical process are derived. The form of the corresponding boundary value problem is also considered.

2.1 The Eulerian Global Form of the Balance Laws

It is assumed that the process under consideration takes place at a constant, uniform temperature and with no heat conduction. Such a process is an isothermal and adiabatic process and is also known as a purely mechanical process. It is assumed that this process takes place in a time interval $\Gamma = [t_0, t_1]$. The body B that is considered is assumed to occupy a regular region R_t at time $t \in \Gamma$, and it is assumed that R_t is a subset of the three-dimensional Euclidean space E_3 . A point or the position vector of a point in R_t is denoted by \mathbf{y} . The traction on the surface with unit normal $\mathbf{n}(\mathbf{y},t)$ is denoted by $\mathbf{t}(\mathbf{y},\mathbf{n},t)$, the body force per unit volume by $\mathbf{b}(\mathbf{y},t)$, and the mass per unit volume by $\bar{\rho}(\mathbf{y},t)$. Also, the Eulerian form of the velocity of the particle of material at $\mathbf{y} \in R_t$ at time $t \in \Gamma$ is denoted by $\bar{\mathbf{v}}(\mathbf{y},t)$. The familiar Eulerian global form of the balance of mass, linear momentum, and angular momentum are

$$\frac{d}{dt} \int_{D_t} \bar{\rho} dV = 0, \qquad (2.1.1)$$

¹ In this thesis, math-italic quantities denote scalars and bold-faced quantities denote tensors, including vectors.

$$\int_{\partial D_t} \mathbf{t} dA + \int_{D_t} \mathbf{b} dV = \frac{d}{dt} \int_{D_t} \bar{\rho} \bar{\mathbf{v}} dV, \qquad (2.1.2)$$

$$\int_{\partial D_t} \mathbf{y} \times \mathbf{t} dA + \int_{D_t} \mathbf{y} \times \mathbf{b} dV = \frac{d}{dt} \int_{D_t} \mathbf{y} \times \bar{\rho} \mathbf{\bar{v}} dV, \tag{2.1.3}$$

respectively, $\forall D_t \subset R_t$ and $\forall t \in \Gamma$.² Equations (2.1.1), (2.1.2), and (2.1.3) can be used to derive the rate of work-energy equation given by

$$\int_{\partial D_t} \mathbf{t} \cdot \bar{\mathbf{v}} dA + \int_{D_t} \mathbf{b} \cdot \bar{\mathbf{v}} dV = \int_{D_t} \boldsymbol{\tau} \cdot \nabla_{\mathbf{y}} \bar{\mathbf{v}} dV + \frac{d}{dt} \int_{D_t} \frac{1}{2} \bar{\rho} \bar{\mathbf{v}} \cdot \bar{\mathbf{v}} dV, \tag{2.1.4}$$

 $\forall D_t \subset R_t$ and $\forall t \in \Gamma$, where $\tau(\mathbf{y},t)$ is the true (or Cauchy) stress tensor, and $\nabla_{\mathbf{y}}\bar{\mathbf{v}}$ denotes the gradient of $\bar{\mathbf{v}}(\mathbf{y},t)$ with respect to \mathbf{y} . The two terms on the left side of (2.1.4) represent the rate of work done on D_t by the traction acting on the boundary of D_t and the body forces acting on D_t , respectively. The first term on the right side of (2.1.4) is referred to as the stress power of D_t , and the second term on the right side of (2.1.4) represents the time rate of change of the kinetic energy of D_t .

2.2 Multiple Reference Configurations

Consider a region R in E_3 that the body B can occupy, in the sense that there exists a suitably smooth and invertible mapping that maps R into R_t . Note that R is not such that the body B has to occupy it at some time $t \in \Gamma$. Such a region R can be used as a reference configuration for the body B.

Most continuum models for materials that can undergo martensitic phase transformations use only one reference configuration, which is taken to be stationary,

In this thesis, unless otherwise stated, whenever a subset of a regular region is considered, it is assumed that the subset is a regular subregion. Similarly, all subregions of regular regions are assumed to be regular.

for the definition of the constitutive equations and for the derivation of the field equations for each phase of the material. This is the case, for example, with the continuum model that uses a single "global" elastic potential and with the continuum model where each phase has its own elastic potential and the shape deformation of each martensite is treated as a finite deformation, which were both described in Section 1.3. This is also the case with the continuum model where each phase has its own linear constitutive equations and the transformation strain of each martensite is treated as an infinitesimal strain, which was also described in Section 1.3. More specifically, in this continuum model, because the shape deformation of each martensite and the deformation of each phase are treated as infinitesimal deformations, there is no distinction between the reference configurations coinciding with the undeformed austenite, the shape deformation of the martensite, and the deformed body, in the sense that the forms of the fields equations with respect to each of these reference configurations are the same.

In the continuum model that is developed in this thesis, each phase has its own constitutive relation. However, these constitutive relations are not all defined with respect to the same fixed reference configuration. Instead, each phase has its own reference configuration for the definition of its constitutive equations. These reference configurations may be independent of time, or they may be special functions of time. Furthermore, the field equations for each phase can be expressed with respect to these reference configurations in a nominal-type form. This can be a very useful and powerful way of setting up the field equations, especially if there exists a configuration for each phase such that the deformations of that phase from this configuration are infinitesimal for all $t \in \Gamma$. In this case, *linear* constitutive equations can be used

if these configurations are used as the reference configurations for the phases of the material.

Using multiple reference configurations for the "nominal" field equations of the different phases of a given material involves only kinematics. However, defining the constitutive equations of the different phases of a material with respect to different reference configurations involves more than just kinematics: It also involves an assumption of the constitutive behavior of the given material. Whether such an assumption is reasonable for a given material depends on the chosen reference configurations for the phases of the material and on the types of constitutive behavior the phases are assumed to exhibit.

It is well known that the solid phases of a metal behave elastically for at least small deformations about a configuration corresponding to an unstressed state. It will be shown later in this chapter that for these types of materials it is reasonable to use multiple reference configurations in the manner described above and that a consistent continuum model can be developed, provided these reference configurations are chosen properly. Whether such a continuum model can be developed for materials with constitutive behavior that is not elastic is an issue that is not considered in this thesis.

2.3 The Kinematics Using Multiple Reference Configurations

For simplicity, a two-phase material will be considered in the following. The corresponding results for a material that consists of more than two phases can be obtained in a similar manner.

As in Section 2.1, consider a body B that occupies a regular region R_t at time $t \in \Gamma$. Additionally, assume that this body consists of two phases, which will

henceforth be referred to as phase 1 and phase 2. Assume that at each $t \in \Gamma$ phase 1 occupies a subregion R_t^- of R_t , and phase 2 occupies a subregion R_t^+ of R_t , where $R_t^- \cup R_t^+ = R_t$ and $R_t^- \cap R_t^+ = \emptyset$ (Figure 2.1). These two subregions of R_t are separated by an interface S_t which can pass over particles of material in R_t . If this occurs, R_t^- will increase in size while R_t^+ decreases in size, or vice-versa, depending on the direction of motion of S_t .

Consider a stationary reference configuration R for R_t (Figure 2.1). Let x denote a point or the position vector of a point in R. Let $\hat{\mathbf{y}}(\mathbf{x},t)$ be the suitably smooth and invertible mapping that maps R into R_t at each $t \in \Gamma$, with $\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x},t) = \mathbf{x} + \hat{\mathbf{u}}(\mathbf{x},t) \ \forall (\mathbf{x},t) \in R \times \Gamma$, where $\mathbf{u} = \hat{\mathbf{u}}(\mathbf{x},t)$ is the displacement of the point $\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x},t)$ from the point \mathbf{x} at time $t \in \Gamma$. The deformation gradient of $\hat{\mathbf{y}}$ is defined as $\mathbf{F}(\mathbf{x},t) = \nabla \hat{\mathbf{y}}(\mathbf{x},t)$, and the Jacobian of \mathbf{F} is defined as $J(\mathbf{x},t) = \det \mathbf{F}(\mathbf{x},t)$, where it is required that J > 0 to exclude reflections.³ The velocity of the particle of material at $\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x},t)$ is defined as $\mathbf{v}(\mathbf{x},t) = \frac{\partial}{\partial t} \hat{\mathbf{y}}(\mathbf{x},t)$, and the Eulerian form of the velocity used in Section 2.1 can be defined as $\bar{\mathbf{v}}(\mathbf{y},t) = \mathbf{v}(\hat{\mathbf{x}}(\mathbf{y},t),t)$, where $\hat{\mathbf{x}}(\cdot,t):R_t \mapsto R$ at each $t \in \Gamma$ is the inverse of $\hat{\mathbf{y}}$. Let $R^- = \hat{\mathbf{x}}(R_t^-,t)$, $R^+ = \hat{\mathbf{x}}(R_t^+,t)$, and $S = \hat{\mathbf{x}}(S_t,t)$. Note that $R^- \cup R^+ = R$, $R^- \cap R^+ = \emptyset$, S is the surface separating R^- from R^+ , and S moves within R as S_t moves within R_t .

Consider a second, not necessarily stationary, reference configuration R_1^+ for phase 2 (Figure 2.1). Let \mathbf{x}_1 denote a point or the position vector of a point in R_1^+ , and let $\tilde{\mathbf{x}}_1(\mathbf{x},t)$ be the suitably smooth and invertible mapping that maps R^+ into R_1^+ at each $t \in \Gamma$, with $\mathbf{x}_1 = \tilde{\mathbf{x}}_1(\mathbf{x},t) \ \forall \ \mathbf{x} \in R^+$ at each $t \in \Gamma$. Let $\tilde{\mathbf{F}}(\mathbf{x},t) = \nabla \tilde{\mathbf{x}}_1(\mathbf{x},t)$ and $\tilde{J}(\mathbf{x},t) = \det \tilde{\mathbf{F}}(\mathbf{x},t)$, with $\tilde{J} > 0$. Let $\hat{\mathbf{y}}_1(\mathbf{x}_1,t)$ be the suitably smooth and invertible mapping that maps R_1^+ into R_t^+ at each $t \in \Gamma$, with

 $^{^3}$ ∇ denotes the gradient operator with respect to $\mathbf{x} \in \mathbf{R}$.

 $\mathbf{y} = \hat{\mathbf{y}}_1(\mathbf{x}_1,t) = \mathbf{x}_1 + \hat{\mathbf{u}}_1(\mathbf{x}_1,t) \ \forall \ \mathbf{x}_1 \in \mathbf{R}_1^+ \ \text{at each} \ t \in \Gamma.$ Note also that $\mathbf{y} = \hat{\mathbf{y}}_1(\tilde{\mathbf{x}}_1(\mathbf{x},t),t) = \hat{\mathbf{y}}(\mathbf{x},t) \ \forall \ \mathbf{x} \in \mathbf{R}^+ \ \text{at each} \ t \in \Gamma.$ Let $\mathbf{F}_1(\mathbf{x}_1,t) = \nabla_1 \hat{\mathbf{y}}_1(\mathbf{x}_1,t)$ and $J_1(\mathbf{x}_1,t) = \det \mathbf{F}_1(\mathbf{x}_1,t)$, with $J_1 > 0$. The velocity field of the particles of material in phase 2 as a function of $\mathbf{x}_1 \in \mathbf{R}_1^+$ is given by $\bar{\mathbf{v}}_1(\mathbf{x}_1,t) = \bar{\mathbf{v}}(\hat{\mathbf{y}}_1(\mathbf{x}_1,t),t) \ \forall \ \mathbf{x}_1 \in \mathbf{R}_1^+$ at each $t \in \Gamma$, or equivalently as $\bar{\mathbf{v}}_1(\mathbf{x}_1,t) = \mathbf{v}(\tilde{\mathbf{x}}(\mathbf{x}_1,t),t) \ \forall \ \mathbf{x}_1 \in \mathbf{R}_1^+$ at each $t \in \Gamma$, where $\tilde{\mathbf{x}}(\cdot,t):\mathbf{R}_1^+ \mapsto \mathbf{R}_1^+$ at each $t \in \Gamma$ is the inverse of $\tilde{\mathbf{x}}_1$. Also, $\hat{\mathbf{x}}_1(\cdot,t):\mathbf{R}_t^+ \mapsto \mathbf{R}_1^+$ at each $t \in \Gamma$ represents the inverse of $\hat{\mathbf{y}}_1$.

As discussed in the Introduction, the displacements at the interface separating the austenite phase from a martensite phase are continuous while the strains at the interface may be discontinuous. We will therefore require that $\hat{\mathbf{y}}(\mathbf{x},t)$, and hence $\mathbf{u}(\mathbf{x},t)$, be continuous on $\mathbf{R}\times \mathbf{\Gamma}$, and allow the first and second derivatives of $\hat{\mathbf{y}}$ and \mathbf{u} to be piecewise continuous on $\mathbf{R}\times \mathbf{\Gamma}$, with discontinuities occurring only at points on S.

Let $N(\mathbf{x},t)$ represent a unit vector normal to S that points into R^+ , and let $L(\mathbf{x},t)$ represent a vector tangent to S, both at a point on S coinciding with the point $\mathbf{x} \in R$ at time $t \in \Gamma$. Also, let $V(\mathbf{x},t)$ represent the velocity of the point on S coinciding with the point $\mathbf{x} \in R$ at time $t \in \Gamma$. In the following, if $g(\mathbf{x},t)$ represents a generic field quantity that is discontinuous at S, then $g^-(\mathbf{x},t)$ and $g^+(\mathbf{x},t)$ denote the limiting values of g at $\mathbf{x} \in S$ as this point \mathbf{x} is approached from negative and positive sides of S, respectively, in directions parallel to $N(\mathbf{x},t)$.

⁴ ∇_1 denotes the gradient operator with respect to $\mathbf{x_1} \in \mathbf{R_1^+}$.

⁵ In the rest of this thesis, a point on the surface S that coincides with the point $x \in R$ at time $t \in \Gamma$ will simply be referred to as the point $x \in S$. Also, note that V represents a nominal-type velocity and not the velocity of a point on S_t .

⁶ If a piecewise continuous field quantity is discontinuous at S, it is sometimes said that the quantity jumps across S, and an equation relating g^- and g^+ is sometimes referred to as a jump condition.

Because the displacement is required to be continuous at each point on the phase boundary, we have

$$\hat{\mathbf{y}}_{1}^{+}(\tilde{\mathbf{x}}_{1}(\mathbf{x},t),t) = \hat{\mathbf{y}}^{-}(\mathbf{x},t), \tag{2.3.1}$$

 $\forall \mathbf{x} \in S$ at each $t \in \Gamma$. Taking the differential of both sides of (2.3.1) while keeping time fixed (and recalling the continuity conditions on $\hat{\mathbf{y}}$) yield

$$\left(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-}\right)\mathbf{L} = \mathbf{0},\tag{2.3.2}$$

 $\forall \mathbf{x} \in S$ at each $t \in \Gamma$, and for every vector **L** tangent to S at $\mathbf{x} \in S$, where $\mathbf{x}_1 = \tilde{\mathbf{x}}_1(\mathbf{x}, t)$ in \mathbf{F}_1^+ . Differentiating (2.3.1) with respect to time yields

$$\bar{\mathbf{v}}_{1}^{+} - \mathbf{v}^{-} + \left(\mathbf{F}_{1}^{+} \tilde{\mathbf{F}}^{+} - \mathbf{F}^{-} \right) \mathbf{V} = \mathbf{0},$$
 (2.3.3)

 $\forall \mathbf{x} \in S$ at each $t \in \Gamma$, where $\mathbf{x}_1 = \tilde{\mathbf{x}}_1(\mathbf{x}, t)$ in $\bar{\mathbf{v}}_1^+$ and $\mathbf{F}_1^{+,7}$

It can be shown that if given an $\mathbf{F}^-, \mathbf{F}_1^+$, and an $\tilde{\mathbf{F}}^+$ such that Equation (2.3.2) is satisfied at a point on some surface, there exist vectors $\hat{\mathbf{a}}$ and \mathbf{N} defined at that point such that

$$\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-} = \hat{\mathbf{a}} \otimes \mathbf{N}, \tag{2.3.4}$$

where N is normal to the surface at that point. Also, note that $\hat{a} \otimes N$ in this equation is a rank-one two-tensor.

⁷ The corresponding forms of Equations (2.3.2) and (2.3.3) involving only one reference configuration are well known and can be found, e.g., in [2].

⁸ The corresponding form of this equation with $\mathbf{F}_{1}^{+}\mathbf{\tilde{F}}^{+}$ replaced with \mathbf{F}^{+} , where $\mathbf{F}^{+}=\mathbf{F}_{1}^{+}\mathbf{\tilde{F}}^{+}$, is well known and can be found, e.g., in [16].

2.4 The Nominal Form of the Field Equations Using Multiple Reference Configurations

Consider the two-phase material described in Section 2.3. In addition to the continuity requirements on $\hat{\mathbf{y}}$ and \mathbf{u} discussed in that section, it is assumed that \mathbf{b} is continuous $\forall \mathbf{y} \in R_t$ and $\forall t \in \Gamma$, and that $\boldsymbol{\tau}$ and its gradient are piecewise continuous $\forall \mathbf{y} \in R_t$ and $\forall t \in \Gamma$, with discontinuities occurring only at points on S_t .

The global form of the balance of mass given by Equation (2.1.1) can be expressed with respect to R as

$$\frac{d}{dt} \int_{D} \rho dV = 0, \tag{2.4.1}$$

where $D = \hat{\mathbf{x}}(D_t, t)$, and $\rho = J\bar{\rho}$ represents the mass per unit volume of R. Note that since (2.1.1) is valid $\forall D_t \subset R_t$, (2.4.1) is valid $\forall D \subset R$. We require that ρ be continuous $\forall \mathbf{x} \in R$. Localizing Equation (2.4.1) yields the familiar result that ρ must be independent of time $\forall \mathbf{x} \in R$. Thus,

$$\rho(\mathbf{x}) = J(\mathbf{x}, t)\bar{\rho}(\hat{\mathbf{y}}(\mathbf{x}, t), t), \tag{2.4.2}$$

 $\forall (\mathbf{x},t) \in \mathbb{R} \times \Gamma$. Note that the global field equations given by (2.1.1)-(2.1.3) are still valid in the regions of space and time indicated there, for the case where ρ , τ , and \mathbf{b} have the continuity conditions specified in this section, and $\hat{\mathbf{y}}$ has the continuity conditions specified in the previous section. However, for these continuity conditions, the work-energy equation given by (2.1.4) is valid only for subregions of R_t not containing a portion of S_t , as will be discussed further in Section 2.9.

For subregions D_t^- of R_t^- , the global forms of the balance of linear and angular momentum for phase 1 given by (2.1.2) and (2.1.3), respectively, can be expressed with respect to R^- as

$$\int_{\partial D^{-}} \sigma \mathbf{n} dA + \int_{D^{-}} \mathbf{f} dV = \frac{d}{dt} \int_{D^{-}} \rho \mathbf{v} dV, \tag{2.4.3}$$

$$\int_{\partial D^{-}} \hat{\mathbf{y}} \times \boldsymbol{\sigma} \mathbf{n} dA + \int_{D^{-}} \hat{\mathbf{y}} \times \mathbf{f} dV = \frac{d}{dt} \int_{D^{-}} \hat{\mathbf{y}} \times \rho \mathbf{v} dV, \tag{2.4.4}$$

respectively, where $D^- = \hat{\mathbf{x}}(D_t^-, t)$, $\sigma(\mathbf{x}, t) = J(\mathbf{x}, t)\tau(\hat{\mathbf{y}}(\mathbf{x}, t), t)\mathbf{F}^{-T}(\mathbf{x}, t)$ is the nominal stress tensor with respect to R^- , $\mathbf{f}(\mathbf{x}, t) = J(\mathbf{x}, t)\mathbf{b}(\hat{\mathbf{y}}(\mathbf{x}, t), t)$ is the nominal body force per unit volume of R^- , and $\mathbf{n}(\mathbf{x})$ is the outward unit normal vector field on the boundary of D^- . These nominal field equations can be obtained in the usual way from Equations (2.1.2) and (2.1.3), respectively (see, e.g., [15]).

For subregions D_t^+ of R_t^+ , the global forms of the balance of linear and angular momentum for phase 2 given by (2.1.2) and (2.1.3), respectively, can be expressed with respect to R_1^+ as

$$\int_{\partial D_{1}^{+}} \sigma_{1} \mathbf{n}_{1} dA + \int_{D_{1}^{+}} \mathbf{f}_{1} dV = \frac{d}{dt} \int_{D_{1}^{+}} \bar{\rho}_{1} \bar{\mathbf{v}}_{1} dV, \qquad (2.4.5)$$

$$\int_{\partial D_1^+} \hat{\mathbf{y}}_1 \times \sigma_1 \mathbf{n}_1 dA + \int_{D_1^+} \hat{\mathbf{y}}_1 \times \mathbf{f}_1 dV = \frac{d}{dt} \int_{D_1^+} \hat{\mathbf{y}}_1 \times \bar{\rho}_1 \overline{\mathbf{v}}_1 dV, \tag{2.4.6}$$

respectively, where $D_1^+ = \hat{\mathbf{x}}_1(D_t^+,t)$, $\bar{\rho}_1(\mathbf{x}_1,t) = J_1(\mathbf{x}_1,t)\bar{\rho}(\hat{\mathbf{y}}_1(\mathbf{x}_1,t),t)$ is the mass per unit volume of R_1^+ , $\sigma_1(\mathbf{x}_1,t) = J_1(\mathbf{x}_1,t)\tau_1(\hat{\mathbf{y}}_1(\mathbf{x}_1,t),t)\mathbf{F}_1^{-T}(\mathbf{x}_1,t)$ represents the stress tensor with respect to R_1^+ , $\mathbf{f}_1(\mathbf{x}_1,t) = J_1(\mathbf{x}_1,t)\mathbf{b}(\hat{\mathbf{y}}_1(\mathbf{x}_1,t),t)$ represents the body force per unit volume of R_1^+ , and $\mathbf{n}_1(\mathbf{x}_1,t)$ is the outward unit normal vector field on the boundary of D_1^+ . Also, $\bar{\rho}_1$ is related to ρ by

$$\rho(\mathbf{x}) = \tilde{J}(\mathbf{x}, t)\bar{\rho}_1(\tilde{\mathbf{x}}_1(\mathbf{x}, t), t), \tag{2.4.7}$$

 $\forall \mathbf{x} \in \mathbb{R}^+$ at each $t \in \Gamma$. Note that σ_1 , $\mathbf{f_1}$, and $\bar{\rho}_1$ do not have a true nominal form since $\tilde{\mathbf{x}}_1$ is a function of time. In fact, because of this time dependence, these quantities are closer to having an Eulerian form. Note also that Equations (2.4.5) and (2.4.6) can be obtained from Equations (2.1.2) and (2.1.3) in a manner completely analogous to that used to obtain Equations (2.4.3) and (2.4.4), regardless of whether \mathbf{R}_1^+ is stationary or whether points in \mathbf{R}_1^+ are moving, which is the case if $\tilde{\mathbf{x}}_1$ is a function of time.

Localization of the global nominal balance laws given by (2.4.3) and (2.4.4) using (2.4.2) yields

$$div \boldsymbol{\sigma} + \mathbf{f} = \rho \mathbf{a},$$

$$\boldsymbol{\sigma} \mathbf{F}^{\mathrm{T}} = \mathbf{F} \boldsymbol{\sigma}^{\mathrm{T}},$$
 (2.4.8)⁹

respectively, $\forall \mathbf{x} \in \mathbf{R}^-$ at each $t \in \Gamma$, where $\mathbf{a}(\mathbf{x},t) = \frac{\partial}{\partial t}\mathbf{v}(\mathbf{x},t)$ is the acceleration of the particle of material in \mathbf{R}_t^- that corresponds to the point $\mathbf{x} \in \mathbf{R}^-$.

Localization of the global nominal balance laws given by (2.4.5) and (2.4.6) using (2.4.7) yields

$$div_{1}\sigma_{1} + \mathbf{f}_{1} = \bar{\rho}_{1}\bar{\mathbf{a}}_{1},$$

$$\sigma_{1}\mathbf{F}_{1}^{\mathrm{T}} = \mathbf{F}_{1}\sigma_{1}^{\mathrm{T}},$$

$$(2.4.9)^{10}$$

respectively, $\forall \mathbf{x}_1 \in \mathbf{R}_1^+$ at each $t \in \Gamma$, where $\mathbf{\bar{a}_1}(\mathbf{x}_1,t) = \left[\frac{\partial}{\partial t}\mathbf{\bar{v}_1}(\mathbf{\tilde{x}_1}(\mathbf{x},t),t)\right]_{\mathbf{\tilde{x}(x_1,t)}}$ is the acceleration of the particle of material in \mathbf{R}_t^+ that corresponds to the point $\mathbf{x}_1 = \mathbf{\tilde{x}_1}(\mathbf{x},t)$ in \mathbf{R}_1^+ .

For subregions D_t of R_t , which contain a portion of S_t , the global form of the balance of linear momentum given by Equation (2.1.2) can be expressed with respect

 $^{^9}$ div denotes the divergence operator with respect to $\mathbf{x} \in \mathrm{R.}$

¹⁰ div₁ denotes the divergence operator with respect to $\mathbf{x}_1 \in \mathbf{R}_1^+$.

to R in terms of the field quantities defined on R⁻ and R₁⁺. Localizing this equation at points on S would then yield

$$\left(\left(\tilde{J}\sigma_{1}\tilde{\mathbf{F}}^{-\mathbf{T}} \right)^{+} - \sigma^{-} \right) \mathbf{N} + \rho \left(\bar{\mathbf{v}}_{1}^{+} - \mathbf{v}^{-} \right) (\mathbf{V} \cdot \mathbf{N}) = 0, \tag{2.4.10}$$

 $\forall \mathbf{x} \in S$ at each $t \in \Gamma$, where $\mathbf{x}_1 = \mathbf{\tilde{x}}_1(\mathbf{x},t)$ in σ_1^+ and $\mathbf{\bar{v}}_1^+$.11

The balance of angular momentum given by Equation (2.1.3) for a subregion D_t of R_t containing a portion of S_t is automatically satisfied if the jump conditions (2.3.2), (2.3.3), and (2.4.10) are satisfied at the points on S corresponding to the points on the portion of S_t contained in D_t . Also, the local field equations given by (2.4.2) and (2.4.7)-(2.4.9), the kinematic jump condition (2.3.1), or (2.3.2) and (2.3.3), and the linear momentum jump condition (2.4.10) are altogether equivalent to the global field equations given by (2.1.1)-(2.1.3).

2.5 Elastic Materials

In this section, a brief introduction to elastic materials will be given. In particular, a formal definition of elastic materials will be presented, and some of the restrictions on the functional forms of the corresponding elastic potentials will be investigated. The form of the stress power for an elastic material will also be considered. For convenience, the notation used to describe the material considered in Sections 2.3 and 2.4 will be used for the materials considered in this section, with the exception that the materials considered here are assumed to be entirely in one phase, which corresponds to phase 1 for the material considered in Sections 2.3 and 2.4.

¹¹ The corresponding form of this jump condition involving only one reference configuration is well known and can be found, e.g., in [2]. In fact, the jump conditions (2.3.2), (2.3.3), and (2.4.10) can be obtained formally from the jump conditions presented in [2] by replacing \mathbf{F}^+ , \mathbf{v}^+ , and σ^+ with $\mathbf{F}_1^+\mathbf{\tilde{F}}^+$, \mathbf{v}_1^+ , and $\left(\tilde{J}\sigma^+\mathbf{\tilde{F}}^{-T}\right)^+$, respectively.

The type of constitutive behavior that a material is said to have is determined by the quantities that the stress response function of the material depends on.¹² For a simple material without memory, the stress response function has the form

$$\tau(\hat{\mathbf{y}}(\mathbf{x},t),t) = \mathbf{g}(\mathbf{F}(\mathbf{x},t),\mathbf{x}). \tag{2.5.1}$$

The term simple is used in this description because the stress depends only on the first gradient of \hat{y} , and the term without memory is used because the stress does not depend on the history of the deformation of the material. Additionally, this constitutive relation is usually defined for only a subset $\tilde{\mathcal{L}}^+$ of \mathcal{L}^+ , where \mathcal{L}^+ denotes the set of all two-tensors with positive determinants. The set $\tilde{\mathcal{L}}^+$ represents the range of deformations for which the material has such constitutive behavior. Also, although the specific functional form of the stress response function in (2.5.1) depends on the particular reference configuration that it is with respect to, the corresponding true stress $\tau(y,t)$ is independent of the reference configuration and depends only on the current configuration of the material.

An *elastic* (or *hyperelastic*) material is a special type of simple material without memory. In particular, such a material possesses an elastic potential

$$W = W(\mathbf{F}(\mathbf{x}, t), \mathbf{x}), \tag{2.5.2}$$

 $\forall \mathbf{x} \in R$ and $\forall \mathbf{F} \in \bar{\mathcal{L}}^+$, such that the nominal stress tensor for the material is given by

$$\sigma(\mathbf{x}, t) = W_{\mathbf{F}}(\mathbf{F}(\mathbf{x}, t), \mathbf{x}), \tag{2.5.3}$$

 $\forall \mathbf{x} \in \mathbb{R}$ and $\forall \mathbf{F} \in \bar{\mathcal{L}}^+$, where the \mathbf{F} subscript on W denotes the tensor gradient with respect to \mathbf{F} , and $\bar{\mathcal{L}}^+$ is a subset of \mathcal{L}^+ and represents the range of deformations

¹² For the case where thermal effects are considered, the quantities that the internal energy, entropy, and heat flux vector depend on also determine what type of constitutive behavior the material is said to have (see [15]).

about R for which the material behaves elastically. The elastic potential given by (2.5.2) also represents the strain energy of the material per unit volume of R. In the rest of this section, an elastic material with an elastic potential that, for simplicity, is defined for every $\mathbf{F} \in \mathcal{L}^+$, as opposed to only a subset of \mathcal{L}^+ , is considered.

It is assumed that the elastic material under consideration is objective. In particular, it is assumed that at each $\mathbf{x} \in R$

$$W(\mathbf{QF}, \mathbf{x}) = W(\mathbf{F}, \mathbf{x}) \quad \forall \, \mathbf{Q} \in O^+, \, \forall \, \mathbf{F} \in \mathcal{L}^+,$$
 (2.5.4)

where O^+ denotes the set of all proper orthogonal two-tensors.¹³ It can be shown that the assumptions of hyperelasticity and objectivity are sufficient for $\sigma \mathbf{F}^T = \mathbf{F} \sigma^T$.¹⁴ A necessary condition for objectivity is that at each $\mathbf{x} \in \mathbf{R}$

$$W(\mathbf{F}, \mathbf{x}) = W(\mathbf{U}, \mathbf{x}) \quad \forall \, \mathbf{F} \in \mathcal{L}^+, \tag{2.5.5}$$

where $\mathbf{U} = \sqrt{\mathbf{F}^{\mathrm{T}}\mathbf{F}} \in \mathcal{S}^{+}$, $\mathbf{F} = \mathbf{R}\mathbf{U}$ represents the right polar decomposition of \mathbf{F} with $\mathbf{R} \in O^{+}$, and \mathcal{S}^{+} denotes the set of all symmetric, positive definite two-tensors. Considering this, we can define a function $\widehat{W} : \mathcal{S}^{+} \times \mathbf{R} \mapsto \Re$ as

$$\widehat{W}(\mathbf{C}, \mathbf{x}) = W(\mathbf{U}, \mathbf{x}), \tag{2.5.6}$$

where $C = U^2 \in S^+$, and \Re denotes the set of all real numbers.

Another restriction on the functional form of W is imposed by the material symmetry group $\mathcal G$ of the material. As mentioned in Section 1.3, for a crystalline solid the transformations that comprise $\mathcal G$ reflect the crystal symmetry of the solid. It is also required that the transformations in $\mathcal G$ be unimodular, so that they preserve

¹³ Note that QF represents the deformation gradient with respect to x of the composition mapping $p \circ q(x)$ of the two mappings p = Qq and q = Fx.

¹⁴ Recall that this is equivalent to the balance of angular momentum at points not on a surface of discontinuity.

volume.¹⁵ For an inhomogeneous material, $\mathcal G$ is a function of $\mathbf x$, and at each $\mathbf x \in R$ the elastic potential must be such that

$$W(\mathbf{FH}, \mathbf{x}) = W(\mathbf{F}, \mathbf{x}) \quad \forall \mathbf{H} \in \mathcal{G}(\mathbf{x}), \ \forall \mathbf{F} \in \mathcal{L}^+.$$
 (2.5.7)

In terms of \widehat{W} , (2.5.7) is equivalent to

$$\widehat{W}(\mathbf{H}^{\mathrm{T}}\mathbf{C}\mathbf{H}, \mathbf{x}) = \widehat{W}(\mathbf{C}, \mathbf{x}) \quad \forall \, \mathbf{H} \in \mathcal{G}(\mathbf{x}), \, \forall \, \mathbf{C} \in \mathcal{S}^{+}, \tag{2.5.8}$$

at each $x \in R$.

Consider next a second reference configuration R^* for the elastic material that can be obtained from R by the mapping with deformation gradient $P(\mathbf{x},t)$. It can be shown that the elastic potential of the material with respect to R^* is given by

$$W^*(\mathbf{F}^*) = \frac{1}{\det \mathbf{P}} W(\mathbf{F}^* \mathbf{P}), \qquad (2.5.9)$$

where \mathbf{F}^* is the deformation gradient of the mapping that maps \mathbf{R}^* into \mathbf{R}_t (see [15])¹⁶. It can also be shown that if \mathcal{G} is the material symmetry group of W, then the material symmetry group of W^* is

$$G^* = PGP^{-1}. (2.5.10)^{17}$$

¹⁵ By definition, a unimodular tensor has a determinant equal to one.

¹⁶ Note, however, that in [15] the factor detP will be missing since the potentials there are defined per unit mass of the material.

¹⁷ With regard to the continuum model that uses a single "global" elastic potential that was described in Section 1.3, if \mathcal{G} is the crystallographic point group of the austenite phase and if \mathbf{P} represents the shape deformation of a martensite phase, then \mathcal{G}^* will not be the crystallographic point group of the martensite phase that \mathbf{P} is supposed to represent (in fact, in general, \mathcal{G}^* will not be any crystallographic point group, and will not even be a subset of the orthogonal group). The only exception to this is the case where the austenite and martensite have crystal symmetries that differ only by a rotation and \mathbf{P} is the deformation gradient of a mapping that is the composition of a mapping that preserves the material symmetry group of the austenite and the mapping that is the rotation by which the two crystal lattices differ.

We next consider the nominal form of the work-energy equation. This equation can be obtained in the usual way from Equation (2.1.4) and is given by

$$\int_{\partial D} \boldsymbol{\sigma} \mathbf{n} \cdot \mathbf{v} dA + \int_{D} \mathbf{f} \cdot \mathbf{v} dV = \int_{D} \boldsymbol{\sigma} \cdot \nabla \mathbf{v} dV + \frac{d}{dt} \int_{D} \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} dV, \qquad (2.5.11)$$

 \forall D \subset R and \forall $t \in \Gamma$. For the material under consideration, the stress power can be written as

$$\int_{D} \boldsymbol{\sigma} \cdot \nabla \mathbf{v} dV = \frac{d}{dt} \int_{D} W dV. \tag{2.5.12}$$

Using this result, it is easy to show that the change in the total strain energy and kinetic energy of any $D \subset R$ in a complete cycle is zero.

2.6 Elastic Materials and Multiple Reference Configurations

It will be shown in this section that for materials with phases that behave elastically for some ranges of deformations about undeformed configurations, a reasonable continuum model using multiple reference configurations in the manner described in Section 2.2 can be developed, provided these reference configurations have the proper form. The material described in Sections 2.3 and 2.4 will be considered. Additionally, it is assumed that R⁻ and R₁⁺ for this material are such that phase 1 and phase 2 have elastic-type constitutive behavior for ranges of deformation about these configurations, respectively.

Since R^- is stationary, in the sense that points $x \in R^-$ are stationary, the elastic-type constitutive behavior of phase 1 is assumed to be the elastic constitutive

¹⁸ Note that it has been assumed here that all quantities in this equation have the continuity conditions necessary for its derivation.

behavior described in the previous section. In particular, it is assumed that phase 1 possesses an elastic potential

$$W = W(\mathbf{F}(\mathbf{x}, t), \mathbf{x}), \tag{2.6.1}$$

 $\forall x \in R^-$ and $\forall F \in \widehat{\mathcal{L}}^+$, such that the nominal stress tensor for this phase is given by

$$\sigma(\mathbf{x}, t) = W_{\mathbf{F}}(\mathbf{F}(\mathbf{x}, t), \mathbf{x}), \tag{2.6.2}$$

 $\forall \mathbf{x} \in \mathbb{R}^- \text{ and } \forall \mathbf{F} \in \widehat{\mathcal{L}}^+$, where $\widehat{\mathcal{L}}^+$ is a subset of \mathcal{L}^+ and represents the range of deformations about \mathbb{R}^- for which phase 1 behaves elastically.

Assume that there exists an elastic potential W_1 for phase 2 defined with respect to R_1^+ . It is assumed that W_1 is a function of F_1 . Additionally, as one might expect, it is required that the inhomogeneity of W_1 remain the same for each particle of material in phase 2 as time progresses. If $\tilde{\mathbf{x}}_1$ is a function of time, the reference point $\mathbf{x}_1 \in R_1^+$ for a given particle of material in phase 2 is changing as time progresses, and a different particle of material occupies a given point $\mathbf{x}_1 \in R_1^+$ at different times $t \in \Gamma$. Because of this, the inhomogeneity of W_1 cannot be expressed with respect to points $\mathbf{x}_1 \in R_1^+$ if $\tilde{\mathbf{x}}_1$ is a function of time. Instead, the inhomogeneity of W_1 must be represented with respect to points \mathbf{x} in the stationary reference configuration R^+ , so that the effect of the inhomogeneity of W_1 on a given particle of material in phase 2 follows that particle for all $t \in \Gamma$. Thus, we assume that W_1 has the form

$$W_1 = W_1(\mathbf{F}_1(\mathbf{x}_1, t), \tilde{\mathbf{x}}(\mathbf{x}_1, t)), \tag{2.6.3}$$

 $\forall \mathbf{x_1} \in \mathbf{R_1^+}, \forall t \in \Gamma$, and $\forall \mathbf{F_1} \in \widehat{\mathcal{L}}_1^+$, where $\widehat{\mathcal{L}}_1^+$ is a subset of \mathcal{L}^+ and represents the range of deformations about $\mathbf{R_1^+}$ for which phase 2 behaves elastically. It is

¹⁹ However, if $\tilde{\mathbf{x}}_1$ is not a function of time, which would be appropriate for the static case, the reference configuration \mathbf{R}_1^+ is stationary, and consequently the inhomogeneity of W_1 can be expressed explicitly with respect to points $\mathbf{x}_1 \in \mathbf{R}_1^+$.

further assumed that W_1 is such that the stress tensor for phase 2 with respect to R_1^+ is given by

$$\sigma_1(\mathbf{x}_1, t) = W_{1_{\mathbf{F}_1}}(\mathbf{F}_1(\mathbf{x}_1, t), \tilde{\mathbf{x}}(\mathbf{x}_1, t))$$
 (2.6.4)

 $\forall \mathbf{x}_1 \in \mathbf{R}_1^+, \forall t \in \Gamma$, and $\forall \mathbf{F}_1 \in \widehat{\mathcal{L}}_1^+$. The material symmetry group for phase 2 is also defined with respect to \mathbf{R}_1^+ . We note that since the material symmetry groups for phase 1 and phase 2 can be chosen independently of each other and arbitrarily, with the exception that they must be subsets of the unimodular group, the material symmetry group of each phase can be chosen to reflect any type of crystal symmetry with any orientation. Therefore, the change in crystal structure that takes place during a martensitic phase transformation and the orientation relation between the crystal lattices of the austenite and the martensite can be accurately represented. We next require that $\tilde{\mathbf{x}}_1$ be such that

$$\nabla_{\mathbf{1}} \left[\frac{\partial}{\partial t} \hat{\mathbf{y}}_{\mathbf{1}} (\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x}, t), t) \right]_{\tilde{\mathbf{x}}(\mathbf{x}_{\mathbf{1}}, t)} = \left[\frac{\partial}{\partial t} [\nabla_{\mathbf{1}} \hat{\mathbf{y}}_{\mathbf{1}}(\mathbf{x}_{\mathbf{1}}, t)]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x}, t)} \right]_{\tilde{\mathbf{x}}(\mathbf{x}_{\mathbf{1}}, t)}$$
(2.6.5)

 $\forall \mathbf{x}_1 \in \mathbf{R}_1^+$ at each $t \in \Gamma$. It is easy to show that a necessary and sufficient condition for (2.6.5) is that $\tilde{\mathbf{x}}_1$ has the form

$$\tilde{\mathbf{x}}_1(\mathbf{x}, t) = \Psi(\mathbf{x}) + \Theta(t), \tag{2.6.6}$$

 $\forall \mathbf{x} \in \mathbf{R}^+ \text{ at each } t \in \Gamma.$

If $\tilde{\mathbf{x}}_1$ has the form given by (2.6.6), the constitutive behavior for phase 2 given by (2.6.3) and (2.6.4) results in the stress power for any subregion of phase 2 being equal

²⁰ The orientation relation that a given material has can be determined experimentally, or from the phenomenological theory of martensite (see [13, 17]), for materials to which this phenomenological theory is applicable.

to the time rate of change of the integral of W_1 over that subregion. To show this, we first note that the stress power of phase 2 can be expressed with respect to R_1^+ as

$$\int_{D_1^+} \sigma_1 \cdot \nabla_1 \bar{\mathbf{v}}_1 dV, \tag{2.6.7}$$

 $\forall D_1^+ \subset R_1^+$ and $\forall t \in \Gamma$. This equation can be expressed with respect to R^+ as

$$\int_{D^{+}} \tilde{J} \left[\sigma_{1} \cdot \nabla_{1} \bar{\mathbf{v}}_{1} \right]_{\bar{\mathbf{x}}_{1}(\mathbf{x},t)} dV, \tag{2.6.8}$$

where $D^+ = \tilde{\mathbf{x}}(D_1^+, t)$. For the moment, we will assume that $\tilde{\mathbf{x}}_1$ is a general function of time. In this case, using (2.6.4) and expanding the term $\nabla_1 \bar{\mathbf{v}}_1$, the above equation can be written as

$$\int_{D^{+}} \tilde{J}(\mathbf{x},t) \left[W_{1_{\mathbf{F}_{1}}} \cdot \nabla_{1} \left(\mathbf{F}_{1} \left[\frac{\partial \tilde{\mathbf{x}}_{1}}{\partial t} \right]_{\tilde{\mathbf{x}}(\mathbf{x}_{1},t)} + \frac{\partial \hat{\mathbf{y}}_{1}}{\partial t} \right) \right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)} dV$$

$$= \int_{D^{+}} \tilde{J} \left\{ \left[W_{1_{\mathbf{F}_{1}}} \cdot \left((\nabla_{1}\mathbf{F}_{1})\tilde{\mathbf{v}}_{1} + \frac{\partial}{\partial t}\mathbf{F}_{1} \right) \right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)} + \left[\left(\mathbf{F}_{1}^{\mathsf{T}}\boldsymbol{\sigma}_{1} \right) \cdot (\nabla_{1}\tilde{\mathbf{v}}_{1}) \right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)} \right\} dV, \tag{2.6.9}$$

where $\tilde{\mathbf{v}}_1(\mathbf{x}_1,t) = \left[\frac{\partial}{\partial t}\tilde{\mathbf{x}}_1(\mathbf{x},t)\right]_{\tilde{\mathbf{x}}(\mathbf{x}_1,t)}$.²² We next note that

$$\frac{\partial}{\partial t}W_{1}(\mathbf{F}_{1}(\tilde{\mathbf{x}}_{1}(\mathbf{x},t),t),\mathbf{x}) = W_{1_{\mathbf{F}_{1}}} \cdot \frac{\partial}{\partial t}\mathbf{F}_{1}(\tilde{\mathbf{x}}_{1}(\mathbf{x},t),t)$$

$$= W_{1_{\mathbf{F}_{1}}} \cdot \left((\nabla_{1}\mathbf{F}_{1})\frac{\partial \tilde{\mathbf{x}}_{1}}{\partial t} + \frac{\partial}{\partial t}\mathbf{F}_{1}\right).$$
(2.6.10)²³

²¹ This form of the stress power can be obtained from the Eulerian form of the stress power in Equation (2.1.4) in a manner completely analogous to that used to obtain the stress power with respect to R in Equation (2.5.11). ²² In a given frame, the two-tensor $(\nabla \mathbf{A})\mathbf{b}$, where **A** is a two-tensor and **b** is a vector, has components $((\nabla \mathbf{A})\mathbf{b})_{ij} = A_{ij,k}b_k$.

Note that if the inhomogeneity of W_1 were expressed explicitly in terms of points $\mathbf{x}_1 \in \mathbf{R}_1^+$, there would be the extra term $\frac{\partial}{\partial \mathbf{x}_1} W_1 \cdot \frac{d}{dt} \tilde{\mathbf{x}}_1$ in this equation.

If $\tilde{\mathbf{x}}_1$ has the form given by (2.6.6), $\nabla_1 \tilde{\mathbf{v}}_1 = \mathbf{0} \ \forall \mathbf{x} \in \mathbf{R}^+$ at each $t \in \Gamma$ and $\tilde{J} = \tilde{J}(\mathbf{x})$. In this case, Equation (2.6.9) becomes

$$\int_{D^{+}} \tilde{J}(\mathbf{x}) \left[W_{1_{\mathbf{F}_{1}}} \cdot \left((\nabla_{1} \mathbf{F}_{1}) \tilde{\mathbf{v}}_{1} + \frac{\partial}{\partial t} \mathbf{F}_{1} \right) \right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)} dV. \tag{2.6.11}$$

Substituting (2.6.10) into (2.6.11) and bringing the time-derivative operator outside the integral yields

$$\frac{d}{dt} \int_{D^+} \tilde{J}(\mathbf{x}) W_1(\mathbf{F}_1(\tilde{\mathbf{x}}_1(\mathbf{x},t),t), \mathbf{x}) dV = \frac{d}{dt} \int_{D_1^+} W_1(\mathbf{F}_1(\mathbf{x}_1,t), \tilde{\mathbf{x}}(\mathbf{x}_1,t)) dV. \quad (2.6.12)$$

Thus, if $\tilde{\mathbf{x}}_1$ has the form given by (2.6.6),

$$\int_{D_1^+} \boldsymbol{\sigma_1} \cdot \nabla_1 \overline{\mathbf{v}}_1 dV = \frac{d}{dt} \int_{D_1^+} W_1 dV, \qquad (2.6.13)$$

 $\forall D_1^+ \subset R_1^+ \text{ and } \forall t \in \Gamma.$

Equation (2.6.13) can be interpreted as a statement that the stress power of any subregion of phase 2 equals the time rate of change of the strain energy of that subregion of phase 2. It can easily be shown that for this case the change in the total strain energy and kinetic energy of any subregion of phase 2 in a complete cycle is zero. Since this is the most important property of elastic materials, the constitutive behavior described by (2.6.3) and (2.6.4) along with the requirement that $\tilde{\mathbf{x}}_1$ has the form given by (2.6.6) can be considered to be included in a generalization of the definition of elastic materials, which was formally given in the previous section. We will henceforth assume that the mapping $\tilde{\mathbf{x}}_1$ has the form given by (2.6.6).

2.7 The Mapping $\tilde{\mathbf{x}}_1$ and Invariant Plane Strain Deformations

As discussed in the Introduction, the martensite has a shape deformation relative to the undeformed austenite. Additionally, because this shape deformation corresponds to an unstressed state of the martensite, it can be considered to represent an undeformed configuration of the martensite, and the martensite will behave elastically for at least small deformations about this configuration. Motivated by this, it will henceforth be assumed that R^- corresponds to an unstressed, undeformed configuration of phase 1 and that there exists a shape deformation for phase 2 with respect to R^+ , which can be considered to represent an unstressed, undeformed configuration of that phase. It will be assumed that R_1^+ coincides with this shape deformation of phase 2. Note that the mapping $\tilde{\mathbf{x}}_1$ corresponding to this shape deformation is assumed to be given in a problem. Note also that because it has been assumed that $\tilde{\mathbf{x}}_1$ has the form given by (2.6.6), the transformation strain for phase 2 is independent of time, which is probably most appropriate for the case considered here (i.e., for the case where phase 2 represents a phase that is in a purely mechanical process and behaves elastically).

As discussed in the Introduction, the shape deformation of many martensites has the macroscopic form of an invariant plane strain. By definition, such a deformation has a deformation gradient of the form

$$1 + c \otimes m, \tag{2.7.1}$$

where 1 is the identity tensor and c and m are both vectors. Consider next the homogeneous invariant plane strain deformation $\mathbf{q} = \mathbf{\hat{q}}(\mathbf{p})$ with

$$\mathbf{q} = \mathbf{\hat{q}}(\mathbf{p}) = (\mathbf{1} + \mathbf{c} \otimes \mathbf{m})\mathbf{p}$$
$$= \mathbf{p} + (\mathbf{p} \cdot \mathbf{m})\mathbf{c}.$$
 (2.7.2)

From this, it can be seen that points \mathbf{p} on the plane that goes through the origin and has a unit normal \mathbf{m} remain fixed under this mapping, since $\mathbf{p} \cdot \mathbf{m} = 0$ for these points. This plane is therefore invariant under this mapping. It can also be observed from (2.7.2) that a point \mathbf{p} is displaced in the direction \mathbf{c} a distance proportional to its distance from the invariant plane. The vector \mathbf{c} is sometimes referred to as the amplitude vector of this type of deformation. Also, note that a simple shear is a special case of an invariant plane strain and exists when $\mathbf{c} \cdot \mathbf{m} = 0$. A homogeneous invariant plane strain is also the type of macroscopic deformation that is assumed to exist in the phenomenological theory of martensite (see [13, 17]). In fact, for some problems, the deformation determined from this theory might be a good choice for $\tilde{\mathbf{x}}_1$.

For the case where phase 1 and phase 2 coexist with continuous displacements at their interface in an unstressed, undeformed state, $\tilde{\mathbf{F}}$ must have the form of an invariant plane strain locally at each point on the interface, as can be seen by substituting $\mathbf{F}^- = \mathbf{F}_1^+ = \mathbf{1}$ into Equation (2.3.4). In this case and when $\tilde{\mathbf{F}}$ is a homogeneous invariant plane stain, $\tilde{\mathbf{x}}_1$ must necessarily have the form

$$\tilde{\mathbf{x}}_{1}(\mathbf{x},t) = (1 + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}})\mathbf{x} + \mathbf{x}_{1}^{*}(t),$$
(2.7.3)²⁴

where \mathbf{x}_1^* is chosen such that (2.7.3) satisfies Equation (2.3.3), when $\mathbf{F}^- = \mathbf{F}_1^+ = \mathbf{1}$. Alternatively, \mathbf{x}_1^* can be determined from Equation (2.3.1). Either way, both of these equations will be satisfied, and consequently the displacements will be continuous at the interface when $\mathbf{F} = \mathbf{1} \ \forall \ \mathbf{x} \in \mathbf{R}^-$ and $\mathbf{F}_1 = \mathbf{1} \ \forall \ \mathbf{x}_1 \in \mathbf{R}_1^+$, if and only if \mathbf{x}_1^* has the form $\mathbf{x}_1^*(t) = -(\mathbf{\tilde{a}} \otimes \mathbf{\tilde{n}})\mathbf{\bar{x}}(t)$, which results in

$$\tilde{\mathbf{x}}_{1}(\mathbf{x},t) = \mathbf{x} + ([\mathbf{x} - \bar{\mathbf{x}}(t)] \cdot \tilde{\mathbf{n}})\tilde{\mathbf{a}}, \tag{2.7.4}$$

Note that for the general case of a homogeneous deformation, the deformation gradient may be a function of time. Here, however, it is not since \bar{x}_1 is also required to have the form given by (2.6.6).

where $\bar{\mathbf{x}}(t)$ is any point on the interface S. We note that for the $\tilde{\mathbf{x}}_1$ given by (2.7.4) and when $\mathbf{F} = \mathbf{1} \ \forall \ \mathbf{x} \in \mathbf{R}^-$ and $\mathbf{F}_1 = \mathbf{1} \ \forall \ \mathbf{x}_1 \in \mathbf{R}_1^+$, at each $t \in \Gamma$, the interface S is a plane with unit normal $\tilde{\mathbf{n}}$ and translates with velocity $\mathbf{V}(t) = \frac{d}{dt}\bar{\mathbf{x}}(t)$. Also, in this case, all points in phase 2 translate with velocity $\tilde{\mathbf{v}}(t) = -(\mathbf{V}(t) \cdot \tilde{\mathbf{n}})\tilde{\mathbf{a}}$.

2.8 The Domains of the Elastic Potentials

As indicated in Section 2.6, the elastic potentials given by (2.6.1) and (2.6.3) are defined for finite deformations in $\widehat{\mathcal{L}}^+ \subset \mathcal{L}^+$ and $\widehat{\mathcal{L}}_1^+ \subset \mathcal{L}^+$, respectively. Additionally, $\widehat{\mathcal{L}}_1^+$ is with respect to R_1^+ in the sense that the two-tensors in $\widehat{\mathcal{L}}_1^+$ represent deformations \mathbf{F}_1 with respect to R_1^+ . The corresponding subset of \mathcal{L}^+ that represents $\widehat{\mathcal{L}}_1^+$ with respect to R can be defined as

$$\bar{\mathcal{L}}_{1}^{+} = \left\{ \bar{\mathbf{F}} / \bar{\mathbf{F}} = \mathbf{F}_{1} \tilde{\mathbf{F}}, \text{ where } \mathbf{F}_{1} \in \widehat{\mathcal{L}}_{1}^{+} \right\}. \tag{2.8.1}$$

In the space S^+ , the deformations with respect to R corresponding to the undeformed configurations of phase 1 and phase 2 are C = 1 and $\tilde{C} = \tilde{F}^T \tilde{F}$, respectively. Considering this, the sets

$$\widehat{S}^{+} = \left\{ \mathbf{C} / \mathbf{C} = \mathbf{F}^{T} \mathbf{F}, \text{ where } \mathbf{F} \in \widehat{\mathcal{L}}^{+} \right\},$$

$$\bar{S}_{1}^{+} = \left\{ \bar{\mathbf{C}} / \bar{\mathbf{C}} = \bar{\mathbf{F}}^{T} \bar{\mathbf{F}}, \text{ where } \bar{\mathbf{F}} \in \bar{\mathcal{L}}_{1}^{+} \right\}$$
(2.8.2)

represent the domains with respect to R about C = 1 and $\tilde{C} = \tilde{F}^T \tilde{F}$ in S^+ for which phase 1 and phase 2, respectively, behave elastically. We note that if \hat{S}^+ and \bar{S}_1^+ are relatively large and 1 and \tilde{C} are relatively close, these two phase domains may intersect in S^+ . In this case, some might consider this constitutive model to be multivalued. Either way, an intersection of these two phase domains will not present any difficulties in setting up or solving a boundary value problem.

Most metals, however, have phases that are not elastic for finite deformations about their undeformed configurations. Instead, they have phases that have elastic-plastic constitutive behaviors with yield stresses corresponding to infinitesimal

deformations. If the material under consideration represents such a material and if the stresses within phase 1 and phase 2 are less than the yield stresses of these phases, respectively, for all $t \in \Gamma$, both of these phases will behave elastically in this time interval. Additionally, in this case, because the deformations are infinitesimal for all $t \in \Gamma$, the linearized forms of the constitutive equations given by (2.6.1) and (2.6.2) about F = 1 and (2.6.3) and (2.6.4) about $F_1 = 1$ can be used. This is probably most appropriate in the temperature interval containing the temperature M_s , where the stress necessary to induce nucleation or growth of a variant of martensite is less than the yield stresses of both phases. In this case, the material will deform by a martensitic phase transformation before it will deform by plastic deformation.²⁵ This martensitic phase transformation may be associated with the austenite phase transforming into a martensite phase, or with one variant of martensite transforming into another variant of the same martensite, which is also known as reorientation. Also, for this case where $\widehat{\mathcal{L}}^+$ and $\widehat{\mathcal{L}}_1^+$ contain only deformations such that $|\nabla \widehat{\mathbf{u}}| \ll 1$ and $|\nabla_{\mathbf{i}}\widehat{\mathbf{u}}_{\mathbf{i}}| \ll 1$, respectively, and if \tilde{x}_1 is a finite deformation, there is no chance that $\widehat{\mathcal{S}}^+$ and $\bar{\mathcal{S}}_1^+$ will intersect.

2.9 The Driving Traction

As mentioned in Section 2.4, the global form of the rate of work-energy equation given by (2.1.4) is not valid for subregions of $R_{\rm t}$ containing a portion of $S_{\rm t}$, since the continuity assumptions that are necessary for the derivation of that equation from Equations (2.1.1)-(2.1.3) do not exist for these subregions. For the two-phase elastic material under consideration, the global form of the rate of work-energy equation for subregions $D_{\rm t}$ of $R_{\rm t}$ containing a portion $S_{\rm t}^*$ of $S_{\rm t}$ can be expressed as

²⁵ A material deforms by a martensitic phase transformation in the sense that the creation of the martensite phase produces a deformation that is due to the shape deformation of that martensite.

$$\int_{\partial D_{t}} \mathbf{t} \cdot \bar{\mathbf{v}} dA + \int_{D_{t}} \mathbf{b} \cdot \bar{\mathbf{v}} dV - \int_{S^{*}} f \mathbf{N} \cdot \mathbf{V} dA$$

$$= \frac{d}{dt} \int_{D^{-}} W dV + \frac{d}{dt} \int_{D_{t}^{+}} W_{1} dV + \frac{d}{dt} \int_{D_{t}} \bar{\rho} \bar{\mathbf{v}} \cdot \bar{\mathbf{v}} dV,$$
(2.9.1)

where $D^- = \hat{\mathbf{x}}(D_t^-, t)$, $D_1^+ = \hat{\mathbf{x}}_1(D_t^+, t)$, $S^* = \hat{\mathbf{x}}(S_t^*, t)$, $D_t^- \cup D_t^+ = D_t$, and

$$f = \left(\tilde{J}^+ W_1^+ - W^-\right) - \frac{1}{2} \left(\left(\tilde{J}\boldsymbol{\sigma}_1 \tilde{\mathbf{F}}^{-T}\right)^+ + \boldsymbol{\sigma}^-\right) \cdot \left(\mathbf{F}_1^+ \tilde{\mathbf{F}}^+ - \mathbf{F}^-\right). \tag{2.9.2}$$

The quantity fN is referred to as the driving traction, and f as the scalar driving traction. The integral

$$\int_{S^*} f \mathbf{N} \cdot \mathbf{V} dA \tag{2.9.3}$$

can be interpreted as representing the rate of work done on the interface S^* by the traction fN exerted by the body on the interface. We require that this integral be positive so that it represents a dissipation of energy. Localizing this equation at points on the interface S then yields

$$f\mathbf{N} \cdot \mathbf{V} \ge 0 \tag{2.9.4}$$

 $\forall \mathbf{x} \in S$ at each $t \in \Gamma^{27}$ Note that energy can be dissipated only at the phase boundary, and that if $f \mathbf{N} \cdot \mathbf{V} = 0 \ \forall \mathbf{x} \in S$ at each $t \in \Gamma$, energy is conserved. Thus,

Refer to [2] and [9] for a more extensive discussion of the driving traction. Also, the scalar driving traction given by (2.9.2) can be obtained formally from the scalar driving traction derived in [2] by replacing W^+ , σ^+ , and F^+ with $\tilde{J}^+W_1^+$, $\left(\tilde{J}\sigma^+\tilde{\mathbf{F}}^{-1}\right)^+$, and $F_1^+\tilde{\mathbf{F}}^+$, respectively.

²⁷ This requirement is also equivalent to the second law of thermodynamics for the type of process under consideration. See [2] and Section 2.12.

by allowing $f \mathbf{N} \cdot \mathbf{V} > 0$, we are in effect considering a nonconservative system even though both phases behave elastically for points not on the interface.

We can also postulate a constitutive relation relating the scalar driving traction to the normal component of the phase boundary velocity at each $x \in S$ (see [2]). More specifically, we can postulate that

$$V_{\rm n} = \Phi(f, \mathbf{x}),\tag{2.9.5}$$

at each $x \in S$, where $\Phi(f, x)$ is given and depends on the material, and $V_n = V \cdot N$. This may be done primarily to provide an extra equation for the extra unknowns — the variables describing the location of the phase boundary.

2.10 The Boundary Value Problem

Upon substituting the constitutive equation given by (2.6.2) into Equation $(2.4.8)_1$ and expressing a in that equation in terms of $\hat{\mathbf{u}}$, we obtain that field equation in terms of the displacement $\hat{\mathbf{u}}$. The resulting equation is as follows:

$$\operatorname{div}(W_{\mathbf{F}}) + \mathbf{f} = \rho \ddot{\hat{\mathbf{u}}}, \tag{2.10.1}$$

 $\forall \mathbf{x} \in \mathbf{R}^- \text{ at each } t \in \Gamma$, where $\mathbf{F} = \mathbf{1} + \nabla \hat{\mathbf{u}} \text{ in } W$, and $\ddot{\hat{\mathbf{u}}}(\mathbf{x}, t) = \frac{\partial^2}{\partial t^2} \hat{\mathbf{u}}(\mathbf{x}, t)$. In a given frame, the term $\operatorname{div}(W_{\mathbf{F}})$ has components

$$\operatorname{div}(W_{\mathbf{F}})_{i} = \frac{\partial^{2} W}{\partial F_{ij} \partial F_{kl}} \frac{\partial^{2} \hat{u}_{k}}{\partial x_{l} \partial x_{j}} + \frac{\partial^{2} W}{\partial F_{ij} \partial x_{j}}.$$
 (2.10.2)

Similarly, upon substituting the constitutive equation given by (2.6.4) into Equation (2.4.9)₁ and expressing $\bar{\mathbf{a}}_1$ in that equation in terms of $\hat{\mathbf{u}}_1$, we obtain that field equation in terms of the displacement $\hat{\mathbf{u}}_1$. The resulting equation is as follows:

$$\operatorname{div}_{\mathbf{1}}\left(W_{\mathbf{1}_{\mathbf{F}_{\mathbf{1}}}}\right) + \mathbf{f}_{\mathbf{1}} = \bar{\rho}_{\mathbf{1}}\left(\ddot{\tilde{\mathbf{x}}}_{\mathbf{1}} + \ddot{\hat{\mathbf{u}}}_{\mathbf{1}}\right),\tag{2.10.3}$$

 $\forall \ \mathbf{x_1} \in \mathbf{R_1^+} \ \text{at each} \ t \in \Gamma, \ \text{where} \ \mathbf{F_1} = \mathbf{1} + \nabla_1 \hat{\mathbf{u}}_1 \ \text{in} \ W_1 \ , \ \ddot{\tilde{\mathbf{x}}}_1(t) = \frac{\partial^2}{\partial t^2} \tilde{\mathbf{x}}_1(\mathbf{x},t) = \frac{d^2}{dt^2} \Theta(t), \ \text{and} \ \ddot{\tilde{\mathbf{u}}}_1(\mathbf{x}_1,t) = \left[\frac{\partial^2}{\partial t^2} \hat{\mathbf{u}}_1(\tilde{\mathbf{x}}_1(\mathbf{x},t),t)\right]_{\tilde{\mathbf{x}}(\mathbf{x}_1,t)}. \ \text{In a given frame, the term} \\ \operatorname{div}_1\left(W_{1_{\mathbf{F_1}}}\right) \ \text{has components}$

$$\operatorname{div}(W_{\mathbf{F}})_{i} = \frac{\partial^{2} W_{\mathbf{1}}}{\partial F_{\mathbf{1}_{ij}} \partial F_{\mathbf{1}_{kl}}} \frac{\partial^{2} \hat{u}_{\mathbf{1}_{k}}}{\partial x_{\mathbf{1}_{l}} \partial x_{\mathbf{1}_{j}}} + \frac{\partial^{2} W_{\mathbf{1}}}{\partial F_{\mathbf{1}_{ij}} \partial x_{k}} \frac{\partial \tilde{x}_{k}}{\partial x_{\mathbf{1}_{j}}}, \qquad (2.10.4)$$

and the term $\ddot{\hat{\mathbf{u}}}_1$ has components

$$\frac{\partial^{2}}{\partial t^{2}}\hat{u}_{1_{i}}(\tilde{\mathbf{x}}_{1}(\mathbf{x},t),t) = \frac{\partial}{\partial t} \left[\left(\frac{\partial \hat{u}_{1_{i}}}{\partial x_{1_{k}}} \tilde{v}_{k} + \frac{\partial \hat{u}_{1_{i}}}{\partial t} \right) \right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)}$$

$$= \left(\frac{\partial^{2} \hat{u}_{1_{i}}}{\partial x_{1_{k}} \partial x_{1_{n}}} \tilde{v}_{k} \tilde{v}_{n} + 2 \frac{\partial^{2} \hat{u}_{1_{i}}}{\partial t \partial x_{1_{k}}} \tilde{v}_{k} + \frac{\partial \hat{u}_{1_{i}}}{\partial x_{1_{k}}} \frac{d\tilde{v}_{k}}{dt} + \frac{\partial^{2} \hat{u}_{1_{i}}}{\partial t^{2}} \right), \tag{2.10.5}$$

where $\tilde{\mathbf{v}}(\mathbf{x},t) = \frac{\partial}{\partial t}\tilde{\mathbf{x}}_1(\mathbf{x},t) = \frac{d}{dt}\Theta(t)$. The inertial-type terms in (2.10.5) obviously occur because points in R_1^+ are moving. This also results in the boundary conditions on the boundary of R_1^+/S_1 , where $S_1 = \hat{\mathbf{x}}_1(S_t,t)$, being with respect to a moving boundary. Both of these issues complicate solving the corresponding boundary value problem, whether it be by using analytical methods or by constructing a finite-difference or a finite-element computer program.

Fortunately, the boundary value problem with the balance of linear momentum for phase 2 in the form given by Equation (2.10.3) does not have to be solved. Instead, Equation (2.10.3) can be transformed into a more tractable equation. In particular, we can use the mapping $\tilde{\mathbf{x}}_1$ and define the function $\bar{\mathbf{u}}_1$ as

$$\bar{\mathbf{u}}_{\mathbf{1}}(\mathbf{x},t) = \hat{\mathbf{u}}_{\mathbf{1}}(\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t),t), \tag{2.10.6}$$

 $\forall \mathbf{x} \in \mathbb{R}^+$ and $\forall t \in \Gamma$, and then solve for $\mathbf{u_1} = \mathbf{\bar{u}_1}(\mathbf{x}, t)$ instead of $\mathbf{u_1} = \mathbf{\hat{u}_1}(\mathbf{x_1}, t)$ in the boundary value problem. This results in Equation (2.10.3) becoming

$$\left[\operatorname{div}_{\mathbf{1}}\left(W_{\mathbf{1}_{\mathbf{F}_{\mathbf{1}}}}\right)\right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)} + \mathbf{f}_{\mathbf{1}}(\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t),t) = \bar{\rho}_{\mathbf{1}}\left(\frac{\partial^{2}}{\partial t^{2}}\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t) + \frac{\partial^{2}}{\partial t^{2}}\bar{\mathbf{u}}_{\mathbf{1}}(\mathbf{x},t)\right), \quad (2.10.7)$$

 $\forall \mathbf{x} \in \mathbb{R}^+$ at each $t \in \Gamma$, where in a given frame, $\left[\operatorname{div}_{\mathbf{1}}\left(W_{\mathbf{1}_{\mathbf{F}_{\mathbf{1}}}}\right)\right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}$ has components

$$\left(\left[\operatorname{div}_{1}\left(W_{1_{\mathbf{F}_{1}}}\right)\right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)}\right)_{i} = \left[\frac{\partial^{2}W_{1}}{\partial F_{1_{ij}}\partial F_{1_{kl}}} \frac{\partial F_{1_{kl}}}{\partial x_{1_{j}}} + \frac{\partial^{2}W_{1}}{\partial F_{1_{ij}}\partial x_{1_{j}}}\right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)}$$

$$= \left[\frac{\partial^{2}W_{1}}{\partial F_{1_{ij}}\partial F_{1_{kl}}}\right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)} \left(\frac{\partial^{2}\bar{u}_{1_{k}}}{\partial x_{m}\partial x_{n}} \left[\frac{\partial \tilde{x}_{m}}{\partial x_{1_{l}}} \frac{\partial \tilde{x}_{n}}{\partial x_{1_{j}}}\right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)} + \frac{\partial \bar{u}_{1_{k}}}{\partial x_{m}} \left[\frac{\partial^{2}\tilde{x}_{m}}{\partial x_{1_{l}}\partial x_{1_{j}}}\right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)}\right)$$

$$+ \left[\frac{\partial^{2}W_{1}}{\partial F_{1_{ij}}\partial x_{k}} \frac{\partial \tilde{x}_{k}}{\partial x_{1_{j}}}\right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)}.$$
(2.10.8)

From these equations we can observe that not only have most of the inertial terms been eliminated, the resulting boundary value problem is in a completely Lagrangian description; i.e., it is completely in terms of the coordinates of the fixed reference configuration. This includes the boundary conditions for phase 2 being specified with respect to a fixed boundary. The only penalty that is paid for this coordinate transformation are the additional terms in Equation (2.10.8). For the special case where $\tilde{\mathbf{x}}_1$ is a homogeneous deformation and phase 2 is a homogeneous material, (2.10.8) reduces to

$$\left(\left[\operatorname{div}_{1} \left(W_{1_{\mathbf{F}_{1}}} \right) \right]_{\tilde{\mathbf{x}}_{1}(\mathbf{x},t)} \right)_{i} = \frac{\partial^{2} W_{1}}{\partial F_{1_{ij}} \partial F_{1_{kl}}} \frac{\partial^{2} \bar{u}_{1_{k}}}{\partial x_{m} \partial x_{n}} \frac{\partial \tilde{x}_{m}}{\partial x_{1_{l}}} \frac{\partial \tilde{x}_{n}}{\partial x_{1_{j}}}, \tag{2.10.9}$$

where $\mathbf{x_1} = \tilde{\mathbf{x}}_1(\mathbf{x}, t)$ in $W_{^{1}\mathbf{F_1}\mathbf{F_1}}$ and $\nabla_{\mathbf{1}}\tilde{\mathbf{x}}$. For this case, the additional terms in (2.10.9) contribute only to the coefficients of the terms involving second spatial

derivatives of $\bar{\mathbf{u}}_1$. Thus, in at least this case, the advantages of using multiple reference configurations along with this coordinate transformation far outweigh their disadvantages. For the static problem, however, points in \mathbf{R}_1^+ are stationary, and it is probably much more convenient to solve for $\mathbf{u}_1 = \hat{\mathbf{u}}_1(\mathbf{x}_1)$ instead of $\mathbf{u}_1 = \bar{\mathbf{u}}_1(\mathbf{x})$ in the boundary value problem. In this case, the inhomogeneity of W_1 can be expressed explicitly with respect to points $\mathbf{x}_1 \in \mathbf{R}_1^+$ and the linear momentum equation for phase 2 would have the same form as (2.10.1), with (2.10.2), except that all quantities would have a 1 subscript and the inertial terms would, of course, be equal to zero. It is also probably much more convenient to solve for $\mathbf{u}_1 = \hat{\mathbf{u}}_1(\mathbf{x}_1)$ instead of $\mathbf{u}_1 = \bar{\mathbf{u}}_1(\mathbf{x})$ in the boundary value problem for the quasi-static case. This type of process will be discussed in the next section.

2.11 A Quasi-Static Process

In this section, a special type of process will be considered. This type of process will be referred to as a quasi-static process, even though it does not conform to the exact definition of such a process. For the process under consideration, $\mathbf{a} = \mathbf{0}$ in Equation (2.4.8)₁, $\bar{\mathbf{a}}_1 = \mathbf{0}$ in Equation (2.4.9)₁, the kinematic jump condition (2.3.3) is considered to be trivially satisfied (and therefore not part of the boundary value problem), and the linear momentum jump condition reduces to

$$\left(\left(\tilde{J}\sigma_{1}\tilde{\mathbf{F}}^{-\mathbf{T}}\right)^{+}-\sigma^{-}\right)\mathbf{N}=\mathbf{0},\tag{2.11.1}$$

which is equivalent to the continuity of tractions across the interface. All of the other field equations and jump conditions in Sections 2.3 and 2.4 remain the same, and condition (2.9.4) is still required.²⁸ Using (2.3.4) and (2.11.1), it can be shown that

²⁸ See [2] for a more extensive discussion about this type of process.

the driving traction for such a process can be written as

$$f = \left(\tilde{J}^+ W_1^+ - W^-\right) - \boldsymbol{\sigma}^- \cdot \left(\mathbf{F}_1^+ \tilde{\mathbf{F}}^+ - \mathbf{F}^-\right). \tag{2.11.2}$$

For this type of process, the only equation in the boundary value problem containing a nonzero time derivative is the kinetic relation with a nonzero V_n . Such a process corresponds to a process where $|V| \ll 1$, and the acceleration of the phase boundary is negligible, for all $t \in \Gamma$. We note that this type of process is not a true quasi-static process because time is not just a parameter in *all* quantities, and consequently the set of all solutions as time is varied does not consist of only static equilibrium solutions. Static equilibrium occurs only when V = 0.

2.12 Thermomechanical Processes

In this section, a brief discussion is given about the continuum model which uses multiple reference configurations for a process involving heat conduction and a nonuniform, nonconstant temperature distribution, and for the case where both phase 1 and phase 2 have thermoelastic constitutive behavior. For this type of process, in addition to the field equations for the balance of mass, linear momentum, and angular momentum given by (2.1.1)-(2.1.3), respectively, we also have the balance of energy equation and the rate of entropy production inequality; i.e., the first and second laws of thermodynamics.

The balance of mass, linear momentum, and angular momentum for phase 1 with respect to ${\rm R}^-$ are given in Section 2.4. The balance of energy and the rate of entropy production for this phase can be expressed with respect to ${\rm R}^-$ as

$$\int_{\partial D^{-}} \sigma \mathbf{n} \cdot \mathbf{v} dA + \int_{D^{-}} \mathbf{f} \cdot \mathbf{v} dV + \int_{\partial D^{-}} \mathbf{q} \cdot \mathbf{n} dA + \int_{D^{-}} r dV$$

$$= \frac{d}{dt} \int_{D^{-}} \varepsilon dV + \frac{d}{dt} \int_{D^{-}} \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} dV,$$
(2.12.1)

$$\frac{d}{dt} \int_{D^{-}} \eta dV - \int_{\partial D^{-}} \frac{1}{\theta} (\mathbf{q} \cdot \mathbf{n}) dA - \int_{D^{-}} \frac{r}{\theta} dV \ge 0, \qquad (2.12.2)$$

respectively, $\forall D^- \subset R^-$ and $\forall t \in \Gamma$, where $\mathbf{q}(\mathbf{x},t)$ is the heat flux vector for phase 1 per unit area of R^- , $r(\mathbf{x},t)$ is the heat source per unit volume of R^- , $\varepsilon(\mathbf{x},t)$ is the internal energy of phase 1 per unit volume of R^- , $\eta(\mathbf{x},t)$ is the entropy of phase 1 per unit volume of R^- , and $\theta(\mathbf{x},t)$ is the temperature field for phase 1. We can also define the Helmholtz free energy for phase 1 as

$$\psi(\mathbf{x},t) = \varepsilon(\mathbf{x},t) - \theta(\mathbf{x},t)\eta(\mathbf{x},t), \tag{2.12.3}$$

and the Gibbs free energy as

$$g(\mathbf{x},t) = \psi(\mathbf{x},t) - \sigma_1(\mathbf{x},t) \cdot \mathbf{F}(\mathbf{x},t). \tag{2.12.4}$$

The balance of mass, linear momentum, and angular momentum for phase 2 with respect to R_1^+ are given in Section 2.4. The balance of energy and the rate of entropy production for this phase can be expressed with respect to R_1^+ as

$$\int_{\partial D_{1}^{+}} \boldsymbol{\sigma}_{1} \mathbf{n}_{1} \cdot \bar{\mathbf{v}}_{1} dA + \int_{D_{1}^{+}} \mathbf{f}_{1} \cdot \bar{\mathbf{v}}_{1} dV + \int_{\partial D_{1}^{+}} \mathbf{q}_{1} \cdot \mathbf{n}_{1} dA + \int_{D_{1}^{+}} r_{1} dV$$

$$= \frac{d}{dt} \int_{D_{1}^{+}} \varepsilon_{1} dV + \frac{d}{dt} \int_{D_{1}^{+}} \frac{1}{2} \bar{\rho}_{1} \bar{\mathbf{v}}_{1} \cdot \bar{\mathbf{v}}_{1} dV,$$
(2.12.5)

$$\frac{d}{dt} \int_{D_1^+} \eta_1 dV - \int_{\partial D_1^+} \frac{1}{\theta_1} (\mathbf{q_1} \cdot \mathbf{n_1}) dA - \int_{D_1^+} \frac{r_1}{\theta_1} dV \ge 0, \qquad (2.12.6)$$

respectively, $\forall D_1^+ \subset R_1^+$ and $\forall t \in \Gamma$, where $\mathbf{q}_1(\mathbf{x}_1,t)$ is the heat flux vector for phase 2 per unit area of R_1^+ , $r_1(\mathbf{x}_1,t)$ is the heat source per unit volume of R_1^+ , $\varepsilon_1(\mathbf{x}_1,t)$ is the internal energy of phase 2 per unit volume of R_1^+ , $\eta_1(\mathbf{x}_1,t)$ is the entropy of phase 2 per unit volume of R_1^+ , and $\theta_1(\mathbf{x}_1,t)$ is the temperature field for phase 2. We can also define the Helmholtz free energy for phase 2 as

$$\psi_1(\mathbf{x}_1, t) = \varepsilon_1(\mathbf{x}_1, t) - \theta_1(\mathbf{x}_1, t)\eta_1(\mathbf{x}_1, t), \qquad (2.12.7)$$

and the Gibbs free energy as

$$g_1(\mathbf{x}_1, t) = \psi_1(\mathbf{x}_1, t) - \sigma_1(\mathbf{x}_1, t) \cdot \mathbf{F}_1(\mathbf{x}_1, t).$$
 (2.12.8)

Localizing Equations (2.12.1) and (2.12.2) yields

$$\sigma \cdot \dot{\mathbf{F}} + \operatorname{div}\mathbf{q} + r = \dot{\varepsilon},$$

$$\operatorname{div}(\mathbf{q}/\theta) + \frac{r}{\theta} \le \dot{\eta},\tag{2.12.9}$$

respectively, $\forall \mathbf{x} \in \mathbf{R}^-$ at each $t \in \Gamma$, where $\dot{\mathbf{F}}(\mathbf{x}, t) = \frac{\partial}{\partial t} \mathbf{F}(\mathbf{x}, t)$, $\dot{\varepsilon}(\mathbf{x}, t) = \frac{\partial}{\partial t} \varepsilon(\mathbf{x}, t)$, and $\dot{\eta}(\mathbf{x}, t) = \frac{\partial}{\partial t} \eta(\mathbf{x}, t)$. Note that $(2.4.8)_1$ was used to obtain $(2.12.9)_1$.

We next require that $\tilde{\mathbf{x}}_1$ have the form given by (2.6.6). In this case, localizing Equations (2.12.5) and (2.12.6) yields

$$\sigma_{1} \cdot \dot{\mathbf{F}}_{1} + \operatorname{div}_{1} \mathbf{q}_{1} + r_{1} = \dot{\varepsilon}_{1},$$

$$\operatorname{div}_{1}(\mathbf{q}_{1}/\theta_{1}) + \frac{r_{1}}{\theta_{1}} \leq \dot{\eta}_{1},$$

$$(2.12.10)$$

respectively, $\forall \mathbf{x}_1 \in \mathbf{R}_1^+$ at each $t \in \Gamma$, where $\dot{\mathbf{F}}_1(\mathbf{x}_1,t) = \left[\frac{\partial}{\partial t}\mathbf{F}_1(\tilde{\mathbf{x}}_1(\mathbf{x},t),t)\right]_{\tilde{\mathbf{x}}(\mathbf{x}_1,t)}$, $\dot{\varepsilon}_1(\mathbf{x}_1,t) = \left[\frac{\partial}{\partial t}\varepsilon_1(\tilde{\mathbf{x}}_1(\mathbf{x},t),t)\right]_{\tilde{\mathbf{x}}(\mathbf{x}_1,t)}$, and $\dot{\eta}_1(\mathbf{x}_1,t) = \left[\frac{\partial}{\partial t}\eta_1(\tilde{\mathbf{x}}_1(\mathbf{x},t),t)\right]_{\tilde{\mathbf{x}}(\mathbf{x}_1,t)}$. Note that $(2.4.9)_1$ was used to obtain $(2.12.10)_1$.

For points on the phase boundary, the kinematic jump conditions given by (2.3.1), or (2.3.2) and (2.3.3), and the linear momentum jump condition given by (2.4.10) must be satisfied at each $t \in \Gamma$. We also require that the temperature be continuous at all points on the phase boundary; i.e., we require

$$\theta^{-}(\mathbf{x},t) = \theta_{1}^{+}(\tilde{\mathbf{x}}_{1}(\mathbf{x},t),t) \tag{2.12.11}$$

 $\forall x \in S$ at each $t \in \Gamma$. For subregions of the body containing a portion of the phase boundary, the global forms of the balance of energy and the rate of entropy production can be expressed with respect to R in terms of the field quantities defined on R^- and R_1^+ . These equations can then be localized at points on S, and the resulting equations can be manipulated to yield

$$\theta\left(\left(\tilde{J}\eta_{1}\right)^{+}-\eta^{-}\right)V_{n}=-fV_{n}-\left(\left(\tilde{J}\tilde{\mathbf{F}}^{-1}\mathbf{q}_{1}\right)^{+}-\mathbf{q}^{-}\right),\tag{2.12.12}$$

$$fV_{\rm n} \geq 0$$
,

respectively, $\forall x \in S$ at each $t \in \Gamma$, where

$$f = \left(\tilde{J}^{+}\psi_{1}^{+} - \psi^{-}\right) - \frac{1}{2}\left(\left(\tilde{J}\boldsymbol{\sigma}_{1}\tilde{\mathbf{F}}^{-T}\right)^{+} + \boldsymbol{\sigma}^{-}\right) \cdot \left(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-}\right)$$
(2.12.13)

represents the driving traction for a thermomechanical process.²⁹ Also, note that $(2.12.12)_2$ has the same form as the requirement (2.9.4) for a purely mechanical process. In fact, $(2.12.12)_2$ reduces to (2.9.4) for such a process.

For the case where phase 1 of the material under consideration behaves thermoelastically, we assume that its Helmholtz free energy potential has the form

$$\psi = \psi(\mathbf{F}, \theta, \mathbf{x}), \tag{2.12.14}$$

and is such that the nominal stress tensor and entropy for phase 1 are given by

$$\sigma(\mathbf{x}, t) = \psi_{\mathbf{F}}(\mathbf{F}(\mathbf{x}, t), \theta(\mathbf{x}, t), \mathbf{x}),$$

$$\eta(\mathbf{x}, t) = -\psi_{\theta}(\mathbf{F}(\mathbf{x}, t), \theta(\mathbf{x}, t), \mathbf{x}),$$
(2.12.15)

respectively, $\forall x \in \mathbb{R}^-$ at each $t \in \Gamma^{30}$ Additionally, for this type of constitutive behavior, we assume that the heat flux vector for phase 1 has the form

$$\mathbf{q}(\mathbf{x},t) = \hat{\mathbf{q}}(\mathbf{F}(\mathbf{x},t), \nabla \theta(\mathbf{x},t), \theta(\mathbf{x},t), \mathbf{x}), \tag{2.12.16}$$

 $\forall \mathbf{x} \in \mathbf{R}^- \text{ at each } t \in \Gamma.$

For the case where phase 2 of the material under consideration behaves thermoelastically, we can assume that its Helmholtz free energy potential has the form

$$\psi_1 = \psi_1(\mathbf{F}_1, \theta_1, \tilde{\mathbf{x}}(\mathbf{x}_1, t)), \tag{2.12.17}$$

²⁹ See [2] for the forms of the field equations and jump conditions that were presented in this section that correspond to a continuum model that uses a single elastic potential and uses only one reference configuration.

³⁰ Usually, there will also be restrictions on the domains of **F** and θ .

and is such that the stress tensor and entropy for phase 2 are given by

$$\sigma_{1}(\mathbf{x}_{1},t) = \psi_{1_{\mathbf{F}_{1}}}(\mathbf{F}_{1}(\mathbf{x}_{1},t),\theta_{1}(\mathbf{x}_{1},t),\tilde{\mathbf{x}}(\mathbf{x}_{1},t)),$$

$$\eta_{1}(\mathbf{x}_{1},t) = -\psi_{1_{\theta_{1}}}(\mathbf{F}_{1}(\mathbf{x}_{1},t),\theta_{1}(\mathbf{x}_{1},t),\tilde{\mathbf{x}}(\mathbf{x}_{1},t)),$$
(2.12.18)

respectively, $\forall \mathbf{x}_1 \in \mathbf{R}_1^+$ at each $t \in \Gamma^{31}$ Additionally, for this type of constitutive behavior, we can assume that the heat flux vector for phase 2 has the form

$$\mathbf{q}_{1}(\mathbf{x}_{1},t) = \hat{\mathbf{q}}_{1}(\mathbf{F}_{1}(\mathbf{x}_{1},t), \nabla_{1}\theta_{1}(\mathbf{x}_{1},t), \theta_{1}(\mathbf{x}_{1},t), \tilde{\mathbf{x}}(\mathbf{x}_{1},t)), \tag{2.12.19}$$

 $\forall \mathbf{x_1} \in \mathbf{R_1^+} \text{ at each } t \in \Gamma^{32}$

For the thermoelastic material under consideration, we can also postulate a kinetic relation of the form

$$V_{\rm n} = \Phi(f, \theta, \mathbf{x}), \tag{2.12.20}$$

 $\forall \mathbf{x} \in S \text{ at each } t \in \Gamma \text{ (see [2])}.$

³¹ Usually, there will also be restrictions on the domains of $\mathbf{F_1}$ and θ_1 .

³² The functional dependencies of the constitutive relations for a thermoelastic material defined with respect to a single reference configuration are well known and can be found, e.g., in [15].

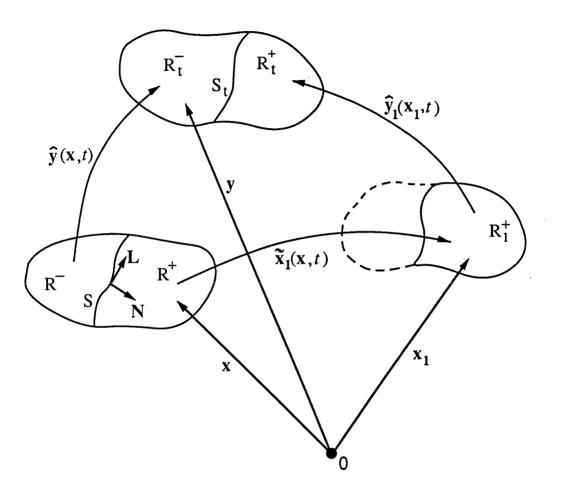


Figure 2.1. The two reference configurations and the deformed body at time $t \in \Gamma$.

CHAPTER 3

THE LINEARIZED PROBLEM

In this chapter, the linearized forms of the field equations and jump conditions for a purely mechanical process are presented and discussed. Some linear problems are then studied. In particular, the issue of which variant of martensite is preferred during the growth process, when a boundary traction is applied, is considered, and a two-phase material subjected to a uniform hydrostatic pressure is studied.

3.1 The Linearized Boundary Value Problem

One of the main advantages of working with multiple reference configurations where the field quantities and equations for each phase are expressed with respect to the reference configuration corresponding to an unstressed, undeformed state of that phase is that the field quantities and equations are in forms that permit direct linearization.¹ This is the case since the displacements for each phase are measured from the reference configuration for that phase, and consequently, for the appropriate boundary and initial conditions, the displacement gradients can be considered infinitesimal.² Another advantage of using multiple reference configurations in this manner is that for the linear case the nominal stress for each phase is approximately equal to the true stress for that phase.³ This is very convenient for solving certain

¹ It is also assumed here that the unstressed, undeformed configuration of each phase corresponds to a local minimum of the elastic potential for that phase.

² Note that if a different potential for each phase is used, where all of the potentials and the field equations for each phase are expressed with respect to the same fixed reference configuration corresponding to the undeformed austenite, the field equations for the martensites are not in forms that permit direct linearization, since the displacements from that reference configuration are not such that their gradients can be considered infinitesimal. In this case, one must at least make a transformation such that the differential equations and jump conditions are in terms of the displacements from the unstressed state of each phase.

³ Note that this is not the case if a different potential for each phase is used and all of the field quantities are with respect to the same fixed reference configuration.

types of boundary value problems, as will become more apparent in Sections 3.2 and 3.3, where several of these types of problems are considered. Also, we note that when using this continuum model, linearizing the field equations for each phase in no way restricts the magnitude or form of the shape deformation for that phase, since the displacements for that phase are measured from this shape deformation.

3.1.1 The Linearized Field Equations

In the following, a purely mechanical process occurring in a time interval $\Gamma = [t_0, t_1]$ is considered. The two-phase body described in Section 2.3 is considered, and the corresponding notation in Chapter 2 will be used. It is assumed that R^- corresponds to an unstressed, undeformed configuration of phase 1 and that R_1^+ corresponds to an unstressed, undeformed configuration of phase 2. It is assumed that both phase 1 and phase 2 have elastic constitutive behavior with $\tilde{\mathbf{x}}_1$ having the form given by (2.6.6). It is further assumed that the undeformed configurations of phase 1 and phase 2 correspond to local minima of their respective elastic potentials.

For the linear problem, we assume that $|\nabla \hat{\mathbf{u}}| \ll 1 \ \forall \mathbf{x} \in \mathbb{R}^-$ and $|\nabla \hat{\mathbf{u}}_1| \ll 1 \ \forall \mathbf{x}_1 \in \mathbb{R}_1^+$ at each $t \in \Gamma$. In this case, we have for phase 1

$$egin{align} W &= W^* + rac{1}{2}
abla \hat{\mathbf{u}} \cdot (\mathbf{C}
abla \hat{\mathbf{u}}) + \mathrm{O}ig(|
abla \hat{\mathbf{u}}|^3ig) \ &= W^* + rac{1}{2} \, oldsymbol{arepsilon} \cdot (\mathbf{C} \, oldsymbol{arepsilon}) + \mathrm{O}ig(|\, oldsymbol{arepsilon}\,|^3ig), \end{split}$$

$$\sigma = \mathbf{C}\nabla\hat{\mathbf{u}} + O(|\nabla\hat{\mathbf{u}}|^2)$$

$$= \mathbf{C}\varepsilon + O(|\varepsilon|^2),$$
(3.1.1)

$$\tau(\hat{\mathbf{y}}(\mathbf{x},t),t) = \sigma(\mathbf{x},t) + O(|\nabla \hat{\mathbf{u}}|^2),$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{T}} + \mathrm{O}(|\nabla \hat{\mathbf{u}}|^2),$$

 $\forall \mathbf{x} \in \mathbf{R}^-$ at each $t \in \Gamma$, where $\varepsilon = \frac{1}{2} \left(\nabla \hat{\mathbf{u}} + (\nabla \hat{\mathbf{u}})^{\mathrm{T}} \right)$ is the infinitesimal strain tensor for phase 1, $W^*(\mathbf{x}) = W(\mathbf{1}, \mathbf{x})$, and $\mathbf{C}(\mathbf{x})$ with $C_{ijkl} = \frac{\partial^2 W}{\partial F_{ij} \partial F_{kl}} \Big|_{\mathbf{F}=\mathbf{1}}$ is the elasticity four-tensor for phase 1.⁴ For phase 2, we have

$$W_{1} = W_{1}^{*} + \frac{1}{2} \nabla_{1} \hat{\mathbf{u}}_{1} \cdot (\mathbf{C}_{1} \nabla_{1} \hat{\mathbf{u}}_{1}) + \mathcal{O}(|\nabla_{1} \hat{\mathbf{u}}_{1}|^{3})$$
$$= W_{1}^{*} + \frac{1}{2} \varepsilon_{1} \cdot (\mathbf{C}_{1} \varepsilon_{1}) + \mathcal{O}(|\varepsilon_{1}|^{3}),$$

$$\sigma_{1} = \mathbf{C}_{1} \nabla_{1} \hat{\mathbf{u}}_{1} + \mathcal{O}(|\nabla_{1} \hat{\mathbf{u}}_{1}|^{2})$$

$$= \mathbf{C}_{1} \varepsilon_{1} + \mathcal{O}(|\varepsilon_{1}|^{2}), \tag{3.1.2}$$

$$\tau(\hat{\mathbf{y}}_1(\mathbf{x}_1,t),t) = \sigma_1(\mathbf{x}_1,t) + O(|\nabla_1 \hat{\mathbf{u}}_1|^2),$$

$$\sigma_1 = \sigma_1^{\mathrm{T}} + \mathrm{O}(|\nabla_1 \hat{\mathbf{u}}_1|^2),$$

 $\forall \ \mathbf{x_1} \in \mathbf{R_1^+}$ at each $t \in \Gamma$, where $\boldsymbol{\varepsilon_1} = \frac{1}{2} \Big(\nabla_1 \hat{\mathbf{u}}_1 + (\nabla_1 \hat{\mathbf{u}}_1)^T \Big)$ is the infinitesimal strain tensor for phase 2, $W_1^*(\tilde{\mathbf{x}}(\mathbf{x}_1,t)) = W_1(\mathbf{1},\tilde{\mathbf{x}}(\mathbf{x}_1,t))$, and $\mathbf{C_1}(\tilde{\mathbf{x}}(\mathbf{x}_1,t))$ with $C_{\mathbf{1}_{ijkl}} = \frac{\partial^2 W_1}{\partial F_{\mathbf{1}_{ij}} \partial F_{\mathbf{1}_{kl}}} \Big|_{\mathbf{F_1}=\mathbf{1}}$ is the elasticity four-tensor for phase 2. We can also express the linear elastic potential and stress tensor for phase 2 in terms of $\tilde{\mathbf{u}}_1$. In this case, Equations (3.1.2)₁ and (3.1.2)₂ become

⁴ In a given frame, the two-tensor Ab, where A is a four-tensor and b is a two-tensor, has components $(Ab)_{ij} = A_{ijkl}b_{kl}$.

$$W_{1} = W_{1}^{*} + \frac{1}{2} (\nabla \bar{\mathbf{u}}_{1} \nabla_{1} \tilde{\mathbf{x}}) \cdot [\mathbf{C}_{1} (\nabla \bar{\mathbf{u}}_{1} \nabla_{1} \tilde{\mathbf{x}})] + \mathcal{O}(|\nabla \bar{\mathbf{u}}_{1}|^{3}),$$

$$\sigma_{1} = \mathbf{C}_{1} (\nabla \bar{\mathbf{u}}_{1} \nabla_{1} \tilde{\mathbf{x}}) + \mathcal{O}(|\nabla \bar{\mathbf{u}}_{1}|^{2}),$$
(3.1.3)

respectively, $\forall \mathbf{x} \in \mathbf{R}^+$ at each $t \in \Gamma$, where $\mathbf{x_1} = \tilde{\mathbf{x}_1}(\mathbf{x}, t)$ in $\nabla_1 \tilde{\mathbf{x}}$. The elasticity tensors \mathbf{C} and $\mathbf{C_1}$ are both four-tensors, which contain the material coefficients and reflect the material symmetry of phase 1 and phase 2, respectively. Additionally, both \mathbf{C} and $\mathbf{C_1}$ are positive definite, since it has been assumed that the undeformed configuration of each phase corresponds to a relative minimum of the elastic potential for that phase. These four-tensors also have the usual major and minor symmetries.

In a given coordinate frame, substituting $(3.1.1)_2$ into the equation representing the balance of linear momentum for phase 1 given by $(2.4.8)_1$ yields

$$\frac{\partial C_{ijkl}}{\partial x_j} \frac{\partial \hat{u}_k}{\partial x_l} + C_{ijkl} \frac{\partial^2 \hat{u}_k}{\partial x_l \partial x_j} + f_i = \rho \frac{\partial^2 \hat{u}_i}{\partial t^2}, \qquad (3.1.4)$$

 $\forall \mathbf{x} \in \mathbb{R}^-$ at each $t \in \Gamma$. Substituting (3.1.3)₂ into the equation representing the balance of linear momentum for phase 2 given by (2.4.9)₁ yields

$$\frac{\partial C_{\mathbf{1}_{ijkl}}}{\partial x_{n}} \left[\frac{\partial \tilde{x}_{n}}{\partial x_{\mathbf{1}_{j}}} \right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}^{\underline{\partial u_{\mathbf{1}_{k}}}} \left[\frac{\partial \tilde{x}_{m}}{\partial x_{\mathbf{1}_{l}}} \right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}^{\underline{\partial u_{\mathbf{1}_{k}}}} \left[\frac{\partial \tilde{x}_{m}}{\partial x_{\mathbf{1}_{l}}} \frac{\partial \tilde{x}_{m}}{\partial x_{\mathbf{1}_{l}}} \right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}^{\underline{\partial u_{\mathbf{1}_{k}}}} + \frac{\partial \bar{u}_{\mathbf{1}_{k}}}{\partial x_{\mathbf{1}_{l}}} \left[\frac{\partial^{2} \tilde{x}_{m}}{\partial x_{\mathbf{1}_{l}} \partial x_{\mathbf{1}_{l}}} \right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}^{\underline{\partial u_{\mathbf{1}_{k}}}} + \left[f_{\mathbf{1}_{i}} \right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}^{\underline{\partial u_{\mathbf{1}_{k}}}} + \left[f_{\mathbf{1}_{i}} \right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}^{\underline{\partial u_{\mathbf{1}_{k}}}} \right] + \left[f_{\mathbf{1}_{i}} \right]_{\tilde{\mathbf{x}}_{\mathbf{1}}(\mathbf{x},t)}^{\underline{\partial u_{\mathbf{1}_{k}}}} + \frac{\partial^{2} \bar{u}_{\mathbf{1}_{k}}}{\partial t^{2}} \right], \tag{3.1.5}$$

 $\forall \mathbf{x} \in \mathbb{R}^+$ at each $t \in \Gamma$. For the important special case where $\tilde{\mathbf{x}}_1$ is a homogeneous deformation, phase 2 is a homogeneous material (i.e., \mathbf{C}_1 is independent of \mathbf{x}), and

 $f_1 = 0$, Equation (3.1.5) given above reduces to

$$C_{\mathbf{1}_{ijkl}} \frac{\partial^2 \bar{u}_{\mathbf{1}_k}}{\partial x_m \partial x_n} \frac{\partial \tilde{x}_m}{\partial x_{\mathbf{1}_l}} \frac{\partial \tilde{x}_n}{\partial x_{\mathbf{1}_i}} = \frac{\rho}{\tilde{J}} \left(\frac{\partial^2 \tilde{x}_{\mathbf{1}_i}}{\partial t^2} + \frac{\partial^2 \bar{u}_{\mathbf{1}_i}}{\partial t^2} \right), \tag{3.1.6}$$

where $\mathbf{x}_1 = \tilde{\mathbf{x}}_1(\mathbf{x}, t)$ in $\nabla_1 \tilde{\mathbf{x}}$.

For the static problem, points in R_1^+ are stationary, and it is probably much more convenient to work in terms of $\mathbf{u}_1 = \hat{\mathbf{u}}_1(\mathbf{x}_1)$ instead of $\mathbf{u}_1 = \bar{\mathbf{u}}_1(\mathbf{x})$ for phase 2. In this case the inhomogeneity of W_1 can be expressed explicitly in terms of points $\mathbf{x}_1 \in R_1^+$, and the equation representing the balance of linear momentum for phase 2 would have the same form as the equation representing the balance of linear momentum for phase 1 given by (3.1.4), except that all of the quantities would have 1 subscripts and the inertial terms would, of course, be equal to zero.

For the linear problem where it is assumed that $|\nabla \hat{\mathbf{u}}| \ll 1 \ \forall \ \mathbf{x} \in \mathbb{R}^-$ and $|\nabla \hat{\mathbf{u}}_1| \ll 1 \ \forall \ \mathbf{x}_1 \in \mathbb{R}^+_1$ at each $t \in \Gamma$, we define a quasi-static process as a process where the first and second time derivatives of $\hat{\mathbf{u}}$ and $\bar{\mathbf{u}}_1$ are negligible $\forall \ \mathbf{x} \in \mathbb{R}^-$ and $\forall \ \mathbf{x} \in \mathbb{R}^+$, respectively, $|\mathbf{V}| \ll 1$, and $d\mathbf{V}/dt$ is negligible, for all $t \in \Gamma$. Such a process corresponds to a process where the strains of each phase are infinitesimal, the motions of each particle of each phase relative to the undeformed configuration of that phase are negligible, the magnitude of the phase boundary velocity is infinitesimal, and the acceleration of the phase boundary is negligible, for all $t \in \Gamma$. For this type of process, it is probably much more convenient to solve for $\mathbf{u}_1 = \hat{\mathbf{u}}_1(\mathbf{x}_1)$ instead of $\mathbf{u}_1 = \bar{\mathbf{u}}_1(\mathbf{x})$ in the boundary value problem. However, unlike the static problem, points in \mathbb{R}_1^+ are moving. Therefore, the inhomogeneity of W_1

⁵ Note that such a process is not a true quasi-static process since time is not just a parameter in *all* variables of the problem, and consequently, the set of all solutions as time is varied does not consist of only static equilibrium solutions.

still needs to be expressed with respect to points $\mathbf{x} \in \mathbf{R}^+$ (see Section 2.6). Thus, for a quasi-static process the balance of linear momentum for phase 2 would have the same form as it would have for the static case, except that $\partial C_{\mathbf{1}_{ijkl}}/\partial x_{\mathbf{1}_{j}}$ would be replaced by $\left(\partial C_{\mathbf{1}_{ijkl}}/\partial x_{n}\right)\left(\partial \tilde{x}_{n}/\partial x_{\mathbf{1}_{j}}\right)$.

3.1.2 The Linearized Jump Conditions

As was partially discussed in Section 2.3, at each point $x \in S$, at each $t \in \Gamma$, the displacements are required to be continuous, and we therefore have

$$\hat{\mathbf{y}}_{1}^{+}(\tilde{\mathbf{x}}_{1}(\mathbf{x},t),t) = \hat{\mathbf{y}}^{-}(\mathbf{x},t), \tag{3.1.7}$$

where $\hat{\mathbf{y}}_1(\tilde{\mathbf{x}}_1(\mathbf{x},t),t) = \tilde{\mathbf{x}}_1(\mathbf{x},t) + \bar{\mathbf{u}}_1(\mathbf{x},t)$ and $\hat{\mathbf{y}}(\mathbf{x},t) = \mathbf{x} + \hat{\mathbf{u}}(\mathbf{x},t)$. If we work with the continuity-of-displacements condition in this form, there is nothing to linearize. However, the jump conditions

$$(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-})\mathbf{L} = \mathbf{0},$$

$$\mathbf{\bar{v}}_{1}^{+} - \mathbf{v}^{-} + (\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-})\mathbf{V} = \mathbf{0},$$

$$(3.1.8)$$

which together represent the continuity of displacements,⁶ are such that they or equations equivalent to them can be linearized. In particular, as was mentioned in Section 2.3, Equation (3.1.8)₁ is equivalent to

$$\mathbf{F}_{\mathbf{1}}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-} = \hat{\mathbf{a}} \otimes \mathbf{N}. \tag{3.1.9}^{7}$$

Since both $\hat{\mathbf{a}}$ and \mathbf{N} are real quantities, we can conclude that the two-tensor $\hat{\mathbf{a}} \otimes \mathbf{N}$, and hence $\mathbf{F}_1^+\tilde{\mathbf{F}}^+ - \mathbf{F}^-$, has two zero eigenvalues and one real not necessarily zero eigenvalue.⁸ Thus, we can write the characteristic equation for $\mathbf{F}_1^+\tilde{\mathbf{F}}^+ - \mathbf{F}^-$ as

$$-\lambda^3 + I_1\lambda^2 - I_2\lambda + I_3 = 0, (3.1.10)$$

⁶ These two equations can be used in place of (3.1.7) in the boundary value problem.

⁷ This equation can be used in place of (3.1.8)₁ in the boundary value problem.

⁸ This can easily be seen by working in the coordinate frame where either N or a coincides with a basis vector.

where

$$I_{1} = \operatorname{tr}\left(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-}\right),$$

$$I_{2} = \frac{1}{2}\left\{\left[\operatorname{tr}\left(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-}\right)\right]^{2} - \operatorname{tr}\left(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-}\right)^{2}\right\},$$

$$I_{3} = \operatorname{det}\left(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-}\right),$$
(3.1.11)

and

$$\mathbf{F}_{1}^{+}\mathbf{\tilde{F}}^{+} - \mathbf{F}^{-} = (\nabla \tilde{\mathbf{u}}_{1})^{+} + (\nabla \bar{\mathbf{u}}_{1} \nabla_{1} \tilde{\mathbf{x}} \nabla \tilde{\mathbf{u}}_{1})^{+} + (\nabla \bar{\mathbf{u}}_{1} \nabla_{1} \tilde{\mathbf{x}})^{+} - (\nabla \hat{\mathbf{u}})^{-}.$$
(3.1.12)

A necessary condition for the existence of two zero eigenvalues of ${\bf F_1^+ \tilde F^+ - F^-}$ is that

$$I_2 = 0, I_3 = 0. (3.1.13)$$

Equations (3.1.13) can both be linearized with respect to $\nabla \mathbf{u}$ and $\nabla \bar{\mathbf{u}}_1$. The set of all vectors \mathbf{L} that satisfy (3.1.8)₁ can then be determined.

As was discussed in Section 2.4, the linear momentum jump condition is

$$\left(\left(\tilde{J} \, \boldsymbol{\sigma}_1 \tilde{\mathbf{F}}^{-T} \right)^+ - \boldsymbol{\sigma}^- \right) \mathbf{N} + \rho (\bar{\mathbf{v}}_1^+ - \mathbf{v}^-) V_n = \mathbf{0}, \tag{3.1.14}$$

which must hold $\forall \mathbf{x} \in S$ at each $t \in \Gamma$, where $\mathbf{x}_1 = \tilde{\mathbf{x}}_1(\mathbf{x}, t)$ in σ_1^+ and $\bar{\mathbf{v}}_1^+$. Once the set of all $\mathbf{L}(\mathbf{x}, t)$ is obtained from $(3.1.8)_1$, $\mathbf{N}(\mathbf{x}, t)$ can be determined such that $\mathbf{N} \cdot \mathbf{L} = 0 \ \forall \mathbf{x} \in S$ at each $t \in \Gamma$. N can then be substituted into (3.1.14), yielding three scalar equations, which can be linearized with respect to $\nabla \mathbf{u}$ and $\nabla \bar{\mathbf{u}}$.

Consider the path of the phase boundary during a motion in the time interval Γ . Next consider the special case where we assume that at each location of the phase boundary in this path there is continuity of displacements at all points on the phase boundary for $\hat{\mathbf{u}} = \mathbf{0} \ \forall \ \mathbf{x} \in \mathbb{R}^-$ and $\hat{\mathbf{u}}_1 = \mathbf{0} \ \forall \ \mathbf{x}_1 \in \mathbb{R}_1^+$. In this case, as discussed in Section 2.7, $\tilde{\mathbf{F}}^+$ must have the form

$$\tilde{\mathbf{F}}^+ = \mathbf{1} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}},\tag{3.1.15}$$

at each point on the phase boundary at each $t \in \Gamma$, where $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{n}}$ may both be functions of $\mathbf{x} \in S$. In this case, we can conclude from substituting (3.1.15) into (3.1.8)₁ that the first-order approximation of \mathbf{L} is $\tilde{\mathbf{L}}$, where $\tilde{\mathbf{L}} \cdot \tilde{\mathbf{n}} = 0$. Additionally, in this case, the first-order approximation of the linear momentum jump condition given by (3.1.14) is

$$(\boldsymbol{\sigma}_{1}^{+} - \boldsymbol{\sigma}^{-})\tilde{\mathbf{n}} + \rho(\bar{\mathbf{v}}_{1}^{+} - \mathbf{v}^{-})V_{n} = \mathbf{0}, \tag{3.1.16}$$

where σ and σ_1 are given by their respective linear constitutive relations. ¹⁰

For the static case, jump conditions (3.1.7) and $(3.1.8)_1$ are the same, jump condition $(3.1.8)_2$ is trivially satisfied, and the linear momentum jump condition given by (3.1.14) reduces to

$$\left(\left(\tilde{J}\,\boldsymbol{\sigma}_{1}\tilde{\mathbf{F}}^{-T}\right)^{+}-\boldsymbol{\sigma}^{-}\right)\mathbf{N}=\mathbf{0},\tag{3.1.17}$$

which is equivalent to the continuity of traction across the interface. For the case where $\tilde{\mathbf{F}} = \mathbf{1} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$, (3.1.17) reduces to

$$(\boldsymbol{\sigma}_1^+ - \boldsymbol{\sigma}^-)\tilde{\mathbf{n}} = \mathbf{0}. \tag{3.1.18}$$

For a quasi-static process, jump conditions (3.1.7) and $(3.1.8)_1$ are the same. However, for this type of process, the first-order approximation of jump condition $(3.1.8)_2$ is

$$\left(\frac{\partial \tilde{\mathbf{x}}_1}{\partial t}\right)^+ = -(\nabla \tilde{\mathbf{u}}_1)^+ \mathbf{V}. \tag{3.1.19}$$

⁹ This may be a good assumption for a material that has continuity of displacements at the phase boundary and is unstressed when it is in static equilibrium with no applied boundary tractions.

¹⁰ Note, however, that because all the jump conditions are evaluated at points on phase boundary and the location of the phase boundary is part of the solution of the boundary value problem, the jump conditions are inherently nonlinear with respect to the variables representing the location of the phase boundary. For the static or quasi-static case, however, this does not present any difficulties.

If the displacements are to be continuous at the phase boundary for all $t \in \Gamma$ with respect to a first-order approximation, the mapping $\tilde{\mathbf{x}}_1$ should be chosen such that (3.1.19) is satisfied. For the case where the shape deformation is a homogeneous invariant plane strain for all $t \in \Gamma$, $\tilde{\mathbf{x}}_1$ must have the following form in order for (3.1.19) to be satisfied at each $t \in \Gamma$:

$$\tilde{\mathbf{x}}_{1}(\mathbf{x},t) = \mathbf{x} + ([\mathbf{x} - \bar{\mathbf{x}}(t)] \cdot \tilde{\mathbf{n}})\tilde{\mathbf{a}}, \qquad (3.1.20)$$

where $\bar{\mathbf{x}}(t)$ is any point on the interface S (see Section 2.7). Also, for a quasi-static process, the first-order approximation of the linear momentum jump condition is the same as that for the static case.

For the static or quasi-static case, when $\hat{\mathbf{u}}_1(\mathbf{x}_1)$ is being solved for instead of $\bar{\mathbf{u}}_1(\mathbf{x})$, the jump conditions would have the same form as described above, with the exception that $\nabla \bar{\mathbf{u}}_1 \nabla_1 \tilde{\mathbf{x}}$ would be replaced by $\nabla_1 \hat{\mathbf{u}}_1$. Consequently, $\mathbf{F}_1^+ \tilde{\mathbf{F}}^+ - \mathbf{F}^-$ in Equations (3.1.8)₁, (3.1.9)-(3.1.11), and (3.1.13) becomes

$$\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}^{+} - \mathbf{F}^{-} = (\nabla \tilde{\mathbf{u}}_{1})^{+} + (\nabla_{1}\hat{\mathbf{u}}_{1}\nabla \tilde{\mathbf{u}}_{1})^{+} + (\nabla_{1}\hat{\mathbf{u}}_{1})^{+} - (\nabla \hat{\mathbf{u}})^{-}, \tag{3.1.21}$$

where $\mathbf{x}_1 = \mathbf{\tilde{x}}_1(\mathbf{x}, t)$ in $\nabla_1 \mathbf{\hat{u}}_1$.¹¹

3.1.3 The Linearized Driving Traction and Kinetic Relation

The driving traction acting on the phase boundary was presented and discussed in Section 2.9. For the linear case where we assume that $\tilde{\mathbf{F}}$ has the form $\tilde{\mathbf{F}} = \mathbf{1} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$, at each point on the phase boundary at each $t \in \Gamma$, the driving traction given by (2.9.2) becomes

$$f = \left(\left(\tilde{J} W_{\mathbf{1}}^* \right)^+ - (W^*)^- \right) - \frac{1}{2} \left[\left(\boldsymbol{\sigma}_{\mathbf{1}}^+ + \boldsymbol{\sigma}^- \right) \tilde{\mathbf{n}} \right] \cdot \tilde{\mathbf{a}} + \mathcal{O} \left(|\nabla \hat{\mathbf{u}}|^2, |\nabla \bar{\mathbf{u}}_{\mathbf{1}}|^2 \right). \quad (3.1.22)$$

¹¹ Note that for the static case, $\tilde{\mathbf{x}}_1$ in (3.1.21) is independent of time. However, for the quasi-static case, the phase boundary velocity is assumed to be nonzero, and consequently, $\tilde{\mathbf{x}}_1$ is a function of time in (3.1.21).

The driving traction for the quasi-static case is given by (2.11.2). For the linear case and when $\tilde{\mathbf{F}} = \mathbf{1} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$, this driving traction becomes

$$f = \left(\left(\tilde{J} W_{\mathbf{1}}^* \right)^+ - \left(W^* \right)^- \right) - \left(\boldsymbol{\sigma}^- \tilde{\mathbf{n}} \right) \cdot \tilde{\mathbf{a}} + \mathcal{O}\left(|\nabla \hat{\mathbf{u}}|^2, |\nabla_{\mathbf{1}} \hat{\mathbf{u}}_{\mathbf{1}}|^2 \right). \tag{3.1.23}$$

The implications of this form of the driving traction for the quasi-static case will be discussed further in Section 3.2.

In Section 2.9, it was mentioned that a kinetic relation

$$V_n = \Phi(f, \mathbf{x}) \tag{3.1.24}$$

at points $x \in S$ can be postulated with the requirement that

$$\Phi(f, \mathbf{x})f \ge 0,\tag{3.1.25}$$

 $\forall \mathbf{x} \in S$ at each $t \in \Gamma$. This kinetic relation is a constitutive relation in the sense that Φ depends on the given material [1, 2]. Consider a kinetic relation, which is such that

$$\Phi(f) \begin{cases}
> 0, & f > f_2 \\
= 0, & \text{for } f_1 \le f \le f_2 ,\\
< 0, & f < f_1
\end{cases} \tag{3.1.26}$$

where the constants f_1 and f_2 are material-dependent and are such that $f_1 \leq 0$ and $f_2 \geq 0$.¹² We note that such a kinetic relation satisfies (3.1.25). Before presenting the linearized form of (3.1.26), we will first consider some motivation for the general form of (3.1.26).

¹² Kinetic relations of this form have been studied in [1].

As was discussed in the Introduction, for most materials, $M_{\rm s} < T_{\rm o} < A_{\rm s}$. Assume that phase 1 represents the austenite and phase 2 represents the martensite. In this case, $T_{\rm o}$ corresponds to the Gibbs free energies of both phases being equal (i.e., $g(\mathbf{1},T_{\rm o})=\tilde{J}g_{1}(\mathbf{1},T_{\rm o})$), 13 $A_{\rm s}$ corresponds to $g(\mathbf{1},A_{\rm s})<\tilde{J}g_{1}(\mathbf{1},A_{\rm s})$, and $M_{\rm s}$ corresponds to $\tilde{J}g_{1}(\mathbf{1},M_{\rm s})< g(\mathbf{1},M_{\rm s})$. Let

$$f_{A} = \tilde{J}g_{1}(\mathbf{1}, A_{s}) - g(\mathbf{1}, A_{s}),$$

$$f_{M} = \tilde{J}g_{1}(\mathbf{1}, M_{s}) - g(\mathbf{1}, M_{s}).$$
(3.1.27)

Note that $f_A > 0$ and $f_M < 0$.

For the case where each phase is unstressed in its undeformed configuration, $g(\mathbf{1},\theta)=\psi(\mathbf{1},\theta)$ and $g_1(\mathbf{1},\theta_1)=\psi_1(\mathbf{1},\theta_1)$. Thus, in this case, $\tilde{J}\psi_1(\mathbf{1},A_s)-\psi(\mathbf{1},A_s)=f_A$ and $\tilde{J}\psi_1(\mathbf{1},M_s)-\psi(\mathbf{1},M_s)=f_M$. Additionally, as was discussed in the Introduction, a thermally-induced martensitic phase transformation will not occur unless $\theta < M_s$, and this corresponds to $\tilde{J}g_1(\mathbf{1},\theta)-g(\mathbf{1},\theta)<\tilde{J}g_1(\mathbf{1},M_s)-g(\mathbf{1},M_s)$, or equivalently $\tilde{J}\psi_1(\mathbf{1},\theta)-\psi(\mathbf{1},\theta)< f_M$. Thus, for an unstressed material at a temperature $\theta < M_s$, $f' < f_M$, where f' represents the driving traction for a thermomechanical process given by (2.12.13), and this corresponds to a nonzero phase boundary velocity with $V_n < 0.^{14}$ Similarly, for an unstressed material at a temperature $\theta > A_s$, $f' > f_A$, and this corresponds to a nonzero phase boundary velocity with $V_n > 0$. Additionally, for an unstressed material at a temperature $M_s < \theta < A_s$, we have $f_M < f' < f_A$, which corresponds to a zero phase boundary velocity, since a thermally-induced martensitic phase transformation does not occur in this temperature interval.

¹³ For this comparison of the Gibbs free energies of both phases, the Gibbs free energies are considered to be with respect to the same reference configuration. Also, in the rest of this section, the spatial dependence of the potentials and kinetic relation will not be displayed in the notation.

¹⁴ Note that if phase 1 is the austenite and phase 2 is the martensite, $V_n < 0$ corresponds to a martensite phase transformation, and $V_n > 0$ corresponds to an austenite phase transformation.

For an isothermal process occurring at the temperature θ_0 , $\psi(\mathbf{F},\theta_0)=W(\mathbf{F})$ and $\psi_1(\mathbf{F_1}, \theta_0) = W_1(\mathbf{F_1})$. Thus, for an isothermal process occurring at $\theta = M_s$, $\tilde{J}W_1(1)-W(1)=f_{\mathrm{M}}$, and for an isothermal process occurring at $\theta=A_{\mathrm{s}}$, $\tilde{J}W_1(1)-W(1)=f_A$. Motivated by this, the above discussion, the fact that it takes a finite applied boundary traction to induce a martensite or austenite phase transformation for $heta > M_{\scriptscriptstyle \rm B}$ and $heta < A_{\scriptscriptstyle \rm B}$, respectively, and considering (3.1.25), one might postulate a kinetic relation of the form given by (3.1.26). Additionally, for an isothermal process occurring at $\theta = M_s$ one might choose f_1 such that $f_1 = f_M$, and for an isothermal process occurring at $\theta=A_{\mathrm{s}}$ one might choose f_2 such that $f_2=f_{\mathrm{A}}$. An example of when it might be appropriate to choose $f_1=f_2\ (=0)$ is for the case where phase 1 and phase 2 represent two different variants of the same martensite in an isothermal process at a temperature near a transformation temperature, since in this case $\tilde{J}W_1(1) = W(1)$, and it has been observed from experiments that at such a temperature, reorientation¹⁵ occurs for any nonzero applied boundary traction. More generally, f_2-f_1 might be chosen to be proportional to the difference in the free energies of phase 1 and phase 2 at the transformation temperatures.

For the linear case, the kinetic relation of the form (3.1.26) is given by

$$\Phi(f) = \begin{cases} \frac{1}{\nu_2} (f - f_2), & f > f_2 \\ 0, & \text{for } f_1 \le f \le f_2 \\ \frac{1}{\nu_1} (f - f_1), & f < f_1 \end{cases}$$
(3.1.28)

where f is the linearized driving traction, and ν_1 and ν_2 are constants that depend on the given material. We note that as ν_1 and $\nu_2 \to \infty$, $V_n \to 0$ and the phase boundary moves with the particles of material at the interface but does not pass over them, converting them from one phase to the other.

¹⁵ Refer to Sections 2.8 and 3.2 for discussions of this phenomenon.

3.2 Reorientation

As discussed in Section 2.8, the phenomenon where a boundary traction is applied, resulting in the phase boundary separating two variants of the same martensite moving and transforming one variant into the other, is known as reorientation. In a material that is fully martensitic, reorientation takes place until the material consists of only one variant of martensite, or the boundary traction is removed.¹⁶

The issue of which variant of martensite is preferred during the growth process, whether the process is reorientation or simply an austenite-martensite phase transformation where several variants of martensite nucleate at different points in the material, is an issue that has received much attention. For the case where a uniaxial tensile traction is applied, it has been observed from experiments in [14] that for 18R martensitic alloys, the variant of martensite that is preferred during the growth process is the variant that yields the largest amount of extension because of its shape deformation in the direction of the uniaxial tensile traction. The consistency of this experimental observation with a minimum energy criterion is shown and discussed in [8]. There have also been proposed criteria involving the shear traction on the interface of the martensite, ¹⁷ and criteria based on the shear stress on the plane of slip for internally slipped martensites.

Consider the quasi-static case where the shape deformation of phase 2 is a homogeneous invariant plane strain. In this case, the driving traction is a special case of the driving traction given by (3.1.23) and is as follows:

$$f = \left(\left(\tilde{J} W_{\mathbf{1}}^* \right)^+ - (W^*)^- \right) - \left(\sigma^- \tilde{\mathbf{n}} \right) \cdot \tilde{\mathbf{a}}, \tag{3.2.1}$$

¹⁶ More specifically, for a material initially consisting of many crystals of austenite, there will usually be many crystals of the same variant of the martensite, and not one crystal of one variant, since phase boundaries cannot, in general, cross grain boundaries.

¹⁷ Such a criterion is discussed, e.g., in [10].

where the second-order terms have been neglected. 18 We next assume that all of the variants of martensite of the material under consideration have the same value for their elastic potentials in their undeformed states, 19 and we assume that the material has a kinetic relation of the form (3.1.28). To consider the case of an austenite-martensite phase transformation, we let phase 1 represent the austenite and phase 2 represent a variant of martensite. From the assumptions given above, we can conclude that $(\tilde{J}W_1^*)^+ - (W^*)^-$ has the same value regardless of which variant of martensite phase 2 represents. We next note that $\sigma^{-}\tilde{\mathbf{n}}$ is the traction on the interface and that $(\sigma^-\tilde{\mathbf{n}}) \cdot \tilde{\mathbf{a}}$ is the component of this traction in the direction of the amplitude vector of the variant of martensite that phase 2 represents, multiplied by the magnitude of this amplitude vector. We also note that the variant that has the largest negative value for its driving traction will grow at the fastest rate. From the discussion above, we can conclude that this variant is the variant with the largest value of $(\sigma^-\tilde{\mathbf{n}}) \cdot \tilde{\mathbf{a}}$. Thus, for the case under consideration, we can conclude that the variant of martensite with the largest value of the component of traction on its interface in the direction of its amplitude vector multiplied by the magnitude of its amplitude vector will be the variant preferred during the growth process in a stress-induced austenite to martensite phase transformation. To consider the case of reorientation, we let phase 1 and phase 2 represent two different variants of the same martensite. From the assumptions given previously, we can conclude that $(\tilde{J}W_1^*)^+ - (W^*)^- = 0$ for every combination of variants that phase 1 and phase 2 can represent. Therefore, the variant with an amplitude vector $\tilde{\mathbf{a}}$ and an interface normal $\tilde{\mathbf{n}}$ that result in $(\boldsymbol{\sigma}^{-}\tilde{\mathbf{n}}) \cdot \tilde{\mathbf{a}}$ having the largest value will grow at the fastest rate. We note, however, that in this

¹⁸ The only difference between (3.1.23) and (3.2.1) is that $\tilde{\bf a}$ and $\tilde{\bf n}$ in (3.1.23) may be functions of $\bf x$.

¹⁹ For this comparison of the elastic potentials, they are all considered to be with respect to the same reference configuration.

case $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{n}}$ for the variant under consideration are measured with respect to the neighboring variant across the interface with normal $\tilde{\mathbf{n}}$.

Consider next a cylindrical body parallel to the unit vector $\mathbf{e_1}$. Assume that a tensile traction $\mathbf{t} = -\sigma_0 \mathbf{e_1}$ is applied at the end with unit normal $-\mathbf{e_1}$, a tensile traction $\mathbf{t} = \sigma_0 \mathbf{e_1}$ is applied at the end with unit normal $\mathbf{e_1}$, and the remaining surface of the cylindrical body is traction-free. For this case, the stress tensor

$$\boldsymbol{\tau} = \sigma_0 \mathbf{e_1} \otimes \mathbf{e_1} \tag{3.2.2}$$

is a solution of the field equations, the traction jump condition, and the boundary conditions for the quasi-static process under consideration.²⁰ Considering (3.1.1)₃, the first-order approximation of σ^- is

$$\boldsymbol{\sigma}^- = \sigma_0 \mathbf{e_1} \otimes \mathbf{e_1}. \tag{3.2.3}$$

For this special case, the linearized driving traction given by (3.2.1) becomes

$$f = f_{\rm cr} - \sigma_0 a \cos\phi \cos\alpha, \tag{3.2.4}$$

where $f_{\rm cr} = \left(\tilde{J} W_1^*\right)^+ - (W^*)^-$, $a = |\tilde{\mathbf{a}}|$, $a\cos\phi = \tilde{\mathbf{a}} \cdot \mathbf{e_1}$, and $\cos\alpha = \tilde{\mathbf{n}} \cdot \mathbf{e_1}$.

We next note that the extension of a unit fiber of material originally parallel to e₁ that is due only to the shape deformation is

$$\delta = \left| \tilde{\mathbf{F}} \mathbf{e_1} \right| - \left| \mathbf{e_1} \right| = \sqrt{\mathbf{e_1} \cdot \tilde{\mathbf{C}} \mathbf{e_1}} - 1, \tag{3.2.5}$$

where $\tilde{\mathbf{C}} = \tilde{\mathbf{F}}^T \tilde{\mathbf{F}}$. The component of extension in the direction of the tensile traction is

$$\delta' = \mathbf{e_1} \cdot \tilde{\mathbf{F}} \mathbf{e_1} - \mathbf{e_1} \cdot \mathbf{e_1} = a \cos\phi \cos\alpha. \tag{3.2.6}$$

²⁰ This can be readily seen by expressing these equations in there Eulerian form.

This is also equal to the extension given by (3.2.5) if rotations are neglected or do not occur. From this, we can write the driving traction given by (3.2.4) as

$$f = f_{\rm cr} - \sigma_0 \delta'. \tag{3.2.7}$$

Thus, for a given σ_0 , the variant of martensite that yields the largest component of extension in the direction of the uniaxial tensile traction will be preferred during the growth process. This corresponds to the experimental observations presented in [14].

Let $\tilde{\mathbf{e}}$ be a unit vector in the $(\tilde{\mathbf{a}}, \tilde{\mathbf{n}})$ plane such that $\tilde{\mathbf{e}} \cdot \tilde{\mathbf{n}} = 0$ and $\tilde{\mathbf{e}} \cdot \tilde{\mathbf{a}} > 0$. For the case of a uniaxial tensile traction described above, the (shear) component of traction on the interface in the direction of $\tilde{\mathbf{e}}$ is

$$\tilde{S} = \tilde{\mathbf{e}} \cdot [(\sigma_0 \mathbf{e_1} \otimes \mathbf{e_1}) \tilde{\mathbf{n}}] = \sigma_0 \cos \lambda \cos \alpha, \tag{3.2.8}$$

where $\tilde{\mathbf{e}} \cdot \mathbf{e_1} = \cos \lambda$. For the case where $\tilde{\mathbf{F}}$ is a simple shear, $\tilde{\mathbf{e}}$ is parallel to $\tilde{\mathbf{a}}$, resulting in $\lambda = \phi$, and (3.2.8) becomes

$$\tilde{S} = \sigma_0 \cos\phi \cos\alpha. \tag{3.2.9}$$

Thus, for this case, the driving traction given by (3.2.4) can be written as

$$f = f_{\rm cr} - a\tilde{S}. \tag{3.2.10}$$

From this, we can conclude that the variant that is predicted to be preferred, by a shear-stress criterion stating that the preferred variant is the variant with the largest value of \tilde{S} , will correspond to the variant with the largest negative driving traction for a given σ_0 , only if each variant has a simple-shear shape deformation and has the same value for the magnitude of its amplitude vector.

3.3 The Case of a Uniform Hydrostatic Pressure

In this section, the effect that an applied hydrostatic pressure has on a martensitic phase transformation in a given material is studied.²¹ The two-phase material described in Section 3.1 is considered. If a given loading results in an increase in the driving traction, that loading is considered to favor the growth of phase 1, and if a given loading results in a decrease in the driving traction, that loading is considered to favor the growth of phase 2. If, on the other hand, the given loading results in no change in the value of the driving traction, neither phase is favored by that loading. For the problem under consideration, it is assumed that a hydrostatic pressure exists such that

$$\tau = -p\mathbf{1},\tag{3.3.1}$$

at every point of the deformed body, where p > 0. A quasi-static process is considered where $|\nabla \hat{\mathbf{u}}| \ll 1 \ \forall \ \mathbf{x} \in \mathbf{R}^-$ and $|\nabla \hat{\mathbf{u}}_1| \ll 1 \ \forall \ \mathbf{x}_1 \in \mathbf{R}_1^+$. For this case, we can conclude from $(3.1.1)_3$ that the first-order approximation of σ^- is

$$\boldsymbol{\sigma}^- = -p\mathbf{1}. \tag{3.3.2}$$

It is assumed that the shape deformation of phase 2 is homogeneous and has the form $\tilde{\mathbf{F}} = \mathbf{1} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$. For the following, let $(\pi/2) - \delta$ denote the angle between $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{n}}$. Note that δ is a measure of the dilatation (or volume expansion) of the shape deformation of phase 2. For the case under consideration and when δ is not infinitesimal, the linearized driving traction given by (3.1.23) becomes

$$f = \left(\left(\tilde{J} W_{\mathbf{1}}^{*} \right)^{+} - \left(W^{*} \right)^{-} \right) + p \,\tilde{\mathbf{a}} \cdot \tilde{\mathbf{n}} + O\left(\left| \nabla \hat{\mathbf{u}} \right|^{2}, \left| \nabla_{\mathbf{1}} \hat{\mathbf{u}}_{\mathbf{1}} \right|^{2} \right)$$

$$= f_{cr} + p a \sin \delta + O\left(\left| \nabla \hat{\mathbf{u}} \right|^{2}, \left| \nabla_{\mathbf{1}} \hat{\mathbf{u}}_{\mathbf{1}} \right|^{2} \right). \tag{3.3.3}$$

²¹ See [13] for a discussion of this type of problem and for a list of some references where such problems are considered.

Thus, if δ is not infinitesimal, we can conclude from (3.3.3) that a hydrostatic pressure favors the austenite phase transformation in a material where the martensite phase is such that $\sin \delta > 0$, 22 and a hydrostatic pressure favors a martensite phase transformation in a material where the martensite phase is such that $\sin \delta < 0$. Additionally, as can be observed from (3.3.3), these results are independent of the material coefficients of both the austenite and martensite. However, for the case where $|\delta| << 1$, the term $pa\sin \delta$ becomes a second-order term. Therefore, in this case, the lowest-order approximation of $f - f_{cr}$ is a second-order approximation, and the second-order terms that have been neglected in (3.3.3) must be retained to obtain a lowest-order approximation of $f - f_{cr}$. We note that these second-order terms contain the material coefficients of both phases.

In the rest of this section, the case where $|\delta| << 1$ is considered. The strains in each phase corresponding to the hydrostatic pressure are calculated, and the continuity-of-displacements condition (the only nontrivial portion of the boundary value problem) is enforced. The driving traction is then calculated to determine what values of the material coefficients of both phases will yield a driving traction that will favor the martensite phase transformation. Additionally, the case where phase 1 and phase 2 represent two different variants of the same martensite that are twin-related is considered, and a result that is expected from physical considerations is obtained. These problems not only demonstrate the convenience of using multiple reference configurations in the manner that they are used in this thesis, but the result that is obtained involving the two different variants of the same martensite serves as a very good check of the continuum model.

²² This corresponds with the well-known result that a hydrostatic pressure stabilizes the austenite phase in many iron alloys [13]. The martensite phases in these iron alloys have small, but not infinitesimal, volume expansions. ²³ Note that because p in (3.3.3) is related to the infinitesimal strains through the constitutive equations, p is considered to be a first-order term in (3.3.3).

3.3.1 The Material Symmetry of the Phases

For the problems considered in this section, the two-phase material that was considered in the previous sections of this chapter is considered. It is assumed that both phase 1 and phase 2 are homogeneous and have tetragonal symmetry.²⁴ The case of cubic symmetry for phase 1 and/or phase 2 can be considered as a special case, once the general results are obtained. It is assumed that each phase has preferred directions [15]. For the case considered here where the tetragonal symmetry reflects the symmetry of a tetragonal crystal lattice, the three preferred directions {h₁, h₂, h₃} of each phase can be considered to be in the [1 0 0], [0 1 0], [0 0 1] directions of a tetragonal unit cell of each phase, respectively. The material symmetry group of a material with tetragonal symmetry can be generated by the set

$$\mathcal{G}_{\mathrm{T}}^{\prime} = \left\{ \mathbf{R}_{\mathbf{1}}^{\pi}, \mathbf{R}_{\mathbf{2}}^{\pi/2} \right\},\tag{3.3.4}$$

where $\mathbf{R}_{\mathbf{k}}^{\phi}$ denotes a right-handed rotation by an angle ϕ about an axis parallel to $\mathbf{h}_{\mathbf{k}}$.²⁵ The eight distinct elements of the tetragonal material symmetry group $\mathcal{G}_{\mathbf{T}}$, which the elements of $\mathcal{G}_{\mathbf{T}}'$ generate, are

$$\mathcal{G}_{\mathrm{T}} = \left\{ 1, \mathbf{R}_{1}^{\pi}, \mathbf{R}_{3}^{\pi}, \mathbf{R}_{2}^{\pi/2}, \mathbf{R}_{2}^{\pi}, \mathbf{R}_{2}^{3\pi/2}, \mathbf{R}_{3}^{\pi} \mathbf{R}_{2}^{\pi/2}, \mathbf{R}_{3}^{\pi} \mathbf{R}_{2}^{3\pi/2} \right\}. \tag{3.3.5}$$

The elements of \mathcal{G}_T map the preferred directions of the phase into equivalent positions, and as discussed in Section 2.5, we require that the elastic potential of the corresponding phase be invariant with respect to these rotations.

3.3.2 The Remaining Assumptions

Let $\{e_1, e_2, e_3\}$ form an orthonormal basis for vectors in E_3 . For the following problem, a state of plane strain is assumed, with e_3 normal to the plane of plane strain,

²⁴ Note that tetragonal symmetry is equivalent to orthotropic symmetry.

²⁵ If the elements of \mathcal{H}^* generate the elements of \mathcal{H} , all of the elements of \mathcal{H} can be obtained by multiplying the elements of \mathcal{H}^* with each other and their inverses.

and a quasi-static process is considered. It is assumed that $|\nabla \hat{\mathbf{u}}| << 1 \ \forall \mathbf{x} \in \mathbf{R}^-$ and $|\nabla \hat{\mathbf{u}}_1| << 1 \ \forall \mathbf{x}_1 \in \mathbf{R}_1^+$. Let $\{\mathbf{h}_1^+, \mathbf{h}_2^+, \mathbf{h}_3^+\}$ represent the preferred directions of phase 2 and assume that $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are such that they are aligned with $\{\mathbf{h}_1^+, \mathbf{h}_2^+, \mathbf{h}_3^+\}$, respectively. Let $\{\mathbf{h}_1^-, \mathbf{h}_2^-, \mathbf{h}_3^-\}$ represent the preferred directions of phase 1, with \mathbf{h}_3^- in the direction of \mathbf{e}_3 and the angle between \mathbf{h}_1^- and \mathbf{e}_1 denoted by α (Figure 3.1). It is assumed that $\tilde{\mathbf{F}} = \mathbf{1} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$. Let ϕ denote the angle between $\tilde{\mathbf{n}}$ and \mathbf{e}_1 , and let δ be defined as it was in the beginning of this section. As mentioned above, it is assumed that $|\delta| << 1$. It is also assumed that a plane-strain hydrostatic pressure exists such that

$$\tau = -p\mathbf{1},\tag{3.3.6}$$

at every point of the deformed body. Additionally, in the following analysis, we will decompose the displacement gradients into their symmetric and skew-symmetric parts as follows

$$\nabla \hat{\mathbf{u}} = \boldsymbol{\varepsilon} + \boldsymbol{\omega},$$

$$\nabla_1 \hat{\mathbf{u}}_1 = \boldsymbol{\varepsilon}_1 + \boldsymbol{\omega}_1,$$
(3.3.7)

where $\omega = \operatorname{skew} \nabla \hat{\mathbf{u}}$, and $\omega_1 = \operatorname{skew} \nabla_1 \hat{\mathbf{u}}_1$.

3.3.3 The Stress and Infinitesimal Strain Tensors

Considering (3.3.6), (3.1.1)₃, and (3.1.2)₃, we can conclude that the first-order approximations of σ and σ_1 are

$$\sigma = -p\mathbf{1},$$

$$\sigma_{\mathbf{1}} = -p\mathbf{1},$$
(3.3.8)

²⁶ Unless otherwise indicated, for the following plane-strain problem, it is assumed that all tensors correspond to the two-dimensional Euclidean space containing $\{e_1, e_2\}$.

respectively.²⁷ For the linear case of plane strain and tetragonal symmetry considered here, the inplane components of stress for phase 1, in the frame coinciding with $\{\mathbf{h}_1^-, \mathbf{h}_2^-\}$, are given by

(see, e.g., [7, 11]), where $\sigma_{\alpha\beta}^-$ and $\varepsilon_{\alpha\beta}^-$ denote the components of σ and ε , respectively, in the $\{\mathbf{h}_1^-,\mathbf{h}_2^-\}$ frame. These equations can be inverted to obtain

$$\begin{cases}
\varepsilon_{11}^{-} \\
\varepsilon_{22}^{-} \\
\varepsilon_{12}^{-}
\end{cases} = \begin{bmatrix}
K_{1111}^{-} & K_{1122}^{-} & 0 \\
K_{1122}^{-} & K_{2222}^{-} & 0 \\
0 & 0 & 2K_{1212}^{-}
\end{bmatrix} \begin{cases}
\sigma_{11}^{-} \\
\sigma_{22}^{-} \\
\sigma_{12}^{-}
\end{cases},$$
(3.3.10)

where $K_{1111}^- = C_{2222}^-/\eta$, $K_{1122}^- = -C_{1122}^-/\eta$, $K_{2222}^- = C_{1111}^-/\eta$, $2K_{1212}^- = 1/(2C_{1212}^-)$, and $\eta = C_{1111}^-C_{2222}^- - (C_{1122}^-)^2$. For the case where $\sigma = -p\mathbf{1}$, the inplane components of strain given by (3.3.10) become

$$[\varepsilon] = -p \begin{bmatrix} \left(K_{1111}^{-} + K_{1122}^{-} \right) & 0 \\ 0 & \left(K_{1122}^{-} + K_{2222}^{-} \right) \end{bmatrix}.$$
 (3.3.11)

The components $\varepsilon'_{\alpha\beta}$ of ε in the $\{e_1, e_2\}$ frame can be obtained from (3.3.11) in the usual way and are given by

Note that since σ , σ_1 , ε , and ε_1 are homogeneous, $\sigma^- = \sigma$, $\sigma_1^+ = \sigma_1$, $\varepsilon^- = \varepsilon$, and $\varepsilon_1^+ = \varepsilon_1$.

Note that $K_{\alpha\beta\gamma\delta}^-$ are the components of the compliance four-tensor **K** for phase 1 in the $\{\mathbf{h}_1^-,\mathbf{h}_2^-\}$ frame.

$$[\boldsymbol{\varepsilon}]' = -p \begin{bmatrix} \left\{ K_{1111}^{-}(\cos\alpha)^{2} + K_{2222}^{-}(\sin\alpha)^{2} + K_{1122}^{-} \right\} & \frac{1}{2} \left(K_{1111}^{-} - K_{2222}^{-} \right) \sin 2\alpha \\ \frac{1}{2} \left(K_{1111}^{-} - K_{2222}^{-} \right) \sin 2\alpha & \left\{ K_{1111}^{-}(\sin\alpha)^{2} + K_{2222}^{-}(\cos\alpha)^{2} + K_{1122}^{-} \right\} \end{bmatrix}.$$
(3.3.12)

Since $\{e_1,e_2\}$ coincide with $\{h_1^+,h_2^+\}$, the inplane components of σ_1 for phase 2 in the $\{e_1,e_2\}$ frame are given by

where $\sigma_{\alpha\beta}^+$ and $\varepsilon_{\alpha\beta}^+$ denote the components of σ_1 and ε_1 , respectively, in the $\{\mathbf{h}_1^+, \mathbf{h}_2^+\}$ (or, in this case, the $\{\mathbf{e}_1, \mathbf{e}_2\}$) frame. Solving the above equations for $\varepsilon_{\alpha\beta}^+$ and substituting (3.3.8)₂ yield

$$[\varepsilon_{1}] = -p \begin{bmatrix} (K_{1111}^{+} + K_{1122}^{+}) & 0\\ 0 & (K_{1122}^{+} + K_{2222}^{+}) \end{bmatrix},$$
(3.3.14)

where $K_{\alpha\beta\gamma\delta}^+$ are the components of the compliance four-tensor K_1 for phase 2 in the $\{\mathbf{h}_1^+, \mathbf{h}_2^+\}$ (or $\{\mathbf{e}_1, \mathbf{e}_2\}$) frame.

3.3.4 The Continuity of Displacements

Because the true stress is assumed to be uniform and constant throughout the body, the linear momentum field equations and the traction jump condition are trivially satisfied. A necessary condition for the continuity of displacements at the phase boundary is that

$$\det\left(\mathbf{F}_{1}^{+}\tilde{\mathbf{F}}-\mathbf{F}^{-}\right)=0. \tag{3.3.15}$$

For the case where $\tilde{\mathbf{F}} = \mathbf{1} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$ that is considered here, the first-order approximation of \mathbf{L} is $\tilde{\mathbf{L}}$, where $\tilde{\mathbf{L}} \cdot \tilde{\mathbf{n}} = 0$. In terms of the displacement gradients, the above equation becomes

$$\det(\tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}} + \nabla_1 \hat{\mathbf{u}}_1^+ (\tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}) + \nabla_1 \hat{\mathbf{u}}_1^+ - \nabla \hat{\mathbf{u}}^-) = 0. \tag{3.3.16}$$

In the $\{e_1, e_2\}$ frame,

$$\{\tilde{\mathbf{n}}\} = \begin{Bmatrix} \cos \phi \\ \sin \phi \end{Bmatrix}, \quad \{\tilde{\mathbf{a}}\} = a \begin{Bmatrix} -\sin(\phi - \delta) \\ \cos(\phi - \delta) \end{Bmatrix} = a \begin{Bmatrix} -\sin\phi \\ \cos\phi \end{Bmatrix} + a\delta \begin{Bmatrix} \cos\phi \\ \sin\phi \end{Bmatrix}. \tag{3.3.17}$$

Substituting (3.3.7) and (3.3.17) into (3.3.16) and retaining only first-order terms yield

$$\frac{1}{2} \left(\varepsilon_{11}^{+} - \varepsilon_{22}^{+} + \varepsilon_{22}^{\prime -} - \varepsilon_{11}^{\prime -} \right) \sin 2\phi + \varepsilon_{12}^{\prime -} \cos 2\phi + \omega^{\prime -} - \omega^{+} = 0, \tag{3.3.18}$$

where $\varepsilon_{ij}^{\prime-}$ and ε_{ij}^{+} denote the components of ε and ε_{1} in the $\{\mathbf{e_{1}},\mathbf{e_{2}}\}$ frame, respectively, and $\omega^{\prime-}$ and ω^{+} denote the $\omega_{12}^{\prime-}$ and ω_{12}^{+} components of ω and ω_{1} in the $\{\mathbf{e_{1}},\mathbf{e_{2}}\}$ frame, respectively.²⁹ We note that for the linear case under consideration, the symmetric parts of the displacement gradients of $\hat{\mathbf{u}}$ and $\hat{\mathbf{u}}_{1}$ are completely determined by the stress distribution and are given by (3.3.12) and (3.3.14), respectively, and Equation (3.3.18) is the only equation that restricts the skew-symmetric parts of these displacement gradients. Substituting (3.3.12) and (3.3.14) into (3.3.18) and solving for $\omega^{+} - \omega^{\prime-}$ yield

$$\omega^{+} - \omega'^{-} = \frac{p}{2} (K_{2222}^{+} - K_{1111}^{+}) \sin 2\phi + \frac{p}{2} (K_{2222}^{-} - K_{1111}^{-}) \sin (2\alpha - 2\phi). \quad (3.3.19)$$

²⁹ Note that because of (3.3.14), ϵ_{12}^+ has been taken to be equal to zero in Equation (3.3.18).

This equation can be written in nondimensional form by using the following nondimensional quantities:

$$\tilde{\omega}^{-} = \frac{2a\omega'^{-}}{pK_{1111}^{+}}, \qquad \tilde{\omega}^{+} = \frac{2a\omega^{+}}{pK_{1111}^{+}}, \qquad \tilde{K}_{2}^{+} = \frac{K_{2222}^{+}}{K_{1111}^{+}},$$

$$\tilde{K}_{1}^{-} = \frac{K_{1111}^{-}}{K_{1111}^{+}} \qquad \tilde{K}_{2}^{-} = \frac{K_{2222}^{-}}{K_{1111}^{+}}.$$
(3.3.20)

The nondimensional form of Equation (3.3.19) is

$$\tilde{\omega}^{+} - \tilde{\omega}^{-} = a \Big(\tilde{K}_{2}^{+} - 1 \Big) \sin 2\phi + a \Big(\tilde{K}_{2}^{-} - \tilde{K}_{1}^{-} \Big) \sin (2\alpha - 2\phi). \tag{3.3.21}$$

3.3.5 The Driving Traction

Considering (3.3.8), $(3.1.1)_1$, and $(3.1.2)_1$, the corresponding second-order approximations of the elastic potentials are

$$W = W^* - \frac{1}{2} \varepsilon \cdot \boldsymbol{\sigma} = W^* - \frac{1}{2} p \operatorname{tr} \varepsilon,$$

$$W = W^* - \frac{1}{2} \varepsilon_1 \cdot \boldsymbol{\sigma}_1 = W_1^* - \frac{1}{2} p \operatorname{tr} \varepsilon_1.$$
(3.3.22)

For the case considered here, the second-order approximation of $-\sigma \cdot \left(\mathbf{F_1^+ \tilde{F} - F^-}\right)$ is

$$p(a\delta + \tilde{\mathbf{n}} \cdot (\nabla_1 \hat{\mathbf{u}}_1 \tilde{\mathbf{a}}) + \operatorname{tr} \boldsymbol{\varepsilon}_1 - \operatorname{tr} \boldsymbol{\varepsilon}), \tag{3.3.23}$$

where the first-order approximations of $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{n}}$ are used. Substituting (3.3.22) and (3.3.23) into (2.11.2) yields the second-order approximation of the driving traction given by

$$f = f_{cr} + p(a\delta + \tilde{\mathbf{n}} \cdot (\nabla_1 \hat{\mathbf{u}}_1 \tilde{\mathbf{a}}) + \frac{1}{2} \operatorname{tr} \boldsymbol{\varepsilon}_1 - \frac{1}{2} \operatorname{tr} \boldsymbol{\varepsilon}). \tag{3.3.24}$$

Retaining only first-order terms, the individual terms in (3.3.24) can be expressed as

$$\tilde{\mathbf{n}} \cdot (\nabla_{\mathbf{1}} \hat{\mathbf{u}}_{\mathbf{1}} \tilde{\mathbf{a}}) = a \left(\omega^{+} - \frac{1}{2} p (K_{2222}^{+} - K_{1111}^{+}) \sin 2\phi \right),$$

$$\operatorname{tr} \boldsymbol{\varepsilon} = -p \operatorname{tr}(\mathbf{K} \mathbf{1}) = -p \left(K_{1111}^{-} + 2K_{1122}^{-} + K_{2222}^{-} \right),$$

$$\operatorname{tr} \boldsymbol{\varepsilon}_{\mathbf{1}} = -p \operatorname{tr}(\mathbf{K}_{\mathbf{1}} \mathbf{1}) = -p \left(K_{1111}^{+} + 2K_{1122}^{+} + K_{2222}^{+} \right).$$

$$(3.3.25)$$

Substituting (3.3.25) into (3.3.24) yields

$$f = f_{cr} + p \left\{ a\delta + a\omega^{+} + \frac{1}{2} ap(K_{1111}^{+} - K_{2222}^{+}) \sin 2\phi + \frac{1}{2} p[\text{tr}(\mathbf{K1}) - \text{tr}(\mathbf{K_{1}1})] \right\}.$$
(3.3.26)

We can put the driving traction given by (3.3.26) in nondimensional form by using the nondimensional quantities given by (3.3.20) and the following additional nondimensional quantities

$$\tilde{f} = \frac{2f}{p^2 K_{1111}^+}, \qquad \tilde{f}_{cr} = \frac{2f_{cr}}{p^2 K_{1111}^+},$$

$$\tilde{\delta} = \frac{2a\delta}{pK_{1111}^+}, \qquad \tilde{\beta} = \frac{1}{K_{1111}^+} [\text{tr}(\mathbf{K1}) - \text{tr}(\mathbf{K_11})].$$
(3.3.27)

The nondimensional driving traction $ilde{f}$ is as follows:

$$\tilde{f} = \tilde{f}_{cr} + \tilde{\delta} + \tilde{\omega}^+ + a\left(1 - \tilde{K}_2^+\right)\sin 2\phi + \tilde{\beta}. \tag{3.3.28}$$

Note that $\tilde{\omega}^+$ is a parameter in the above equation for \tilde{f} . We can obtain \tilde{f} as a function of $\tilde{\omega}^-$ by using (3.3.21). The resulting equation is

$$\tilde{f} = \tilde{f}_{cr} + \tilde{\delta} + \tilde{\omega}^- + a\left(\tilde{K}_2^- - \tilde{K}_1^-\right)\sin(2\alpha - 2\phi) + \tilde{\beta}. \tag{3.3.29}$$

3.3.6 The Austenite-Martensite Phase Transformation

In the following, it is assumed that phase 1 represents the austenite and phase 2 represents the martensite. From the discussion in the beginning of this section, a hydrostatic pressure will favor the austenite phase transformation if it results in $\tilde{f} - \tilde{f}_{\rm cr} > 0$, and a hydrostatic pressure will favor the martensite phase transformation if it results in $\tilde{f} - \tilde{f}_{\rm cr} < 0$. For the case under consideration where $|\delta| << 1$, if $\tilde{\omega}^+$ is used as the parameter, we can conclude from (3.3.28) that the second-order approximation of $f - \tilde{f}_{\rm cr}$ can be negative if and only if

$$\tilde{\delta} + \tilde{\omega}^+ + \tilde{\beta} < -a \left(1 - \tilde{K}_2 \right) \sin 2\phi \,. \tag{3.3.30}$$

Alternatively, if $\tilde{\omega}^-$ is used as the parameter, we can conclude from (3.3.29) that the second-order approximation of $f - \tilde{f}_{cr}$ can be negative if and only if

$$\tilde{\delta} + \tilde{\omega}^- + \tilde{\beta} < -a \Big(\tilde{K}_2^- - \tilde{K}_1^- \Big) \sin(2\alpha - 2\phi) \,. \tag{3.3.31}$$

We note that a value for $\tilde{\omega}^-$ or $\tilde{\omega}^+$ might be prescribed by some displacement boundary condition that is applied to the material in addition to the hydrostatic pressure, and that is consistent with the assumed state of stress within the material. Thus, a hydrostatic pressure will favor the martensite phase transformation if and only if the shape deformation of the martensite, the material coefficients of both phases, the orientation of the phase boundary, and the additional boundary conditions are such that (3.3.30) or (3.3.31) is satisfied. Otherwise, the hydrostatic pressure will favor the austenite phase transformation.

3.3.7 The Case of Twin-Related Variants

For the case where phase 1 and phase 2 represent two variants of the same martensite that are twin-related and the isothermal process is at a temperature near the transformation temperature, we have: (1) $\delta = 0$, since one twin has a simple-shear shape deformation relative to the other twin; (2) $f_{cr} = 0$, since $\tilde{J}W_1(1) = W(1)$ for two variants of the same martensite near the transformation temperature; (3) $K_{ijkl}^+ = K_{ijkl}^-$, since both phases represent the same material; (4) $\tilde{\beta} = 0$, as a result of (3); and (5) $\alpha = 2\phi$, as can be seen from Figure 3.2. In this case, the driving traction given by (3.3.28) becomes

$$\tilde{f} = \tilde{\omega}^+ + a \left(1 - \tilde{K}_2^+ \right) \sin 2\phi, \tag{3.3.32}$$

and Equation (3.3.21) becomes

$$\tilde{\omega}^{+} - \tilde{\omega}^{-} = -2a \Big(1 - \tilde{K}_{2}^{+} \Big) \sin 2\phi \,.$$
 (3.3.33)

If we now require that the deformation of one twin be symmetric with respect to the deformation of the other twin (because of the *symmetric* stress distribution), we must require that

$$\omega^- = -\omega^+. \tag{3.3.34}$$

In this case, substituting (3.3.34) into (3.3.33), solving for $\tilde{\omega}^+$ in the resulting equation, and then substituting the resulting equation for $\tilde{\omega}^+$ into (3.3.32), yield

$$f = 0.$$
 (3.3.35)

This is what should be expected, since everything else in the problem is symmetric, and consequently, one twin should not be preferred over the other.

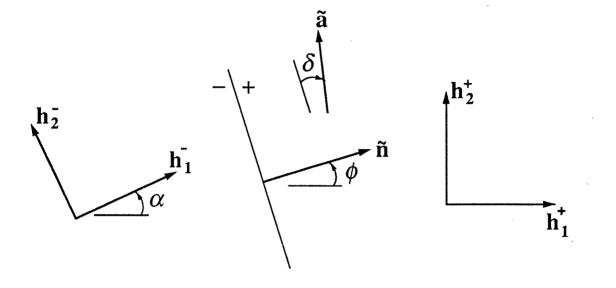


Figure 3.1. The hydrostatic pressure problem.

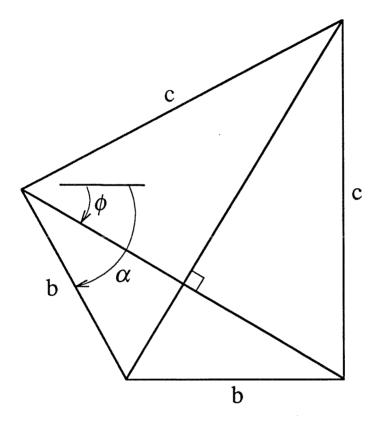


Figure 3.2. Twin-related variants.

CHAPTER 4

A THERMOMECHANICAL PROBLEM

In this chapter, a thermomechanical problem involving a one-dimensional, twophase bar is studied. The bar is subject to different temperatures at each boundary and to a mechanical end-loading. A quasi-static process is considered, and the temperature and static equilibrium positions of the phase boundary are calculated and studied as the material coefficients, temperature boundary conditions, and end-loading are varied.

4.1 The Field Equations and Jump Conditions

A one-dimensional, finite bar that initially consists of two phases is considered. It is assumed that the process under consideration is thermomechanical with no body forces and no heat sources present. It is further assumed that the process occurs in a time interval $\Gamma = [t_0, t_1]$, and in a temperature interval $\Omega = [\theta'_0, \theta'_1]$ containing the temperatures M_s , T_0 , and A_s . Unless otherwise indicated, the notation used in Section 2.12 will be used in the following, with the understanding that it corresponds to the one-dimensional problem under consideration. Let x = s(t) be the location of the phase boundary at time $t \in \Gamma$, and let L be the length of the bar with respect to the reference configuration R. Considering this, $R = \{x/x \in [0, L]\}$, $R^- = \{x/x \in [0, s(t)]\}$, and $R^+ = \{x/x \in [s(t), L]\}$. It is assumed that $\tilde{x}_1(\cdot, t)$: $R^+ \mapsto R_1^+$ at each $t \in \Gamma$ is given by

$$\tilde{x}_1(x,t) = x + \int_{s(t)}^x \tilde{\gamma}(\theta(\xi))d\xi, \qquad (4.1.1)$$

where $\theta(x)$ is the temperature field of the material with respect to the coordinates of R. The displacement gradient (transformation strain) corresponding to this choice of

 \tilde{x}_1 is $\tilde{\gamma}(\theta(x))$, the Jacobian is $\tilde{J}=1+\tilde{\gamma}$, and $R_1^+=\{x_1/x_1\in [\tilde{x}_1(s(t),t),\tilde{x}_1(L,t)]\}=\{x_1/x_1\in [s(t),L_1(t)]\}$, at each $t\in \Gamma$, where $L_1(t)=\tilde{x}_1(L,t)$, and $\tilde{\gamma}>-1$ so that reflections are excluded from (4.1.1). Also, the temperature field for phase 2 with respect to the coordinates of R_1^+ is denoted by $\theta_1(x_1)$. In the following, a quasi-static process is considered. In particular, a process is considered where time is treated as just a parameter in all quantities except for s(t). The dependence of s(t) on time is such that $\left(\frac{ds(t)}{dt}\right)^n$ (n>1) and $\ddot{s}(t)=\frac{\partial^2 s(t)}{\partial t^2}$ are assumed to be negligible for all $t\in \Gamma$, and are therefore taken to be equal to zero. For this type of process, the only time-derivative terms in the boundary value problem that are not identically equal to zero are those that are linear in $\dot{s}(t)=\frac{ds(t)}{dt}$. Such a process corresponds to a process where $|\dot{s}(t)|<<1$ and the acceleration of the phase boundary is negligible for all $t\in \Gamma$.

The balance of linear momentum, the balance of energy (the first law of thermodynamics), and the entropy inequality (the second law of thermodynamics) for phase 1 and for the assumptions given above are

$$\frac{d\sigma}{dx} = 0,$$

$$\frac{dq}{dx} = 0, (4.1.2)$$

$$\frac{d}{dx}\left(\frac{q}{\theta}\right) \le 0,$$

respectively, $\forall x \in (0, s(t))$ at each $t \in \Gamma$. The balance of linear momentum, the

¹ Because of this, the dependence of all quantities, except for s(t) and $\tilde{x}_1(x,t)$, on time will not be displayed in the notation. Also, strictly speaking, such a process is not a true quasi-static process since time is not just a parameter in *all* variables of the problem, and therefore the set of all solutions as time is varied does not consist of only static equilibrium solutions.

balance of energy, and the entropy inequality for phase 2 are given by

$$\frac{d\sigma_1}{dx_1} = 0,$$

$$\frac{dq_1}{dx_1} = 0, (4.1.3)$$

$$\frac{d}{dx_1} \left(\frac{q_1}{\theta_1} \right) \le 0,$$

respectively, $\forall x_1 \in (s(t), L_1(t))$ at each $t \in \Gamma$.

At x=s(t), the continuity-of-displacement and the continuity-of-temperature conditions are

$$u_1^+(s(t)) = u^-(s(t)),$$
 (4.1.4)

$$\theta_1^+(s(t)) = \theta^-(s(t)),$$

respectively, at each $t \in \Gamma$.² The jump conditions at x = s(t) that are equivalent to the balance of linear momentum, the balance of energy, and the entropy inequality are given by

$$\sigma_1^+ - \sigma^- = 0,$$

$$\left\{\theta\left(\tilde{J}\eta_{1}^{+}-\eta^{-}\right)+f\right\}\dot{s}+\left(q_{1}^{+}-q^{-}\right)=0,$$
 (4.1.5)

$$f\dot{s} \geq 0$$
,

respectively, at each $t \in \Gamma$, where

$$f = \tilde{J}\psi_{1}^{+} - \psi^{-} - \sigma^{-}(\tilde{\gamma} + \gamma_{1}^{+}\tilde{\gamma} + \gamma_{1}^{+} - \gamma^{-})$$
 (4.1.6)

Note that the original form of the continuity-of-displacement condition $y_1^+ = y^-$ reduces to (4.1.4)₁ for the \tilde{x}_1 given by (4.1.1).

is the driving traction acting at the interface for the quasi-static process under consideration. We also have at the phase boundary a kinetic relation relating \dot{s} to at least f. This kinetic relation is a constitutive relation and will be discussed in Section 4.3.

The boundary conditions for equations $(4.1.2)_1$ and $(4.1.3)_1$ are

$$u(0) = 0, \quad \sigma_1(L_1(t)) = \sigma_0,$$
 (4.1.7)

respectively, and the boundary conditions for the temperatures $\theta(x)$ and $\theta_1(x_1)$ are

$$\theta(0) = \theta^*, \quad \theta_1(L_1(t)) = \theta_1^*,$$
 (4.1.8)

respectively.

4.2 The Constitutive Assumptions

It is assumed that both phase 1 and phase 2 are homogeneous, thermoelastic materials. In particular, for phase 1 it is assumed that there exists a Helmholtz free energy potential

$$\psi = \psi(\gamma, \theta), \tag{4.2.1}$$

such that

$$\sigma = \frac{\partial \psi}{\partial \gamma},$$

$$\eta = -\frac{\partial \psi}{\partial \theta},$$
(4.2.2)

where $\gamma = \frac{du}{dx}$, and it is assumed that the heat flux response function for phase 1 has the form

$$q = \hat{q}\left(\gamma, \theta, \frac{d\theta}{dx}\right). \tag{4.2.3}$$

Similarly, for phase 2 it is assumed that there exists a Helmholtz free energy potential

$$\psi_1 = \psi_1(\gamma_1, \theta_1), \tag{4.2.4}$$

such that

$$\sigma_1 = \frac{\partial \psi_1}{\partial \gamma_1},$$
 (4.2.5)
$$\eta_1 = -\frac{\partial \psi_1}{\partial \theta_1},$$

where $\gamma_1 = \frac{du_1}{dx_1}$, and it is assumed that the heat flux response function for phase 2 has the form

$$q_1 = \hat{q}_1 \left(\gamma_1, \theta_1, \frac{d\theta_1}{dx_1} \right). \tag{4.2.6}$$

We note that all of the quantities for phase 1 given by (4.2.1)-(4.2.3) are defined with respect to the reference configuration R^- , and all of the quantities for phase 2 given by (4.2.4)-(4.2.6) are defined with respect to the reference configuration R_1^+ .

We next assume that the thermomechanical process under consideration takes place in a neighborhood of a temperature $\theta_0 \in \Omega$. More precisely, letting $\hat{\theta} = (\theta - \theta_0)$ and $\hat{\theta}_1 = (\theta_1 - \theta_0)$, we assume that $|\hat{\theta}| << 1 \ \forall x \in [0, s(t)]$ and $|\hat{\theta}_1| << 1 \ \forall x_1 \in [s(t), L_1(t)]$, at each $t \in \Gamma$. Additionally, we assume that for a given θ_0 , the dependence of $\tilde{\gamma}$ on $\hat{\theta}$ is at least second-order; i.e., we assume

$$\tilde{\gamma} = \gamma_0 + \mathcal{O}(\hat{\theta}^2),\tag{4.2.7}$$

where $\gamma_0 = \tilde{\gamma}(\theta_0) > -1$. For this assumption, the first-order approximation of \tilde{x}_1 is

$$\tilde{x}_1(x,t) = x + \gamma_0(x - s(t)),$$
 (4.2.8)

and the first-order approximation of $L_1(t)$ is $L_1(t) = L + \gamma_0(L - s(t))$. We assume that phase 1 is unstressed at $(\gamma, \theta) = (0, \theta_0)$, and that phase 2 is unstressed at

 $(\gamma_1, \theta_1) = (0, \theta_0)$. We also assume that $|\gamma| << 1 \ \forall x \in [0, s(t))$ and $|\gamma_1| << 1 \ \forall x_1 \in (s(t), L_1(t)]$, at each $t \in \Gamma$. Considering this, ψ for phase 1 can be written as

$$\psi = \psi^* - \eta^* \hat{\theta} + \mathcal{O}\left(\hat{\theta}^2, \gamma \hat{\theta}, \gamma^2\right), \tag{4.2.9}$$

where $\psi^* = \psi(0, \theta_0)$ and $\eta^* = \eta(0, \theta_0) = -\frac{\partial \psi}{\partial \theta}|_{(0, \theta_0)}$. Similarly, ψ_1 for phase 2 can be written as

$$\psi_1 = \psi_1^* - \eta_1^* \hat{\theta}_1 + \mathcal{O}\left(\hat{\theta}_1^2, \gamma_1 \hat{\theta}_1, \gamma_1^2\right), \tag{4.2.10}$$

where $\psi_1^* = \psi_1(0,\theta_0)$ and $\eta_1^* = \eta_1(0,\theta_0) = -\frac{\partial \psi_1}{\partial \theta_1}\Big|_{(0,\theta_0)}$. We next assume that the heat flux q for phase 1 is zero when $\frac{d\theta}{dx} = 0$, and that the heat flux q_1 for phase 2 is zero when $\frac{d\theta_1}{dx_1} = 0$. We additionally assume that $\left|\frac{d\theta}{dx}\right| << 1 \ \forall \ x \in [0,s(t))$ and $\left|\frac{d\theta_1}{dx_1}\right| << 1 \ \forall \ x_1 \in (s(t),L_1(t)]$, at each $t \in \Gamma$. For these assumptions, the first-order approximation of q for phase 1 is

$$q = k \frac{d\theta}{dx}, (4.2.11)$$

where $k=\left[\partial\hat{q}/\partial\left(\frac{d\theta}{dx}\right)\right]_{(0,\theta_0,0)}$, and the first-order approximation of q_1 for phase 2 is

$$q_1 = k_1 \frac{d\theta_1}{dx_1}, (4.2.12)$$

where $k_1 = \left[\partial \hat{q}_1/\partial \left(\frac{d\theta_1}{dx_1}\right)\right]_{(0,\theta_0,0)}$. Using (4.2.9), (4.2.10), and (4.1.4)₂, the first-order approximation of the driving traction given by (4.1.6) is

$$f = \tilde{J}^* \psi_1^* - \psi^* - \left(\tilde{J}^* \eta_1^* - \eta^* \right) \hat{\theta}^{\pm} - \sigma^- \gamma_0 , \qquad (4.2.13)$$

where σ^- is given by the linearized form of (4.2.2)₁, and $\tilde{J}^* = 1 + \tilde{\gamma}(\theta_0) = 1 + \gamma_0$. We must also specify the kinetic relation, which relates \dot{s} and at least f. This will be discussed in the following section.

Note that Equations (4.2.11) and (4.2.12) both have the form of Fourier's Law.

⁴ Note that because both phases are homogeneous, $\psi^-(0,\theta_0) = \psi^*$, $\eta^-(0,\theta_0) = \eta^*$, $\psi_1^+(0,\theta_0) = \psi_1^*$, and $\eta_1^+(0,\theta_0) = \eta_1^*$.

4.3 The Kinetic Relation

It is assumed that the thermoelastic material under consideration has a kinetic relation of the form

$$\dot{s} = \Phi(f, \theta), \tag{4.3.1}$$

where $\theta = \theta(s)$. Because of the entropy inequality (4.1.5)₃, this kinetic relation must be such that

$$f\Phi(f,\theta) \ge 0. \tag{4.3.2}$$

We additionally assume that at each temperature $\theta(s) \in \Omega$, the kinetic relation given by (4.3.1) has the form

$$\Phi(f,\theta) \begin{cases}
> 0, & f > f_2(\theta) \\
= 0, & f_1(\theta) \le f \le f_2(\theta) \\
< 0, & f < f_1(\theta)
\end{cases} (4.3.3)$$

where $f_1(\theta(s))$ and $f_2(\theta(s))$ depend on the material and are such that $f_1 \leq 0$ and $f_2 \geq 0$ $\forall \theta(s) \in \Omega$. We note that this kinetic relation satisfies (4.3.2). A kinetic relation that has the form given by (4.3.3) and is linear in f is

$$\Phi(f,\theta) = \begin{cases} \frac{1}{\nu_2(\theta)} \{f - f_2(\theta)\}, & f > f_2(\theta) \\ 0, & f_1(\theta) \le f \le f_2(\theta) \\ \frac{1}{\nu_1(\theta)} \{f - f_1(\theta)\}, & f < f_1(\theta) \end{cases}$$
(4.3.4)

where $\nu_1(\theta(s)) \geq 0$ and $\nu_2(\theta(s)) \geq 0 \ \forall \ \theta(s) \in \Omega$. We note that because (4.3.4) is linear in f, it is probably most appropriate only for values of f such that $f_1 \leq f \leq f_2$, $|(f-f_2)/f| << 1$, or $|(f-f_1)/f| << 1$. For the

following, let $\mathrm{B}(\theta_0) = \left\{ (\gamma^-, \gamma_1^+, \theta) / \left| \gamma^- \right| << 1, \left| \gamma_1^+ \right| << 1, \left| \hat{\theta} \right| << 1 \right\}$ and $\Lambda(\theta_0) =$ $\{(f(\gamma^-,\gamma_1^+,\theta),\theta)/(\gamma^-,\gamma_1^+,\theta)\in B(\theta_0)\},\ \text{for a given }\theta_0\in\Omega.^5$ Three cases will be considered.

<u>Case I</u>: Consider first the case where the temperature $\theta_0 \in \Omega$ and the material are such that $f(0,0,\theta_0) = f_1(\theta_0) = f_2(\theta_0) = 0.6$ Additionally, assume that $(\gamma^-, \gamma_1^+, \theta) \in B(\theta_0)$ at each $t \in \Gamma$. For this case, $\frac{df_1}{d\theta}\Big|_{\theta_0} = 0$ and $\frac{df_2}{d\theta}\Big|_{\theta_0} = 0$, since $f_1(\theta_0) = f_2(\theta_0) = 0$ and it is required that $f_1 \leq 0$ and $f_2 \geq 0 \ \forall \theta(s) \in \Omega$. Thus, for this case, $f_1 = O(\hat{\theta}^2)$, $f_2 = O(\hat{\theta}^2)$, and the first-order approximation of (4.3.4) is

$$\Phi = \begin{cases} -\frac{1}{\nu_{2}} \left\{ \left(\tilde{J}^{*} \eta_{1}^{*} - \eta^{*} \right) \hat{\theta} + \sigma^{-} \gamma_{0} \right\}, & -\left(\tilde{J}^{*} \eta_{1}^{*} - \eta^{*} \right) \hat{\theta} - \sigma^{-} \gamma_{0} \geq 0 \\ -\frac{1}{\nu_{1}} \left\{ \left(\tilde{J}^{*} \eta_{1}^{*} - \eta^{*} \right) \hat{\theta} + \sigma^{-} \gamma_{0} \right\}, & -\left(\tilde{J}^{*} \eta_{1}^{*} - \eta^{*} \right) \hat{\theta} - \sigma^{-} \gamma_{0} \leq 0 \end{cases}$$
(4.3.5)

 $\forall (\gamma^-, \gamma_1^+, \theta) \in B(\theta_0)$, where $\nu_1 = \nu_1(\theta_0) \ge 0$ and $\nu_2 = \nu_2(\theta_0) \ge 0$.

<u>Case II</u>: Consider the case where the temperature $\theta_0 \in \Omega$ and the material are such that $f(0,0, heta_0)=f_1(heta_0)$ and $f_1(heta_0)$ is not small, in the sense that $|f-f_1|< f_1$ $\forall (f,\theta) \in \Lambda(\theta_0)$. If phase 1 represents the austenite and phase 2 represents the martensite, the temperature θ_0 for this case might be considered to represent the martensitic start temperature of the material. We also assume that $(\gamma^-, \gamma_1^+, \theta) \in B(\theta_0)$ at each $t \in \Gamma$. For this case, the portion of (4.3.4) that corresponds to $(f, \theta) \in \Lambda(\theta_0)$

$$\Phi(f,\theta) = \begin{cases} 0, & f \ge f_1(\theta) \\ \frac{1}{\nu_1(\theta)} \{f - f_1(\theta)\}, & f < f_1(\theta) \end{cases}$$
 (4.3.6)

is

Note that although f depends on $\theta(s)$, it can be varied independently of $\theta(s)$ since it also depends on γ^- and γ_1^+ . Note that $f(0,0,\theta_0) = \tilde{J}^*\psi_1^* - \psi^*$

Substituting (4.2.13) and

$$f_1 = f_1(\theta_0) + \mu_1 \hat{\theta} + O(\hat{\theta}^2),$$
 (4.3.7)

where $\mu_1 = \frac{df_1}{d\theta}\Big|_{\theta_0}$, into (4.3.6) and retaining only first-order terms yield

$$\Phi = \begin{cases}
0, & -\left(\tilde{J}^* \eta_1^* - \eta^*\right) \hat{\theta} - \sigma^- \gamma_0 \ge \mu_1 \hat{\theta} \\
-\frac{1}{\nu_1} \left\{ \left[\mu_1 + \left(\tilde{J}^* \eta_1^* - \eta^*\right) \right] \hat{\theta} + \sigma^- \gamma_0 \right\}, & -\left(\tilde{J}^* \eta_1^* - \eta^*\right) \hat{\theta} - \sigma^- \gamma_0 < \mu_1 \hat{\theta} \end{cases} ,$$
(4.3.8)

 $\forall (\gamma^-, \gamma_1^+, \theta) \in B(\theta_0).$

Case III: We next consider the case where the temperature $\theta_0 \in \Omega$ and the material are such that $f(0,0,\theta_0) = f_2(\theta_0)$ and $f_2(\theta_0)$ is not small, in the sense that $|f - f_2| < f_2$ $\forall (f,\theta) \in \Lambda(\theta_0)$. If phase 1 represents the austenite and phase 2 represents the martensite, the temperature θ_0 for this case might be considered to represent the austenite start temperature of the material. We also assume that $(\gamma^-, \gamma_1^+, \theta) \in B(\theta_0)$ at each $t \in \Gamma$. For this case, the portion of (4.3.4) that corresponds to $(f,\theta) \in \Lambda(\theta_0)$ is

$$\Phi(f,\theta) = \begin{cases} \frac{1}{\nu_2(\theta)} \{ f - f_2(\theta) \}, & f > f_2(\theta) \\ 0, & f \le f_2(\theta) \end{cases}$$
 (4.3.9)

Substituting (4.2.13) and

$$f_2 = f_2(\theta_0) + \mu_2 \hat{\theta} + O(\hat{\theta}^2),$$
 (4.3.10)

where $\mu_2 = \frac{df_2}{d\theta}\Big|_{\theta_0}$, into (4.3.9) and retaining only first-order terms yield

$$\Phi = \begin{cases} -\frac{1}{\nu_{2}} \left\{ \left[\mu_{2} + \left(\tilde{J}^{*} \eta_{1}^{*} - \eta^{*} \right) \right] \hat{\theta} + \sigma^{-} \gamma_{0} \right\}, & -\left(\tilde{J}^{*} \eta_{1}^{*} - \eta^{*} \right) \hat{\theta} - \sigma^{-} \gamma_{0} > \mu_{2} \hat{\theta} \\ 0, & -\left(\tilde{J}^{*} \eta_{1}^{*} - \eta^{*} \right) \hat{\theta} - \sigma^{-} \gamma_{0} \leq \mu_{2} \hat{\theta} \end{cases},$$

$$(4.3.11)$$

$$\forall (\gamma^-, \gamma_1^+, \theta) \in B(\theta_0).^7$$

Another method for obtaining a linear approximation of the nonzero portion of a kinetic relation of the form (4.3.1) is to simply expand it in a Taylor series about $(f,\theta)=(f_0,\theta_0)$, where $f_0=f(0,0,\theta_0)$. For the moment, assume that (4.3.1) and its first derivatives are continuous at $(f,\theta)=(f_0,\theta_0)$. For the case where $\Phi(f_0,\theta_0)=0$, the Taylor series expansion of (4.3.1) about $(f,\theta)=(f_0,\theta_0)$ is

$$\Phi = \alpha_1(f - f_0) + \alpha_2 \hat{\theta} + O\left((f - f_0)^2, (f - f_0)\hat{\theta}, \hat{\theta}^2\right), \tag{4.3.12}$$

where $\alpha_1 = \frac{\partial \Phi}{\partial f}|_{(f_0,\theta_0)}$ and $\alpha_2 = \frac{\partial \Phi}{\partial \theta}|_{(f_0,\theta_0)}$. Substituting (4.2.13) into (4.3.12) and retaining only first-order terms yields

$$\Phi = \left[\alpha_2 - \alpha_1 \left(\tilde{J}^* \eta_1^* - \eta^*\right)\right] \hat{\theta} - \alpha_1 \sigma^- \gamma_0. \tag{4.3.13}$$

For the case where α_1 is not continuous at f_0 , α_1 is taken to be the limiting value of $\frac{\partial \Phi}{\partial f}$ as f approaches f_0 from the side of f corresponding to a nonzero portion of Φ . Comparing (4.3.5) with (4.3.13), we can conclude that $\alpha_1 = \frac{1}{\nu}$ and $\alpha_2 = 0$, where $\nu = \nu_1$ or $\nu = \nu_2$, depending on which branch of (4.3.5) is considered. Comparing (4.3.8) and (4.3.11) with (4.3.13), we can conclude that $\alpha_1 = \frac{1}{\nu}$ and $\alpha_2 = -\frac{\mu}{\nu}$, where $\nu = \nu_1$, $\mu = \mu_1$ or $\nu = \nu_2$, $\mu = \mu_2$, depending on the case considered.

Note that there are other cases concerning the linearized form of (4.3.4) that can be considered. For example, one can consider the case where $f_1(\theta_0)$ and/or $f_2(\theta_0)$ are small and nonzero.

⁸ Note that although $f - f_0$ is not small for a relatively large range of values of $(\gamma^-, \gamma_1^+, \theta) \in B(\theta_0)$, $f - f_0$ does go to zero at the same rate as γ^- , γ_1^+ , and $\hat{\theta}(s)$ go to zero.

4.4 The Solution of the Boundary Value Problem

From Equation $(4.1.3)_1$ and the boundary condition given by $(4.1.7)_2$, we can conclude that

$$\sigma_1(x_1) = \sigma_0 \tag{4.4.1}$$

for $s(t) < x_1 \le L_1(t)$, at each $t \in \Gamma$. From Equation (4.1.2)₁, the jump condition (4.1.5)₁, and (4.4.1) given above, we obtain

$$\sigma(x) = \sigma_0 \,, \tag{4.4.2}$$

for $0 \le x < s(t)$, at each $t \in \Gamma$. Since the objective is to calculate the temperature at the interface and the corresponding kinetic relation, the displacements will not be calculated.

Using (4.2.11), Equation (4.1.2)₂ for phase 1 becomes

$$k\frac{d^2\hat{\theta}}{dx^2} = 0, (4.4.3)$$

 $\forall x \in (0, s(t))$, at each $t \in \Gamma$. Using (4.2.11) and (4.4.3) given above, Equation (4.1.2)₃ becomes

$$-k\left(\frac{1}{\theta}\frac{d\hat{\theta}}{dx}\right)^2 \le 0,\tag{4.4.4}$$

 $\forall x \in (0, s(t))$, at each $t \in \Gamma$. Additionally, the boundary condition (4.1.8)₁ in terms of $\hat{\theta}$ is

$$\hat{\theta}(0) = \bar{\theta},\tag{4.4.5}$$

where $\bar{\theta} = \theta^* - \theta_0$. From (4.4.4), we obtain the well-known result that $k \geq 0$. Assuming that k > 0, the solution of (4.4.3) that satisfies the boundary condition (4.4.5) is

$$\hat{\theta}(x) = C_1 x + \bar{\theta},\tag{4.4.6}$$

for $0 \le x < s(t)$, at each $t \in \Gamma$.

Using (4.2.12), Equation $(4.1.3)_2$ for phase 2 becomes

$$k_1 \frac{d^2 \hat{\theta}_1}{dx_1^2} = 0, (4.4.7)$$

 $\forall x_1 \in (s(t), L_1(t))$, at each $t \in \Gamma$. Using (4.2.12) and (4.4.7) given above, Equation (4.1.3)₃ yields $k_1 \geq 0$. The boundary condition (4.1.8)₂ in terms of $\hat{\theta}_1$ is

$$\hat{\theta}_1(L_1(t)) = \bar{\theta}_1,\tag{4.4.8}$$

where $\bar{\theta}_1 = \theta_1^* - \theta_0$. Assuming that $k_1 > 0$, the solution of (4.4.7) that satisfies the boundary condition (4.4.8) is

$$\hat{\theta}_1(x_1) = C_3(x_1 - L_1(t)) + \bar{\theta}_1, \tag{4.4.9}$$

for $s(t) < x_1 \le L_1(t)$, at each $t \in \Gamma$. From the continuity-of-temperature jump condition, we can solve for C_1 in (4.4.6) in terms of C_3 in (4.4.9) and obtain

$$\hat{\theta}(x) = \left\{ -C_3(1+\gamma_0)(L-s) + \bar{\theta}_1 - \bar{\theta} \right\} \frac{x}{s} + \bar{\theta}, \qquad (4.4.10)$$

for $0 \le x \le s(t)$, at each $t \in \Gamma$.

For the calculation of the first-order approximation of the energy jump condition, a kinetic relation that can have the forms of the kinetic relations given by (4.3.5),

(4.3.8), and (4.3.11) will be used. In particular, we consider the kinetic relation with the form

$$\dot{s} = \frac{1}{\nu(\theta)} \{ f - f^*(\theta) \}. \tag{4.4.11}$$

We next assume that the temperature θ_0 and the material are such that $f(0,0,\theta_0) = f^*(\theta_0)$. Considering this and substituting (4.2.13) and

$$f^* = f^*(\theta_0) + \mu \hat{\theta} + O(\hat{\theta}^2),$$
 (4.4.12)

where $\mu = \frac{df^*}{d\theta}\Big|_{\theta_0}$, into (4.4.11) and retaining only first-order terms yield

$$\dot{s} = -\frac{1}{\nu} \Big\{ \Big[\mu + \Big(\tilde{J}^* \eta_1^* - \eta^* \Big) \Big] \hat{\theta} + \sigma^- \gamma_0 \Big\}, \tag{4.4.13}$$

 $\forall (\gamma^-, \gamma_1^+, \theta) \in B(\theta_0)$, where $\sigma^- = \sigma_0$ for the problem considered here. This kinetic relation will be used for the boundary value problem under consideration. Using (4.2.13), (4.4.13), (4.2.11), and (4.2.12), the first-order approximation of the energy jump condition given by (4.1.5)₂ is

$$-\frac{1}{\nu} \Big\{ \theta_0 \Big(\tilde{J}^* \eta_1^* - \eta^* \Big) + f_0 \Big\} \Big\{ \Big[\mu + \Big(\tilde{J}^* \eta_1^* - \eta^* \Big) \Big] \hat{\theta} + \sigma_0 \gamma_0 \Big\}$$

$$+ \left(k_1 \left(\frac{d\hat{\theta}_1}{dx_1} \right)^+ - k \left(\frac{d\hat{\theta}}{dx} \right)^- \right) = 0.$$

$$(4.4.14)$$

The constant C_3 in Equations (4.4.9) and (4.4.10) will be determined from this equation. We next define the nondimensional quantities

$$\tilde{s} = \frac{s}{L}, \quad \tilde{\theta}(\tilde{s}) = \frac{\hat{\theta}(\tilde{s}L)}{\theta_0}, \quad \tilde{\theta}^* = \frac{\bar{\theta}}{\theta_0}, \quad \tilde{\theta}_1^* = \frac{\bar{\theta}_1}{\theta_0}, \quad \tilde{k} = \frac{k_1}{\tilde{J}^* k}, \quad (4.4.15)$$

$$ilde{\sigma}_0 = rac{\sigma_0 \gamma_0}{ heta_0 \Big[\mu + \Big(ilde{J}^* \eta_1^* - \eta^* \Big) \Big]} \,, \quad ilde{
u} = rac{
u k}{L \Big(ilde{J}^* arepsilon_1^* - arepsilon^* \Big) \Big[\mu + \Big(ilde{J}^* \eta_1^* - \eta^* \Big) \Big]} \,,$$

where ε_1^* is the internal energy of phase 2 evaluated at $(\gamma_1, \theta_1) = (0, \theta_0)$, ε^* is the internal energy of phase 1 evaluated at $(\gamma, \theta) = (0, \theta_0)$, and $(\tilde{J}^* \varepsilon_1^* - \varepsilon^*) = (\tilde{J}^* \psi_1^* - \psi^*) + \theta_0 (\tilde{J}^* \eta_1^* - \eta^*)$. Substituting (4.4.9) and (4.4.10) into (4.4.14), using the nondimensional quantities given by (4.4.15), and then solving for C_3 yield

$$C_{3} = \frac{\theta_{0} \left\{ \tilde{\sigma}_{0} + \tilde{\theta}_{1}^{*} + \frac{\tilde{\nu}(\tilde{\theta}_{1}^{*} - \tilde{\theta}^{*})}{\tilde{s}} \right\}}{L(1 + \gamma_{0})(1 - \tilde{s}) \left\{ 1 + \frac{\tilde{\nu}}{\tilde{s}} + \frac{\tilde{\nu}\tilde{k}}{(1 - \tilde{s})} \right\}}.$$

$$(4.4.16)$$

Substituting (4.4.16) into (4.4.9) or (4.4.10) yields the following for the temperature at the interface:

$$\tilde{\theta}(\tilde{s}) = \frac{\left(\tilde{\nu}\,\tilde{\theta}^* - \tilde{\sigma}_0\tilde{s}\right)(1-\tilde{s}) + \tilde{\nu}\,\tilde{k}\,\tilde{\theta}_1^*\tilde{s}}{(\tilde{\nu}+\tilde{s})(1-\tilde{s}) + \tilde{\nu}\,\tilde{k}\tilde{s}}.$$
(4.4.17)

4.5 The Temperature at the Interface

The temperature at the interface given by (4.4.17) for the three cases described in Section 4.3 will be studied as the material coefficients $\tilde{\nu}$ and \tilde{k} , the temperature boundary conditions $\tilde{\theta}^*$ and $\tilde{\theta}_1^*$, the end-load $\tilde{\sigma}_0$, and the position \tilde{s} of the phase boundary are varied. The temperature at the interface for each of these three cases can be obtained from (4.4.17) by substituting the appropriate values of ν and μ . For Cases II and III, when f is in an interval such that $\dot{s}=0$, the temperature at the interface can be obtained from (4.4.17) by letting $\nu \to \infty$.

Plots of $\tilde{\theta}(\tilde{s})$ vs \tilde{s} for several values of $\tilde{\nu}$ are presented in Figures 4.1 and 4.2. In these figures, and in the rest of the figures in this section, the values of $\tilde{\theta}(\tilde{s})$, $\tilde{\theta}^*$, $\tilde{\theta}_1^*$, and $\tilde{\sigma}_0$ that are shown should all be multiplied by some small number;

e.g., 10^{-5} . We note that such a multiplicative factor can be divided out in (4.4.17). The limiting values of $\tilde{\theta}(\tilde{s})$ as $\tilde{\nu} \to 0$ and $\tilde{\nu} \to \infty$ are

$$\lim_{\tilde{\nu} \to 0} \tilde{\theta}(\tilde{s}) = -\tilde{\sigma}_{0},$$

$$\lim_{\tilde{\nu} \to \infty} \tilde{\theta}(\tilde{s}) = \frac{\tilde{\theta}^{*}(1 - \tilde{s}) + \tilde{\theta}_{1}^{*}\tilde{k}\tilde{s}}{1 - \tilde{s} + \tilde{k}\tilde{s}},$$
(4.5.1)

respectively. An easy calculation shows that as $\tilde{\nu}$ is varied, $\frac{\partial \tilde{\theta}(\tilde{s})}{\partial \tilde{\nu}} \to 0$ only as $\tilde{\nu} \to \infty$, and that $\lim_{\tilde{\nu} \to \infty} \frac{\partial^2 \tilde{\theta}(\tilde{s})}{\partial \tilde{\nu}^2} = 0$. Therefore, as $\tilde{\nu}$ is varied, $\tilde{\theta}(\tilde{s})$ (at a given \tilde{s}) monotonically increases or decreases, depending on the values of the other parameters.⁹ Also, note that $(4.5.1)_2$ is the temperature at the interface for Cases II and III when f is in an interval such that $\dot{s} = 0$.

Plots of $\tilde{\theta}(\tilde{s})$ vs. \tilde{s} for several values of \tilde{k} are presented in Figure 4.3. The limiting values of $\tilde{\theta}(\tilde{s})$ as $\tilde{k} \to 0$ and $\tilde{k} \to \infty$ are

$$\lim_{\tilde{k}\to 0} \tilde{\theta}(\tilde{s}) = \frac{-\tilde{\sigma}_0 \tilde{s} + \tilde{\nu} \tilde{\theta}^*}{\tilde{s} + \tilde{\nu}},$$

$$\lim_{\tilde{k}\to \infty} \tilde{\theta}(\tilde{s}) = \tilde{\theta}_1^*,$$
(4.5.2)

respectively. An easy calculation shows that as \tilde{k} is varied, $\frac{\partial \tilde{\theta}(\tilde{s})}{\partial \tilde{k}} \to 0$ only as $\tilde{k} \to \infty$, and that $\lim_{\tilde{\nu} \to \infty} \frac{\partial^2 \tilde{\theta}(\tilde{s})}{\partial \tilde{k}^2} = 0$. Therefore, as \tilde{k} is varied, $\tilde{\theta}(\tilde{s})$ monotonically increases or decreases, depending on the values of the other parameters.

Plots of $\tilde{\theta}(\tilde{s})$ vs \tilde{s} for several values of $\tilde{\sigma}_0$ are presented in Figures 4.4 and 4.5. The limiting value of $\tilde{\theta}(\tilde{s})$ as $\tilde{\sigma}_0 \to 0$ can be easily observed from (4.4.17), and the limiting value of $\tilde{\theta}(\tilde{s})$ as $\tilde{\sigma}_0 \to \infty$ is ∞ .

⁹ Whether $\tilde{\theta}(\tilde{s})$ monotonically increases or decreases can, of course, be determined by comparing (4.5.1)₁ and (4.5.1)₂ for a given set of parameter values.

The values of $\tilde{\theta}(\tilde{s})$ as $\tilde{s} \to 0$ and $\tilde{s} \to 1$ are

$$\lim_{\tilde{s}\to 0} \tilde{\theta}(\tilde{s}) = \tilde{\theta}^*, \qquad \lim_{\tilde{s}\to 1} \tilde{\theta}(\tilde{s}) = \tilde{\theta}_1^*, \qquad (4.5.3)$$

respectively. These results should be expected. An extremum of $\tilde{\theta}(\tilde{s})$ can, of course, be determined from

$$\frac{d\tilde{\theta}(\tilde{s})}{d\tilde{s}} = 0. {(4.5.4)}$$

For a given set of material coefficients and boundary conditions, the values of \tilde{s} that satisfy (4.5.4) are

$$\tilde{s} = \frac{\tilde{\sigma}_0 + \tilde{\theta}^*}{\tilde{\sigma}_0 \left(1 - \tilde{k}\right) + \tilde{\theta}^* - \tilde{k}\tilde{\theta}_1^*}$$

$$\pm \sqrt{\left(\frac{\tilde{\sigma}_0 + \tilde{\theta}^*}{\tilde{\sigma}_0 \left(1 - \tilde{k}\right) + \tilde{\theta}^* - \tilde{k}\tilde{\theta}_1^*}\right)^2 + \frac{\tilde{\nu}\,\tilde{k}\left(\tilde{\theta}_1^* - \tilde{\theta}^*\right) - \left(\tilde{\sigma}_0 + \tilde{\theta}^*\right)}{\tilde{\sigma}_0 \left(1 - \tilde{k}\right) + \tilde{\theta}^* - \tilde{k}\tilde{\theta}_1^*}} \quad . \tag{4.5.5}$$

Note that for a given set of parameters, \tilde{s} given by (4.5.5) is a physically meaningful solution only if it is real-valued and is such that $0 < \tilde{s} < 1$.

4.6 A Quasi-Static Process

In this section, a quasi-static process will be considered for the three cases described in Section 4.3. The direction of motion of the phase boundary will be considered and the static equilibrium positions of the phase boundary will be determined. For the following cases, let

$$\dot{\tilde{s}} = \frac{d\tilde{s}(\tilde{t})}{d\tilde{t}}, \qquad \tilde{t} = t \left(\frac{k\theta_0}{L^2 \left(\tilde{J}^* \varepsilon_1^* - \varepsilon^* \right)} \right). \tag{4.6.1}$$

Before we consider the three cases, however, we will first consider the signs of some of the variables that have the same signs for all of the cases considered. As is usually done, we assume that the dependence of the Gibbs free energy g^* for an unstressed phase 1 and the Gibbs free energy $\tilde{J}^*g_1^*$ for an unstressed phase 2 (with respect to R⁺) on the temperature is qualitatively like that presented in Figure 4.6.¹⁰ As can be observed from the definitions of the Gibbs free energies of both phases that were given in Section 2.12, $\psi^*=g^*$ and $\psi_1^*=g_1^*$ for all temperatures where the undeformed configurations of both phases are unstressed. From this, we can conclude that $\eta^* > \tilde{J}^*\eta_1^* \ \forall \ \theta \in \Omega$, for the case under consideration. We also always have $L>0,\ \theta_0\geq 0,\ \tilde{J}>0,\ k>0,\ k_1>0,\ \text{and }\nu\geq 0.$ From this, we can conclude that $\tilde{k} \geq 0$. We can also conclude from this, and the kinetic relations presented in Section 4.3, that for a given σ_0 , an increase in temperature will result in an increase in f, and a decrease in temperature will result in a decrease in f. Therefore, if phase 1 represents the austenite and phase 2 represents the martensite, which is what corresponds to Figure 4.6, an increase in temperature favors the austenite, and a decrease in temperature favors the martensite. This corresponds exactly with experimental observations and what was discussed in Section 1.2.1.

<u>Case I</u>: From the description of this case given in Section 4.3, we have $\tilde{J}^*\psi_1^* - \psi^* = 0$ and $\mu = 0$. We next make the additional assumption that $\nu_1 = \nu_2 = \nu$, and we let

$$\tilde{\nu}' = \tilde{\nu}|_{\mu=0}, \quad \tilde{\sigma}'_0 = \tilde{\sigma}_0|_{\mu=0}.$$
 (4.6.2)

For this case, the sign of $\dot{\tilde{s}}$ is opposite the sign of \tilde{s} , the sign of $\tilde{\sigma}'_0$ is opposite the sign of $\sigma_0 \gamma_0$, $\tilde{\nu}' \geq 0$, and the kinetic relation given by (4.3.5) in terms of the nondimensional variables is

$$\dot{\tilde{s}} = -\frac{1}{\tilde{\nu}'} \left(\tilde{\theta}' + \tilde{\sigma}'_0 \right), \tag{4.6.3}$$

¹⁰ See [13] and Section 1.2.1 of this thesis.

where $\tilde{\theta}'$ is the temperature at the interface given by (4.4.17) with $(\tilde{\nu}, \tilde{\sigma}_0) = (\tilde{\nu}', \tilde{\sigma}'_0)$. For the quasi-static process under consideration, static equilibrium occurs when $\dot{\tilde{s}} = 0$. From (4.6.3), we can conclude that this occurs when

$$\tilde{\theta}(\tilde{s}) = -\tilde{\sigma}_0'. \tag{4.6.4}^{11}$$

Using (4.4.17) in (4.6.4), the static equilibrium position of the phase boundary for a given set of material coefficients and boundary conditions will occur at

$$\tilde{s} = \frac{\tilde{\theta}^* + \tilde{\sigma}_0'}{\tilde{\theta}^* - k\tilde{\theta}_1^* + \left(1 - \tilde{k}\right)\tilde{\sigma}_0'},\tag{4.6.5}$$

with the requirement that $0 < \tilde{s} < 1$. We note that in Figures 4.1 and 4.2, where plots of $\tilde{\theta}(\tilde{s})$ vs \tilde{s} for several values of $\tilde{\nu}$ are presented, the static equilibrium positions given by (4.6.5) occur where all of the temperature curves intersect. This is because the static equilibrium position of the phase boundary given by (4.6.5) is independent of $\tilde{\nu}$. From (4.6.3) and the fact that the sign of $\dot{\tilde{s}}$ is opposite the sign of \dot{s} , we can conclude that $\dot{s} > 0$ for $\tilde{\theta}(\tilde{s}) > -\tilde{\sigma}'_0$, and $\dot{s} < 0$ for $\tilde{\theta}(\tilde{s}) < -\tilde{\sigma}'_0$. Because of this, the static equilibrium positions in Figures 4.1 and 4.4 are unstable, in the sense that the phase boundary will move away from these static equilibrium positions for any perturbation away from them, and the static equilibrium positions in Figures 4.2, 4.3, and 4.5 are stable. In Figures 4.4 and 4.5, some values of $\tilde{\sigma}_0$ are used which result in the static equilibrium position determined by (4.6.5) being outside the interval (0,1). Consequently, the static equilibrium states of the bar for these values of $\tilde{\sigma}_0$ consist of only one phase.

In the remainder of this section, the temperature at the interface may sometimes be referred to simply as $\tilde{\theta}(\tilde{s})$, with the understanding that it corresponds to the case under consideration.

The case where $\tilde{J}^*\eta_1^*=\eta^*$ in addition to $\tilde{J}^*\psi_1^*=\psi^*$ can also be considered here. In particular, for this case, the first-order approximation of the energy jump condition reduces to the continuity of heat fluxes across the phase boundary. From (4.4.14), we can conclude that the temperature solution for this case is the same as the temperature solution for the case where $\nu \to \infty$. Thus, the temperature and quasi-static motions for the case where $\tilde{J}^*\psi_1^*=\psi^*$ and $\tilde{J}^*\eta_1^*=\eta^*$ are the same as they are for the cases presented here for Case I, where $\tilde{\nu} \to \infty$.

Case II: For this case, let

$$\tilde{\nu}_1 = \tilde{\nu}|_{(\nu,\mu)=(\nu_1,\mu_1)}, \qquad \tilde{\sigma}_1 = \tilde{\sigma}_0|_{\mu=\mu_1}.$$
 (4.6.6)

From the description of this case given in Section 4.3, we have $\tilde{J}\psi_1^* < \psi^*$. If we also make the assumption that $|\mu| < |J^*\eta_1^* - \eta^*|$, the sign of $\dot{\tilde{s}}$ will be opposite that of \dot{s} , the sign of $\tilde{\sigma}_1$ will be opposite that of $\sigma_0\gamma_0$, and $\tilde{\nu}_1 \geq 0$. The kinetic relation given by (4.3.8) in terms of the nondimensional variables is

$$\dot{\tilde{s}} = \begin{cases} 0, & \left(\tilde{\theta}^{(2)} + \tilde{\sigma}_1\right) \ge 0\\ -\frac{1}{\tilde{\nu}_1} \left(\tilde{\theta}^{(1)} + \tilde{\sigma}_1\right), & \left(\tilde{\theta}^{(1)} + \tilde{\sigma}_1\right) \le 0 \end{cases}, \tag{4.6.7}$$

where $\tilde{\theta}^{(1)}$ is the temperature at the interface given by (4.4.17) with $(\tilde{\nu}, \tilde{\sigma}_0) = (\tilde{\nu}_1, \tilde{\sigma}_1)$, and $\tilde{\theta}^{(2)}$ is given by (4.5.1)₂, which corresponds to (4.4.17) with $\nu \to \infty$. In Figures 4.7 and 4.8, plots of $\tilde{\theta}(\tilde{s})$ vs \tilde{s} for $\tilde{\nu}=0.1$ and $\tilde{\nu}\to\infty$ are presented. The case where $\tilde{\nu}=0.1$ represents $\tilde{\theta}^{(1)}$ with $\tilde{\nu}_1=0.1$, and the case where $\nu\to\infty$ represents $\tilde{\theta}^{(2)}$. Quasi-static processes will be considered for the cases presented in these two figures. The position of the phase boundary corresponding to $\tilde{\theta}(\tilde{s})=-\tilde{\sigma}_0$ is given by (4.6.5) with $\tilde{\sigma}_0'=\tilde{\sigma}_1$. This static equilibrium position also corresponds to the point

¹² These assumptions might be most appropriate for the case where phase 1 and phase 2 represent two different variants of the same martensite.

where $\tilde{\theta}^{(1)}$ and $\tilde{\theta}^{(2)}$ intersect, since it is independent of $\tilde{\nu}$. When $\tilde{\theta}(\tilde{s}(\tilde{t}_0)) < -\tilde{\sigma}_1$, the temperature at the interface is given by $\tilde{\theta}^{(1)}$, and when $\tilde{\theta}(\tilde{s}(\tilde{t}_0)) > -\tilde{\sigma}_1$, the temperature at the interface is given by $\tilde{\theta}^{(2)}$. From (4.6.7), we can conclude that a phase boundary with an initial position of $\tilde{s}(\tilde{t}_0)$ such that $\tilde{\theta}(\tilde{s}(\tilde{t}_0)) > -\tilde{\sigma}_1$ will stay at that position, and a phase transformation will not occur. However, a phase boundary with an initial position such that $\tilde{\theta}(\tilde{s}(\tilde{t}_0)) < -\tilde{\sigma}_1$ will have a $\dot{s} < 0$, and consequently, phase 1 will be converted into phase 2.

Case III: For this case, let

$$\tilde{\nu}_2 = \tilde{\nu}|_{(\nu,\mu)=(\nu_2,\mu_2)}, \qquad \tilde{\sigma}_2 = \tilde{\sigma}_0|_{\mu=\mu_2}.$$
 (4.6.8)

From the description of this case given in Section 4.3, we have $\psi^* < \tilde{J}\psi_1^*$. Also, for the following, we assume that $|\mu| < |J^*\eta_1^* - \eta^*|$. For this case, the sign of $\tilde{\nu}$ and the sign of $\dot{s}(t)$ in relation to $\dot{\tilde{s}}$ depend on the relative values of $(J\psi_1^* - \psi^*)$ and $\theta_0(J\eta_1^* - \eta^*)$. Thus, we cannot make such definite conclusions concerning the sign of $\tilde{\nu}$ and the sign of $\dot{s}(t)$ in relation to $\dot{\tilde{s}}$ for this case, as we were able to do for the two cases discussed previously. The kinetic relation given by (4.3.11) in terms of the nondimensional variables is

$$\dot{\tilde{s}} = \begin{cases} -\frac{1}{\tilde{\nu}_2} \left(\tilde{\theta}^{(2)} + \tilde{\sigma}_2 \right), & \left(\tilde{\theta}^{(2)} + \tilde{\sigma}_2 \right) \ge 0 \\ 0, & \left(\tilde{\theta}^{(1)} + \tilde{\sigma}_2 \right) \le 0 \end{cases}, \tag{4.6.9}$$

where $\tilde{\theta}^{(1)}$ is the temperature at the interface given by $(4.5.1)_2$, which corresponds to (4.4.17) with $\nu \to \infty$, and $\tilde{\theta}^{(2)}$ is the temperature at the interface given by (4.4.17) with $(\tilde{\nu}, \tilde{\sigma}_0) = (\tilde{\nu}_2, \tilde{\sigma}_2)$. For this case, we will consider a quasi-static process for the cases presented in Figures 4.7 and 4.8. The position of the phase boundary corresponding to $\tilde{\theta}(\tilde{s}) = -\tilde{\sigma}_2$ is given by (4.6.5) with $\tilde{\sigma}_0' = \tilde{\sigma}_2$. This static equilibrium position also

corresponds to the point where $\tilde{\theta}^{(1)}$ and $\tilde{\theta}^{(2)}$ intersect, since it is independent of $\tilde{\nu}$. When $\tilde{\theta}(\tilde{s}(\tilde{t}_0))<-\tilde{\sigma}_1$, the temperature at the interface is given by $\tilde{\theta}^{(1)}$, and when $\tilde{\theta}(\tilde{s}(\tilde{t}_0))>-\tilde{\sigma}_1$, the temperature at the interface is given by $\tilde{\theta}^{(2)}$. From (4.6.9), we can conclude that a phase boundary with an initial position of $\tilde{s}(\tilde{t}_0)$ such that $\tilde{\theta}(\tilde{s}(\tilde{t}_0))<-\tilde{\sigma}_2$ will stay at that position, and a phase transformation will not occur. However, a phase boundary with an initial position such that $\tilde{\theta}(\tilde{s}(\tilde{t}_0))>-\tilde{\sigma}_2$ will have a $\dot{s}>0$, and consequently, phase 2 will be converted into phase 1.

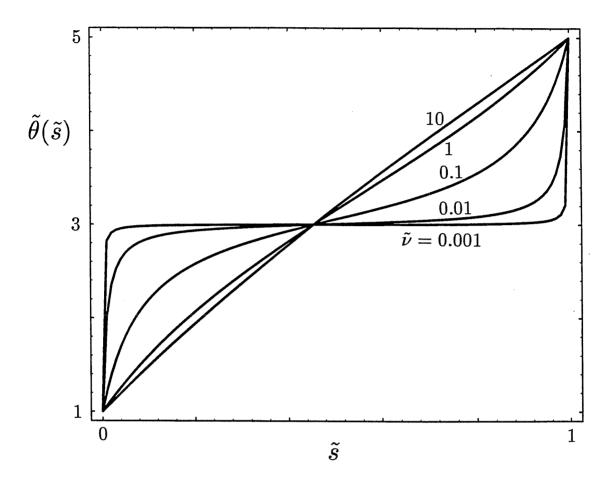


Figure 4.1. The temperature at the interface vs. the position of the interface as $\tilde{\nu}$ varies; $\tilde{\theta}^* = 1$, $\tilde{\theta}_1^* = 5$, $\tilde{\sigma}_0 = -3$, $\tilde{k} = 1.2$.

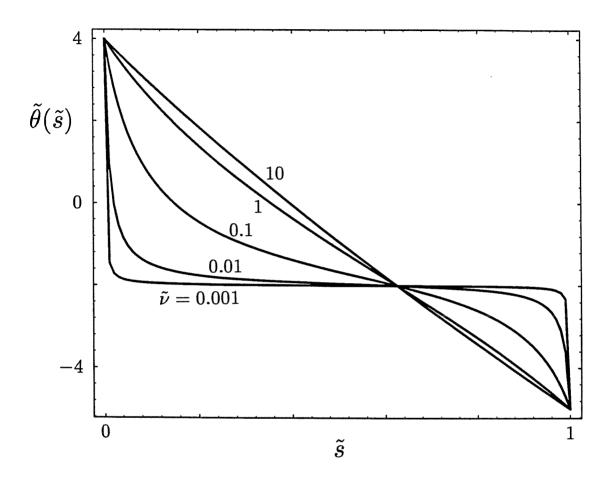


Figure 4.2. The temperature at the interface vs. the position of the interface as $\tilde{\nu}$ varies; $\tilde{\theta}^* = 4$, $\tilde{\theta}_1^* = -5$, $\tilde{\sigma}_0 = 2$, $\tilde{k} = 1.2$.

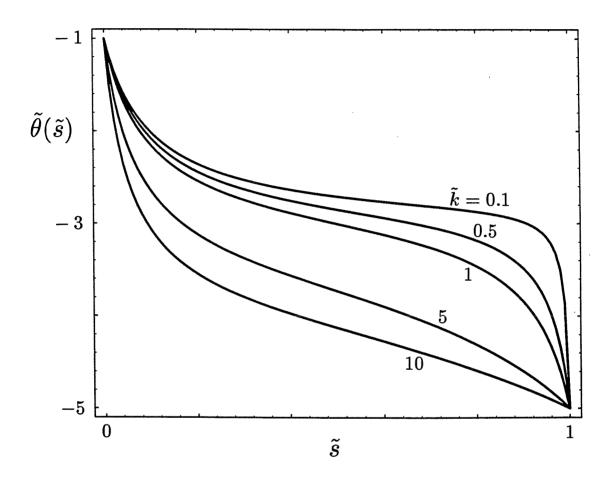


Figure 4.3. The temperature at the interface vs. the position of the interface as \tilde{k} varies; $\tilde{\theta}^* = -1$, $\tilde{\theta}_1^* = -5$, $\tilde{\sigma}_0 = 3$, $\tilde{\nu} = 0.1$.

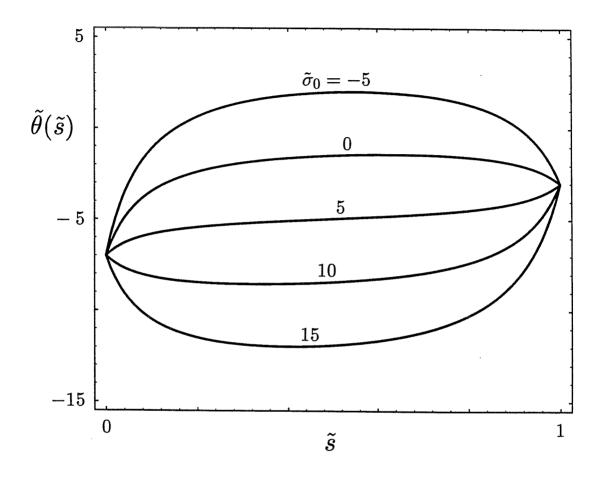


Figure 4.4. The temperature at the interface vs. the position of the interface as $\tilde{\sigma}_0$ varies; $\tilde{\theta}^* = -7$, $\tilde{\theta}_1^* = -3$, $\tilde{\nu} = 0.1$, $\tilde{k} = 1.2$.

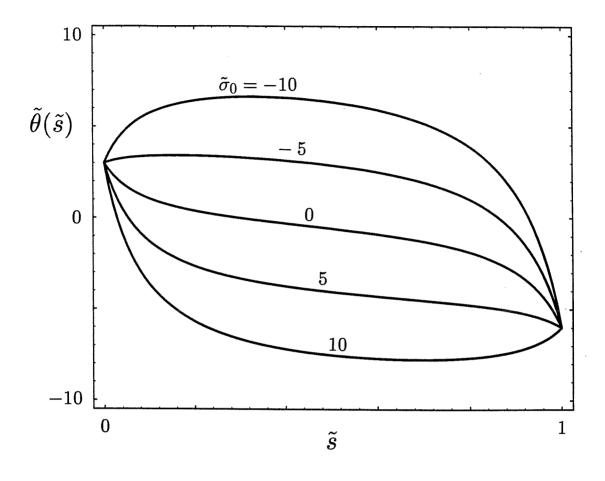


Figure 4.5. The temperature at the interface vs. the position of the interface as $\tilde{\sigma}_0$ varies; $\tilde{\theta}^*=3,~\tilde{\theta}_1^*=-6,~\tilde{\nu}=0.1,~\tilde{k}=1.2.$

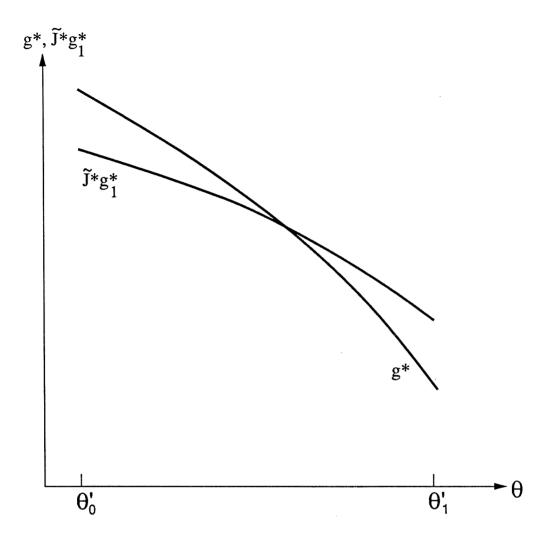


Figure 4.6. The dependence of the Gibbs free energies of the undeformed phase 1 and the undeformed phase 2 on the temperature $\theta \in \Omega$.

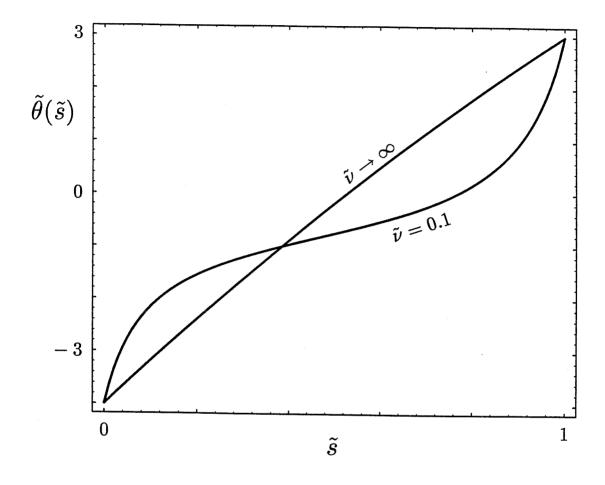


Figure 4.7. The temperature at the interface vs. the position of the interface for $\tilde{\nu}=0.1$ and $\tilde{\nu}\to\infty$; $\tilde{\theta}^*=-4,\ \tilde{\theta}_1^*=3,\ \tilde{\sigma}_0=1,\ \tilde{k}=1.2.$

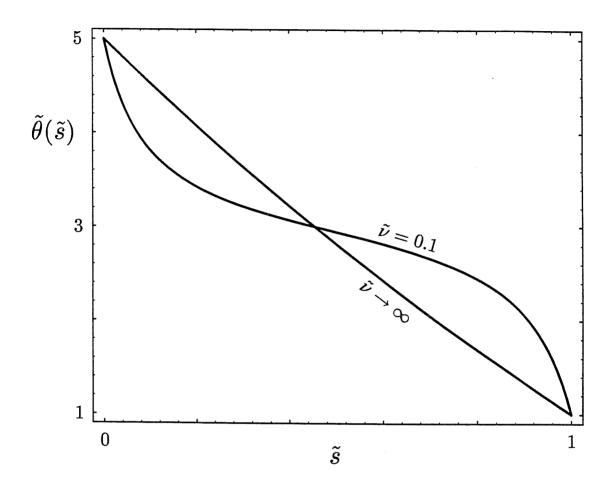


Figure 4.8. The temperature at the interface vs. the position of the interface for $\tilde{\nu}=0.1$ and $\tilde{\nu}\to\infty;~\tilde{\theta}^*=5,~\tilde{\theta}_1^*=1,~\tilde{\sigma}_0=-3,~\tilde{k}=1.2.$

CHAPTER 5

THE FREE VIBRATIONS OF A TWO-PHASE BAR

In this chapter, the longitudinal free vibrations of a fixed-free, two-phase bar are studied. For an elastic bar consisting entirely of one phase, it is well known that during the free vibrations of the bar, the displacement and stress at each point of the bar oscillate as time progresses [12]. If there is damping present, these oscillations will decay and go to zero as time goes to infinity; otherwise, their amplitudes will remain constant in time. Considering this, for a bar that initially consists of two different phases that both behave elastically, one might expect that the displacement and stress at each point of the bar will also have oscillatory-type behavior during the free vibrations of the bar. If this is the case, the driving traction at the interface separating the two phases will oscillate. As a result of this, if the nominal phase boundary velocity is related to the driving traction through a kinetic relation that does not have an interval of the driving traction corresponding to a zero nominal phase boundary velocity, the nominal phase boundary velocity will also oscillate. Since energy is dissipated when the phase boundary moves and passes over particles of material of one phase, converting them into particles of material of the other phase, one might conclude that the oscillatory-type response of the two-phase bar during the free vibrations of the bar should decay as time increases. It is this damping behavior of the two-phase bar that will be the main subject of this chapter. The solutions of the boundary value problem will be determined by a numerical method, and the damping of the two-phase bar will be studied as the material coefficients are varied. The values of the material coefficients resulting in the maximum damping will also be investigated.

5.1 The Field Equations and Jump Conditions

A one-dimensional, finite bar that initially consists of two phases is considered. It is assumed that the process under consideration is a purely mechanical process with no body forces present. It is further assumed that the process occurs in a time interval $\Gamma = [t_0, t_1]$. Unless otherwise indicated, the notation used in Chapter 2 will be used in the following, with the understanding that it corresponds to the one-dimensional problem under consideration. Let x = s(t) be the location of the phase boundary at time $t \in \Gamma$, and let L be the length of the bar with respect to the reference configuration R. Considering this, $R = \{x/x \in [0, L]\}$, $R^- = \{x/x \in [0, s(t)]\}$, and $R^+ = \{x/x \in [s(t), L]\}$. It is assumed that $\tilde{x}_1(\cdot, t) : R^+ \mapsto R_1^+$ at each $t \in \Gamma$ is given by

$$\tilde{x}_1(x,t) = x + \gamma_0(x - s(t)).$$
 (5.1.1)

The displacement gradient (transformation strain) corresponding to this choice of \tilde{x}_1 is γ_0 , the Jacobian is $\tilde{J}=1+\gamma_0$, and $R_1^+=\{x_1/x_1\in [\tilde{x}_1(s(t),t),\tilde{x}_1(L,t)]\}=\{x_1/x_1\in [s(t),L_1(t)]\}$, where $L_1(t)=\tilde{x}_1(L,t)=L+\gamma_0(L-s(t))$. It is also assumed that $\gamma_0>-1$, so that reflections are excluded from (5.1.1). Additionally, the inverse of the \tilde{x}_1 given by (5.1.1) is

$$\tilde{x}(x_1,t) = \frac{1}{1+\gamma_0}(x_1+\gamma_0 s(t)),$$
 (5.1.2)

 $\forall x_1 \in \mathbb{R}_1^+$ at each $t \in \Gamma$. In the following, the phase occupying \mathbb{R}^- at each $t \in \Gamma$ will be referred to as phase 1, and the phase occupying \mathbb{R}_1^+ at each $t \in \Gamma$ will be referred to as phase 2. The suitably smooth and invertible mapping that maps \mathbb{R} into the current deformed configuration of the bar at each $t \in \Gamma$ is $\hat{y}(x,t)$, with $\hat{y}(x,t) = x + \hat{u}(x,t)$, and the suitably smooth and invertible mapping that maps \mathbb{R}_1^+ into the current deformed configuration of phase 2 at each $t \in \Gamma$ is $\hat{y}_1(x_1,t)$, with $\hat{y}_1(x_1,t) = x_1 + \hat{u}_1(x_1,t)$.

The field equations for the problem under consideration consist of the balance of linear momentum for phase 1 and the balance of linear momentum for phase 2. These equations are

$$\frac{\partial \sigma}{\partial x} = \rho a,\tag{5.1.3}$$

 $\forall x \in \mathbb{R}^-$ at each $t \in \Gamma$, and

$$\frac{\partial \sigma_1}{\partial x_1} = \bar{\rho}_1 \bar{a}_1,\tag{5.1.4}$$

 $\forall x_1 \in \mathbb{R}_1^+$ at each $t \in \Gamma$, respectively.

The continuity-of-displacement condition in its most direct form is

$$y_1^+(s(t),t) = y^-(s(t),t).$$
 (5.1.5)

For the \tilde{x}_1 given by (5.1.1), (5.1.5) reduces to

$$\hat{u}_1^+(s(t),t) = \hat{u}^-(s(t),t). \tag{5.1.6}$$

The jump condition at x = s(t) representing the balance of linear momentum is

$$\sigma_1^+ - \sigma^- + \rho(\bar{v}_1^+ - v^-)\dot{s} = 0, \tag{5.1.7}$$

where $\dot{s}(t) = \frac{ds(t)}{dt}$. Differentiating (5.1.5) with respect to time yields

$$(\gamma_0 + \gamma_1^+ \gamma_0 + \gamma_1^+ - \gamma^-) \dot{s} + \bar{v}_1^+ - v^- = 0, \tag{5.1.8}$$

at x=s(t), where $\gamma=\frac{\partial \hat{u}}{\partial x}$ and $\gamma_1=\frac{\partial \hat{u}_1}{\partial x_1}$. Using (5.1.8) in (5.1.7), we can obtain an alternate form for the linear momentum jump condition:

$$\sigma_1^+ - \sigma^- = \rho (\gamma_0 + \gamma_1^+ \gamma_0 + \gamma_1^+ - \gamma^-) (\dot{s})^2. \tag{5.1.9}$$

The remaining equation at the phase boundary is a kinetic relation relating \dot{s} and the driving traction f. This kinetic relation is a constitutive equation and will be discussed

in the next section. For the problem under consideration, the driving traction is given by

$$f = \tilde{J} W_1^+ - W^- - \frac{1}{2} (\sigma_1^+ + \sigma^-) (\gamma_0 + \gamma_1^+ \gamma_0 + \gamma_1^+ - \gamma^-).$$
 (5.1.10)

We also have the boundary conditions at x = 0 and $x_1 = L_1(t)$ (or x = L). For the fixed boundary condition at x = 0, we have

$$u(0,t) = 0, (5.1.11)$$

 $\forall t \in \Gamma$. At the $x_1 = L_1(t)$ boundary, there is nothing applied to the boundary; i.e., it is a free boundary. Therefore, the traction at this boundary is necessarily zero. Thus, the boundary condition at $x_1 = L_1(t)$ is

$$\sigma_1(L_1(t), t) = 0,$$
 (5.1.12)

 $\forall t \in \Gamma$.

5.2 The Constitutive Equations

It is assumed that both phase 1 and phase 2 are homogeneous, hyperelastic materials of the type described in Section 2.6. In particular, for phase 1 we assume that there exists an elastic potential

$$W = W(\gamma), \tag{5.2.1}$$

such that

$$\sigma = \frac{\partial W}{\partial \gamma} \,, \tag{5.2.2}$$

and for phase 2 we assume that there exists an elastic potential

$$W_1 = W_1(\gamma_1), (5.2.3)$$

such that

$$\sigma_1 = \frac{\partial W_1}{\partial \gamma_1}.\tag{5.2.4}$$

If we solve for $u_1 = \hat{u}_1(x_1,t)$ in the dynamic boundary value problem, the acceleration term \bar{u}_1 in Equation (5.1.4) will contain several inertial-type terms that are solely a result of \tilde{x}_1 being a function of time. This was discussed for the general three-dimensional problem in Section 2.10. As was further discussed there, but again for the general three-dimensional problem, these inertial-type terms can be avoided instead by solving for $u_1 = \bar{u}_1(x,t)$ in the boundary value problem, where $\bar{u}_1(x,t) = \hat{u}_1(\tilde{x}_1(x,t),t)$ and $\hat{u}_1(x_1,t) = \bar{u}_1(\tilde{x}_1(x,t),t)$. This will be done in the boundary value problem considered here.

It is assumed that phase 1 is unstressed at $\gamma=0$ and phase 2 is unstressed at $\gamma_1=0$. We next assume that the initial conditions are such that $|\gamma|<<1\ \forall\ x\in[0,s(t))$ and $|\gamma_1|<<1\ \forall\ x\in(s(t),L]$, at each $t\in\Gamma$, where here and in the following, $\gamma_1=\frac{\partial \bar{u}_1}{\partial x_1}=\frac{\partial \bar{u}_1}{\partial x}\frac{\partial \bar{x}}{\partial x_1}$. For the \tilde{x} given by (5.1.2), $\gamma_1=\frac{1}{1+\gamma_0}\frac{\partial \bar{u}_1}{\partial x}$. For these assumptions, W for phase 1 can be written as

$$W = W^* + \frac{1}{2}E\gamma^2 + O(\gamma^3), \tag{5.2.5}$$

where $W^*=W(0)$ and $E=\frac{\partial^2 W}{\partial \gamma^2}|_{\gamma=0}$, and W_1 for phase 2 can be written as

$$W_1 = W_1^* + \frac{1}{2}E_1\gamma_1^2 + \mathcal{O}(\gamma_1^3), \tag{5.2.6}$$

where $W_1^*=W_1(0)$ and $E_1=\frac{\partial^2 W_1}{\partial \gamma_1^2}|_{\gamma_1=0}$. From (5.2.2) and (5.2.5), the first-order approximation of σ for phase 1 is

$$\sigma = E\gamma = E\frac{\partial \hat{u}}{\partial x},\tag{5.2.7}$$

and from (5.2.4) and (5.2.6) the first-order approximation of σ_1 for phase 2 is

$$\sigma_1 = E_1 \gamma_1 = \frac{E_1}{1 + \gamma_0} \frac{\partial \bar{u}_1}{\partial x}. \tag{5.2.8}$$

We note that the constitutive quantities for phase 1 given by (5.2.1), (5.2.2), (5.2.5), and (5.2.7) are defined with respect to R^- , and the constitutive quantities for phase 2 given by (5.2.3), (5.2.4), (5.2.6), and (5.2.8) are defined with respect to R_1^+ , even though (5.2.6) and (5.2.8) are in terms of the independent variable $x \in R^+$.

We next assume that $W^* = \tilde{J} W_1^*$. This assumption might be most appropriate if phase 1 and phase 2 represent two different variants of the same martensite. We note, however, that if this were the case, we need not assume that $\tilde{E}_1 = \tilde{E}$, since in a real three-dimensional material the moduli in a given direction of two variants of martensite separated by a phase boundary are not, in general, the same, and this can be incorporated into a one-dimensional model by assuming that $\tilde{E}_1 \neq \tilde{E}$. For these assumptions and using (5.2.5)-(5.2.8), the first-order approximation of the driving traction given by (5.1.10) is

$$f = -\frac{1}{2} \left\{ \frac{E_1}{1 + \gamma_0} \left(\frac{\partial \bar{u}_1}{\partial x} \right)^{+} + E \left(\frac{\partial \hat{u}}{\partial x} \right)^{-} \right\} \gamma_0.$$
 (5.2.9)

We next postulate a kinetic (constitutive) relation

$$\dot{s} = \Phi(f),\tag{5.2.10}$$

such that

$$\Phi(f)f \ge 0,\tag{5.2.11}$$

for all f. The requirement given by (5.2.11) is imposed so that energy is dissipated (or preserved if the equality sign holds) during a phase transformation, instead of being

created. We further assume that for the problem under consideration, the first-order form of $\Phi(f)$ is

$$\Phi(f) = \frac{1}{\nu}f = -\frac{\gamma_0}{2\nu} \left\{ \frac{E_1}{1+\gamma_0} \left(\frac{\partial \bar{u}_1}{\partial x} \right)^+ + E \left(\frac{\partial \hat{u}}{\partial x} \right)^- \right\}, \tag{5.2.12}$$

where the constant ν depends on the material and is such that $\nu \geq 0$ so that (5.2.11) is satisfied.

5.3 The Boundary Value Problem

Substituting (5.2.7) into (5.1.3) and expressing the acceleration in that equation in terms of \hat{u} , we obtain the following for the balance of linear momentum for phase 1:

$$E\frac{\partial^2 \hat{u}}{\partial x^2} = \rho \frac{\partial^2 \hat{u}}{\partial t^2}, \qquad (5.3.1)$$

 $\forall x \in (0, s(t))$ at each $t \in \Gamma$. Substituting (5.2.8) and $\bar{\rho}_1 = \rho/\tilde{J} = \rho/(1 + \gamma_0)$ into (5.1.4), and calculating \bar{a}_1 in that equation using $\hat{y}_1(\tilde{x}_1(x,t),t) = \tilde{x}_1(x,t) + \bar{u}_1(x,t)$, we obtain the following for the balance of linear momentum for phase 2:

$$\frac{E_1}{(1+\gamma_0)}\frac{\partial^2 \bar{u}_1}{\partial x^2} = \rho \left(-\gamma_0 \frac{d^2 s}{dt^2} + \frac{\partial^2 \bar{u}_1}{\partial t^2}\right),\tag{5.3.2}$$

 $\forall x \in (s(t), L) \text{ at each } t \in \Gamma.$

For the linearized problem, the continuity-of-displacement condition is still given by (5.1.6), since there is nothing to linearize in that equation. We next consider the linearized form of the linear momentum jump condition given by (5.1.9). Because \dot{s} is related to γ and γ_1 through the kinetic relation given by (5.2.12), \dot{s}^2 is second-order in

¹ See Section 2.9.

 γ and γ_1 ; i.e., \dot{s}^2 goes to zero at the same rate as γ^2 , γ_1^2 , and γ_1 go to zero. However, the second-order terms in \dot{s}^2 also contain the constants E^2/ν , E_1^2/ν , and EE_1/ν . Considering the fact that the magnitudes of E and E_1 are very large, if the magnitude of ν is not also large, γ and γ_1 might have to be unrealistically small in order for the terms in \dot{s}^2 to have magnitudes that are negligible in comparison to the magnitudes of the first-order terms. In the following, it will be assumed that the values of the material coefficients are such that the magnitudes of the second-order terms in Equation (5.1.9) are negligible in comparison to the magnitudes of the first-order terms in that equation for realistic values of the infinitesimal strains.² The restrictions that this assumption puts on the relative values of ν and the other material coefficients can best be observed when the linear momentum jump condition and the kinetic relation are in nondimensional form, which will be done in the next section. The true first-order approximation of the linear momentum jump condition given by (5.1.9) is

$$\frac{E_1}{1+\gamma_0} \left[\frac{\partial \bar{u}_1}{\partial x} \right]_{(s(t),t)} - E \left[\frac{\partial \hat{u}}{\partial x} \right]_{(s(t),t)} = 0, \qquad (5.3.3)$$

 $\forall t \in \Gamma$, which is equivalent to the continuity of tractions across the interface. Using (5.3.3) in (5.2.12), the first-order approximation of the kinetic relation for the problem under consideration can be written as

$$\dot{s} = -\frac{\gamma_0 E}{\nu} \left[\frac{\partial \hat{u}}{\partial x} \right]_{(s(t),t)}, \tag{5.3.4}$$

 $\forall t \in \Gamma$.

For the linearized problem, the fixed boundary condition is still given by (5.1.11), and using (5.2.8) in (5.1.12), the first-order approximation of the free boundary

² We note that the values of the strains at the interface as time progresses are proportional to the initial conditions given.

condition is

$$\left. \frac{\partial \bar{u}_1}{\partial x} \right|_{(L,t)} = 0, \qquad (5.3.5)$$

 $\forall t \in \Gamma$.

5.4 The Nondimensional Form of the Boundary Value Problem

For the problem under consideration, we define the following nondimensional variables:

$$\widetilde{x} = rac{x}{L}\,, \quad \ \widetilde{t} = \omega t\,, \quad \ \widetilde{s}(\widetilde{t}) = rac{s(\widetilde{t}/\omega)}{L}\,,$$

$$\tilde{u}(\tilde{x},\tilde{t}) = \frac{\hat{u}(\tilde{x}L,\tilde{t}/\omega)}{L}, \quad \tilde{u}_1(\tilde{x},\tilde{t}) = \frac{\bar{u}_1(\tilde{x}L,\tilde{t}/\omega)}{L}, \quad (5.4.1)$$

$$\tilde{E} = \frac{E_1}{(1+\gamma_0)E}, \qquad \quad \tilde{\nu} = \frac{\nu}{\gamma_0\sqrt{E\rho}},$$

where $\omega = \sqrt{E/(\rho L^2)}$. Using these nondimensional variables, the nondimensional form of the balance of linear momentum for phase 1 is

$$\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} = \frac{\partial^2 \tilde{u}}{\partial \tilde{t}^2},\tag{5.4.2}$$

 $\forall \tilde{x} \in (0, \tilde{s}(\tilde{t}))$ at each $\tilde{t} \in \tilde{\Gamma}$, where $\tilde{\Gamma} = [\tilde{t}_0, \tilde{t}_1] = [\omega t_0, \omega t_1]$, and the nondimensional form of the balance of linear momentum for phase 2 is

$$\tilde{E}\frac{\partial^2 \tilde{u}_1}{\partial \tilde{x}^2} + \gamma_0 \frac{d^2 \tilde{s}}{d\tilde{t}^2} = \frac{\partial^2 \tilde{u}_1}{\partial \tilde{t}^2}, \tag{5.4.3}$$

 $\forall \tilde{x} \in (\tilde{s}(\tilde{t}), 1) \text{ at each } \tilde{t} \in \tilde{\Gamma}.$

In the following, \tilde{x} will denote the nondimensional independent variable defined by (5.4.1)₁, and not the inverse function of the function \tilde{x}_1 , which maps R^+ into R_1^+ at each $t \in \Gamma$.

The nondimensional form of the continuity-of-displacement condition is

$$\tilde{u}(\tilde{s}(\tilde{t}), \tilde{t}) = \tilde{u}_1(\tilde{s}(\tilde{t}), \tilde{t}), \qquad (5.4.4)$$

 $\forall \tilde{t} \in \tilde{\Gamma}$, and the nondimensional form of the first-order form of the linear momentum jump condition given by (5.3.3) is

$$\tilde{E}\left[\frac{\partial \tilde{u}_1}{\partial \tilde{x}}\right]_{\left(\tilde{s}(\tilde{t}),\tilde{t}\right)} - \left[\frac{\partial \tilde{u}}{\partial \tilde{x}}\right]_{\left(\tilde{s}(\tilde{t}),\tilde{t}\right)} = 0, \qquad (5.4.5)$$

 $\forall \ \tilde{t} \in \tilde{\Gamma}$. Additionally, the nondimensional form of the kinetic relation given by (5.3.4) is

$$\frac{d\tilde{s}}{d\tilde{t}} = -\frac{1}{\tilde{\nu}} \left[\frac{\partial \tilde{u}}{\partial \tilde{x}} \right]_{(\tilde{s}(\tilde{t}), \tilde{t})}, \tag{5.4.6}$$

 $\forall \tilde{t} \in \tilde{\Gamma}$. In the previous section, the issue concerning when it is appropriate to neglect the second-order terms in the linear momentum jump condition was discussed. The nondimensional form of the lowest-order term that was neglected in that equation is $\gamma_0 \left(\frac{d\tilde{s}}{d\tilde{t}}\right)^2$. From this, (5.4.6), and the definitions of the nondimensional parameters, we can observe what relative values of the material coefficients are appropriate for the assumption that the magnitude of $\gamma_0 \left(\frac{d\tilde{s}}{d\tilde{t}}\right)^2$ is negligible in comparison to the magnitudes of the terms in (5.4.5), for realistic values of the initial conditions.

The nondimensional form of the fixed boundary condition is

$$\tilde{u}(0,\tilde{t}) = 0, (5.4.7)$$

 $\forall \tilde{t} \in \tilde{\Gamma}$, and the nondimensional form of the free boundary condition is

$$\left. \frac{\partial \tilde{u}_1}{\partial \tilde{x}} \right|_{(1,\tilde{t})} = 0, \tag{5.4.8}$$

 $\forall \, \tilde{t} \in \tilde{\Gamma}.$

We must also specify initial conditions for the two-phase bar. In particular, for phase 1 we specify

$$\tilde{u}(\tilde{x}, \tilde{t}_0) = \tilde{h}(\tilde{x}),$$

$$\frac{\partial \tilde{u}}{\partial \tilde{t}}\Big|_{(\tilde{x}, \tilde{t}_0)} = \tilde{g}(\tilde{x}),$$
(5.4.9)

for $0 \le \tilde{x} < \tilde{s}(\tilde{t})$, and for phase 2 we specify

$$\tilde{u}_{1}(\tilde{x}, \tilde{t}_{0}) = \tilde{h}_{1}(\tilde{x}),$$

$$\frac{\partial \tilde{u}_{1}}{\partial \tilde{t}}\Big|_{(\tilde{x}, \tilde{t}_{0})} = \tilde{g}_{1}(\tilde{x}),$$
(5.4.10)

for $\tilde{s}(\tilde{t}) < \tilde{x} \le 1$. We must also specify an initial position for the phase boundary. In particular, we specify

$$\tilde{s}(\tilde{t}_0) = \tilde{s}_0. \tag{5.4.11}$$

The initial boundary value problem that will be considered consists of the field equations (5.4.2) and (5.4.3), the continuity-of-displacement condition (5.4.4), the linear momentum jump condition given by (5.4.5), the kinetic relation given by (5.4.6), the fixed boundary condition (5.4.7), the free boundary condition (5.4.8), and the initial conditions given by (5.4.9)-(5.4.11).

5.5 The Numerical Method of Solution

We can observe that the differential equations involving time derivatives in the boundary value problem presented in Section 5.4 consist of a wave equation given by (5.4.2), a forced wave equation given by (5.4.3), and an ordinary differential equation given by (5.4.6). The boundary conditions for Equations (5.4.2) and (5.4.3), given by (5.4.7) and (5.4.8), are both with respect to fixed boundaries.⁴ However, the jump conditions given by (5.4.4) and (5.4.5), which are also types of boundary conditions, are with respect to a moving boundary (i.e., the interface). We also note that because $\tilde{s}(\tilde{t})$ is one of the unknown dependent variables in the problem and the jump conditions are evaluated at $\tilde{x} = \tilde{s}(\tilde{t})$, the boundary value problem is inherently nonlinear with respect to $\tilde{s}(\tilde{t})$.

Dynamic boundary value problems involving moving interfaces within finite bodies have been studied before (see [4]). Some of the more well known of these problems are the class of problems considered to be Stephan problems. These types of problems involve melting solids, with a moving interface (or boundary) separating the solid from the liquid. The unknowns in these types of problems are the temperature distributions of both the liquid and solid phases, and the position of the interface separating these two phases. The governing equations for these Stephan problems consist of heat equations for both phases and an equation governing the motion of the interface. There are a variety of numerical methods that have been used to study these Stephan problems (see [4] for an overview and discussion of these methods). Among these numerical methods are several types of finite-difference methods.

For the problem considered here, the type of numerical method that will be used is a finite-difference method. This type of numerical method has been chosen, as opposed, e.g., to a finite-element method, because it is probably the most straightforward to apply to the type of boundary value problem that is being considered. The particular finite-difference method used here, however, does differ somewhat from

⁴ Note that if we were solving for \hat{u}_1 instead of \bar{u}_1 in the boundary value problem, the free boundary condition would be with respect to a moving boundary.

the finite-difference methods that have been used for the Stephan problems that are discussed in [4]. Most of these differences reflect the fact that the field equations in the Stephan problems are of parabolic-type with monotonically decaying solutions, and the field equations in the problem considered here are of hyperbolic-type with decaying oscillatory solutions.

In the following, let $\mathcal{I}[a,b] = \{m \in \mathcal{Z} / a \le m \le b, a \in \mathcal{Z}, b \in \mathcal{Z}\}$, where \mathcal{Z} denotes the set of all integers. For the finite-difference method used here, the bar will be divided into n intervals, each of length h = 1/n. The points x = ih, $i \in \mathcal{I}[0, n]$, will be referred to as the nodes of the bar. In the finite-difference method, the displacements at these nodes will be determined (i.e., approximated). increment is denoted by T, and for convenience we assume in the following that $ilde{t}_0=0.$ Considering this, $ilde{t}=jT,\ j\in\mathcal{I}[0,l_1],$ where $ilde{t}_1$ and l_1 are chosen such that $l_1T = \tilde{t}_1$. We let s(j) represent $\tilde{s}(jT)$, and k(j) denote the node such that $|s(j)-k(j)h| \leq h/2$, at time $\tilde{t}=jT$. Additionally, we let p(j)h represent the distance from the node k(j) - 1 to s(j), at time $\tilde{t} = jT$. Considering this, we can write s(j) as s(j) = [k(j) - 1 + p(j)]h, at each $j \in \mathcal{I}[0, l_1]$. Let u(i, j) represent $\tilde{u}(ih,jT), \ 0 \leq ih \leq s(j)$ at each $j \in \mathcal{I}[0,l_1]$, and let $u_1(i,j)$ represent $\tilde{u}_1(ih,jT)$, $s(j) \le ih \le 1$ at each $j \in \mathcal{I}[0, l_1]$. Additionally, let q(j) denote the displacement at the interface at time $\tilde{t} = jT$; i.e., let q(j) represent $\tilde{u}(\tilde{s}(jT), jT) = \tilde{u}_1(\tilde{s}(jT), jT)$. We also let $\Phi(j)$ represent the nondimensional kinetic relation given by (5.4.6) at time $\tilde{t} = jT$.

At each time increment, the numerical routine begins by calculating s(j+1). We are given s(0) as an initial condition. At j=0, we use Euler's method to approximate Equation (5.4.6) and obtain s(1). In particular, we use

$$p(1) = p(0) + \frac{T}{h}\Phi(0)$$
 (5.5.1)

to obtain p(1). Since k(0) is given when s(0) is given, we can then obtain s(1). For this case where j=0, we can use the initial conditions given by $(5.4.9)_1$ and $(5.4.10)_1$ to obtain the derivative term in $\Phi(0)$. The specific form of these initial conditions will be discussed at a later point in this section. Also, we note that Euler's method has an O(T) numerical error. At j=1, we use an Adams-Bashforth two-step method, which has an $O(T^2)$ error (see [3]), to approximate Equation (5.4.6) and obtain s(2). The resulting equation for p(2) is

$$p(2) = p(1) + \frac{T}{2h} \{3\Phi(1) - \Phi(0)\}, \qquad (5.5.2)$$

which can then be used to obtain s(2). Also, to obtain the derivative term in $\Phi(1)$, we can use the initial conditions given by (5.4.9) and (5.4.10). For $j \in \mathcal{I}[2, l_1 - 1]$, we use an Adams-Bashforth three-step method, which has an $O(T^3)$ error, to approximate Equation (5.4.6) and obtain s(j+1). In particular, we use

$$p(j+1) = p(j) + \frac{T}{12h} \{23\Phi(j) - 16\Phi(j-1) + 5\Phi(j-2)\}$$
 (5.5.3)

to obtain p(j+1) for $j \in \mathcal{I}[2,l_1-1]$. p(j+1) is then used to obtain s(j+1). The specific form of the finite-difference approximation in $\Phi(j)$, $j \in \mathcal{I}[2,l_1]$, will be discussed at a later point in this section. Also, because of the definition of k(j+1), after each p(j+1) is calculated, it must be checked to determine whether it is such that $0.5 \leq p(j+1) \leq 1.5$. If p(j+1) is calculated to be such that p(j+1) < 0.5, k(j+1) must be set to k(j+1) = k(j) - 1, and p(j+1) must be updated to $p(j+1) \to p(j+1) + 1$. If p(j+1) is calculated to be such that p(j+1) > 1.5, k(j+1) must be set to k(j+1) = k(j) + 1, and p(j+1) must be updated to $p(j+1) \to p(j+1) - 1$.

At each time step, once p(j+1), k(j+1), and s(j+1) are determined, and p(j+1) is updated if necessary, the displacements at the nodes are determined.

For each $j \in \mathcal{I}[1, l_1 - 1]$, the displacements u(i, j + 1), $i \in \mathcal{I}[1, k(j + 1) - 1]$, and $u_1(i, j + 1)$, $i \in \mathcal{I}[k(j + 1) + 1, n - 1]$, are determined from centered-type difference equations. It will also be assumed in the following that |s(j + 1) - s(j)| < h/4, $\forall j \in \mathcal{I}[0, l_1]$. This is done so that u(i, j - 1), u(i, j), and u(i, j + 1) in the difference equations representing Equation (5.4.2) all correspond to phase 1, and $u_1(i, j - 1)$, $u_1(i, j)$, and $u_1(i, j + 1)$ in the difference equations representing Equation (5.4.3) all correspond to phase 2.5

To obtain the initial displacements at the nodes, we use the initial conditions given by $(5.4.9)_1$ and $(5.4.10)_1$. We assume that these initial displacements are continuous $\forall \ \tilde{x} \in (0,1)$, satisfy the boundary conditions given by (5.4.7) and (5.4.8), are such that the linear momentum jump condition given by (5.4.5) is satisfied, and have a first-mode-type mode shape. In particular, we assume that

$$\tilde{h}(\tilde{x}) = \varepsilon_0 \tilde{x} \,, \tag{5.5.4}$$

for $0 \le \tilde{x} \le \tilde{s}(0)$, and

$$\tilde{h}_1(\tilde{x}) = \frac{\varepsilon_0}{2\tilde{E}(\tilde{s}(0) - 1)} \left\{ (\tilde{x} - 1)^2 - (\tilde{s}(0) - 1)^2 \right\} + \varepsilon_0 \tilde{s}(0), \qquad (5.5.5)$$

for $\tilde{s}(0) \leq \tilde{x} \leq 1$. The values of the displacements at the next time increment can be approximated by the Taylor series expansion in time of the displacements. In particular, using the initial conditions given by (5.4.9) and (5.4.10), the first-order approximation of \tilde{u} and \tilde{u}_1 at $\tilde{t} = T$ are

$$\tilde{u}(\tilde{x},T) = \tilde{h}(\tilde{x}) + \tilde{g}(\tilde{x})T, \qquad (5.5.6)$$

Note that this is consistent with the assumption that the magnitudes of the terms in $\dot{\tilde{s}}^2$ in the linear momentum jump condition are negligible in comparison to the magnitudes of the first-order terms in that jump condition.

for $0 \le \tilde{x} \le \tilde{s}(0)$, and

$$\tilde{u}_1(\tilde{x},T) = \tilde{h}_1(\tilde{x}) + \tilde{g}_1(\tilde{x})T, \qquad (5.5.7)$$

for $\tilde{s}(0) \leq \tilde{x} \leq 1$, respectively. It is assumed that the initial velocity distribution results in a continuous displacement at the phase boundary at time $\tilde{t} = T$, results in the boundary conditions given by (5.4.7) and (5.4.8) being satisfied at time $\tilde{t} = T$, results in the linear momentum jump condition given by (5.4.5) being approximately satisfied at time $\tilde{t} = T$, and has a first-mode-type velocity profile. Such an initial velocity distribution is given by

$$\tilde{g}(\tilde{x}) = v_0 \tilde{x} \,, \tag{5.5.8}$$

for $0 \le \tilde{x} \le \tilde{s}(0)$, and

$$\tilde{g}_1(\tilde{x}) = \frac{v_0}{2\tilde{E}(\tilde{s}(T) - 1)} \left\{ (\tilde{x} - 1)^2 - (\tilde{s}(T) - 1)^2 \right\} + v_0 \tilde{s}(T), \tag{5.5.9}$$

for $\tilde{s}(0) \leq \tilde{x} \leq 1$. This initial velocity distribution was used in (5.5.6) and (5.5.7), which were then used to obtain the displacements at the nodes at $\tilde{t} = T$.

For $j \in \mathcal{I}[1, l_1 - 1]$, u(0, j + 1) is obtained from the following equation, which represents the fixed boundary condition given by (5.4.7):

$$u(0, j+1) = 0, (5.5.10)$$

 $\forall j \in \mathcal{I}[1, l_1 - 1]$. We can obtain u(i, j + 1), for $i \in \mathcal{I}[1, k(j + 1) - 2]$ at each $j \in \mathcal{I}[1, l_1 - 1]$, from a finite-difference approximation of Equation (5.4.2), which uses centered-difference equations for equally spaced nodes to approximate each term

⁶ We note that $\tilde{s}(T)$ is not a given constant in the problem and therefore cannot be used if an analytical solution was to be obtained. In this case, we could use $\tilde{s}(0)$ instead of $\tilde{s}(T)$ in (5.5.9) as an approximation. For the numerical method, however, we can use $\tilde{s}(T)$.

in that equation. In the following, centered-difference equations for equally spaced nodes will be referred to as *standard* centered-difference equations. The resulting difference equation that is used to obtain u(i, j + 1) is

$$u(i, j + 1) = 2u(i, j) - u(i, j - 1) + \alpha \{u(i + 1, j) - 2u(i, j) + u(i - 1, j)\},$$
(5.5.11)

for $i \in \mathcal{I}[1, k(j+1)-2]$ at each $j \in \mathcal{I}[1, l_1-1]$, where $\alpha = (T/h)^2$. The difference equation given by (5.5.11) is commonly used for the wave equation [3]. It is also well known that a numerical routine using this difference equation is numerically stable if and only if $\alpha \leq 1$, and that the numerical error increases as α decreases from 1 [3]. We can obtain $u_1(i,j+1)$, for $i \in \mathcal{I}[k(j+1)+2,n-1]$ at each $j \in \mathcal{I}[1,l_1-1]$, from a finite-difference approximation of Equation (5.4.3), which uses standard centered-difference equations to approximate each term in that equation. The resulting difference equation that is used to obtain $u_1(i,j+1)$ is

$$u_{1}(i, j + 1) = 2u_{1}(i, j) - u_{1}(i, j - 1) + \tilde{E}\alpha\{u_{1}(i + 1, j) - 2u_{1}(i, j) + u_{1}(i - 1, j)\} + \gamma_{0}\{s(j + 1) - 2s(j) + s(j - 1)\},$$
(5.5.12)

for $i \in \mathcal{I}[k(j+1)+2,n-1]$ at each $j \in \mathcal{I}[1,l_1-1]$. For $j \in \mathcal{I}[1,l_1-1]$, we can obtain u(n,j+1) from an $O(h^2)$ difference equation representing the free boundary condition given by Equation (5.4.8). This difference equation is

$$u_1(n,j+1) = \frac{1}{3} \left\{ 4u_1(n-1,j+1) - u_1(n-2,j+1) \right\}, \tag{5.5.13}$$

for each $j \in \mathcal{I}[1, l_1 - 1]$.

For the displacements u(k(j+1)-1,j+1) and/or $u_1(k(j+1)+1,j+1)$, finite-difference methods using q(j) will be used. For the derivation of the difference equations for these displacements, we first note that the distance separating s(j)

from its nearest nodes is not equal to h. Because of this, difference equations for unequally spaced nodes must be used to represent $\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2}$ and/or $\frac{\partial^2 \tilde{u}_1}{\partial \tilde{x}^2}$. These difference equations will be derived from the second-degree Lagrange interpolating polynomials for \tilde{u} and/or \tilde{u}_1 near the interface. For a function g(x), its second-degree Lagrange polynomial, denoted by P(x), is given by

$$P(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} g(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} g(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} g(x_2),$$
(5.5.14)

where $x_0, x_1, x_2, g(x_0), g(x_1),$ and $g(x_2)$ are given (see [3]). The first derivative of $P(x) \approx g(x)$ is

$$\frac{dP(x)}{dx} = \frac{x - x_1 + x - x_2}{(x_0 - x_1)(x_0 - x_2)} g(x_0) + \frac{x - x_0 + x - x_2}{(x_1 - x_0)(x_1 - x_2)} g(x_1) + \frac{x - x_0 + x - x_1}{(x_2 - x_0)(x_2 - x_1)} g(x_2),$$
(5.5.15)

and the second derivative is

$$\frac{d^{2}P(x)}{dx^{2}} = \frac{2}{(x_{0} - x_{1})(x_{0} - x_{2})}g(x_{0}) + \frac{2}{(x_{1} - x_{0})(x_{1} - x_{2})}g(x_{1}) + \frac{2}{(x_{2} - x_{0})(x_{2} - x_{1})}g(x_{2}).$$
(5.5.16)

If we choose $x = x_0$, x_1 , or x_2 in Equations (5.5.15) and (5.5.16), the errors in these equations are approximately $O(d^2)$, where d is the maximum distance between any of these three points.⁷ Also, we note that when x_0 , x_1 , and x_2 are equally spaced, (5.5.16) reduces to a standard centered-difference equation of the form used in (5.5.11) and (5.5.12).

⁷ See [3] for a more detailed discussion of the error that is involved in the Lagrange interpolating polynomial and its derivatives. Also, difference equations of this type are used in some finite-difference methods for Stephan problems (see [4]).

Case I: Consider the case where $0.5 \le p(j+1) \le 1.5$, before being updated (Figure 5.1a). For this case, k(j+1) = k(j), and for the calculation of u(k(j+1)-1,j+1), a difference equation of the form (5.5.16) will be used to approximate $\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2}$ at $\tilde{t} = jT$ in Equation (5.4.2). Using this difference equation and a standard centered-difference equation for the second-time-derivative term in Equation (5.4.2), we obtain

$$u(k(j+1)-1,j+1) = 2u(k(j+1)-1,j) - u(k(j+1)-1,j-1)$$

$$+ \, 2\alpha \bigg\{ \frac{u(k(j)-2,j)}{1+p(j)} - \frac{u(k(j)-1,j)}{p(j)} + \frac{q(j)}{[1+p(j)]p(j)} \bigg\} \, . \tag{5.5.17}$$

Similarly, for the calculation of $u_1(k(j+1)+1,j+1)$, a difference equation of the form (5.5.16) will be used to approximate $\frac{\partial^2 \tilde{u}_1}{\partial \tilde{x}^2}$ at $\tilde{t}=jT$ in Equation (5.4.3). Using this difference equation and standard centered-difference equations for the second-time-derivative terms in Equation (5.4.3), we obtain

$$u_1(k(j+1)+1,j+1) = 2u_1(k(j+1)+1,j) - u_1(k(j+1)+1,j-1)$$

$$+2\tilde{E}\alpha\left\{\frac{q(j)}{[2-p(j)][3-p(j)]}-\frac{u_1(k(j)+1,j)}{2-p(j)}+\frac{u_1(k(j)+2,j)}{3-p(j)}\right\} \hspace{1cm} (5.5.18)$$

$$+ \gamma_0 \{s(j+1) - 2s(j) + s(j-1)\}.$$

We note that when p(j) = 1, Equations (5.5.17) and (5.5.18) reduce to Equations (5.5.11) and (5.5.12), respectively.

Case II: Consider the case where p(j+1) < 0.5, before being updated (Figure 5.1b). For this case, k(j+1) = k(j) - 1 and $p(j+1) \to p(j+1) + 1$. Additionally, in this case, we can use the difference equation given by (5.5.11) for the calculation

of u(k(j+1)-1,j+1). However, for the calculation of $u_1(k(j+1)+1,j+1)$, a difference equation of the form (5.5.16) will be used to approximate $\frac{\partial^2 \tilde{u}_1}{\partial \tilde{x}^2}$, and standard centered-difference equations will be used to approximate the two time-derivative terms in Equation (5.4.3). The resulting difference equation is

$$u_1(k(j+1)+1,j+1) = 2u_1(k(j+1)+1,j) - u_1(k(j+1)+1,j-1)$$

$$+2\tilde{E}\alpha\left\{\frac{q(j)}{[1-p(j)][2-p(j)]} - \frac{u_1(k(j),j)}{1-p(j)} + \frac{u_1(k(j)+1,j)}{2-p(j)}\right\}$$
(5.5.19)

$$+ \gamma_0 \{s(j+1) - 2s(j) + s(j-1)\}.$$

Case III: The last case that can occur is p(j+1) > 1.5, before being updated (Figure 5.1c). In this case, k(j+1) = k(j) + 1 and $p(j+1) \to p(j+1) - 1$. In this case, for the calculation of u(k(j+1)-1,j+1), a difference equation of the form (5.5.16) will be used to approximate $\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2}$, and a standard centered-difference equation will be used to approximate the second-time-derivative term in Equation (5.4.2). The resulting difference equation is

$$u(k(j+1)-1,j+1) = 2u(k(j+1)-1,j) - u(k(j+1)-1,j-1)$$

$$+2\alpha \left\{ \frac{u(k(j)-1,j)}{p(j)} - \frac{u(k(j),j)}{p(j)-1} + \frac{q(j)}{p(j)[p(j)-1]} \right\}. \tag{5.5.20}$$

For this case, we can use the difference equation given by (5.5.12) for the calculation of $u_1(k(j+1)+1,j+1)$.

Once s(j+1) and the displacements at the nodes $i \in \mathcal{I}[0, k(j+1)-1]$ and $i \in \mathcal{I}[k(j+1)+1, n]$ have been determined, we determine the displacement q(j+1) at

the interface from the difference equation representing the linear momentum jump condition. Using difference equations of the form (5.5.15) to approximate the spatial derivatives in Equation (5.4.5), we obtain

$$q(j+1) = \left\{ \frac{\tilde{E}[2p-5]}{[2-p][3-p]} - \frac{2p+1}{[1+p]p} \right\}^{-1} \left\{ \frac{p}{1+p} u(k-2,j+1) - \frac{1+p}{p} u(k-1,j+1) - \tilde{E} \frac{3-p}{2-p} u_1(k+1,j+1) - \tilde{E} \frac{p-2}{3-p} u_1(k+2,j+1) \right\},$$

$$(5.5.21)$$

where k = k(j+1) and p = p(j+1).

The last displacement that must be calculated at each time increment is the displacement at the node k(j+1). This displacement will be calculated using a second-degree Lagrange interpolating polynomial. In particular, if k(j+1)h < s(j+1), we calculate u(k(j+1),j+1) from

$$u(k, j+1) = \frac{1-p}{1+p}u(k-2, j+1) + \frac{2[p-1]}{p}u(k-1, j+1) + \frac{2q(j+1)}{[1+p]p}, (5.5.22)$$

where k=k(j+1) and p=p(j+1), and if k(j+1)h>s(j+1), we calculate $u_1(k(j+1),j+1)$ from

$$u_1(k,j+1) = \frac{2q(j+1)}{[2-p][3-p]} + \frac{2[1-p]}{2-p}u_1(k+1,j+1) + \frac{p-1}{3-p}u_1(k+2,j+1),$$
(5.5.23)

where k = k(j+1) and p = p(j+1).

The last quantity calculated at each time step is $\Phi(j+1)$. Recall that this quantity is used in the calculation of p(j+1) at the next time step. For the calculation of $\Phi(j+1), \ j \in \mathcal{I}[1,l_1-1],$ a finite-difference equation of the form (5.5.15) is used for the approximation of $\frac{\partial \tilde{u}}{\partial \tilde{x}}\big|_{\left(\tilde{s}(\tilde{t}),\tilde{t}\right)}$. The resulting finite-difference equation for $\Phi(j+1)$ is

$$\Phi(j+1) = -\frac{1}{\tilde{\nu}h} \left\{ \frac{p}{1+p} u(k-2,j+1) - \frac{1+p}{p} u(k-1,j+1) + \frac{2p+1}{[1+p]p} q(j+1) \right\},$$
(5.5.24)

for $j \in \mathcal{I}[1, l_1 - 1]$, where k = k(j + 1) and p = p(j + 1).

The numerical routine discussed above allows for the phase boundary to pass over nodes other than the node k(j). However, for a problem using a kinetic relation of the form given by (5.4.6), most values of the material coefficients that are consistent with the assumption that the second-order terms in the linear momentum jump condition are negligible in comparison to the first-order terms in that equation, and most initial conditions that produce infinitesimal initial strains will result in the phase boundary staying within the interval between the nodes k(j) - 1 and k(j) + 1 for all $\tilde{t} \in \tilde{\Gamma}$. In this case, a simplified numerical routine can be used where k(j) has the same value at each time increment, p(j+1) never needs to be updated (in the sense that it was updated in Cases II and III), and only Case I for the calculation of the displacements near the interface needs to be considered.

5.6 The Free Vibrations and Damping Properties

In this section, the free vibrations of the two-phase bar that were determined from the finite-difference method discussed in the previous section are discussed. As expected, the response of the two-phase bar to the initial conditions given by (5.5.4), (5.5.5), (5.5.8), (5.5.9), and (5.4.11) has a decaying oscillatory form. In particular, the position of the phase boundary oscillates as time progresses and decays to a new position that has a distance and direction from its initial position that is proportional to the magnitude and "direction" of its initial conditions (Figures 5.2–5.4). The displacements also have a decaying oscillatory form, and they go to zero as time goes to infinity (Figures 5.5–5.9). The mode shape of the bar during these free vibrations has a first-mode-type form (Figure 5.10)⁸. This is most likely a result of the fact that first-mode-type initial conditions were given.

5.6.1 The Damping Behavior

The damping of the bar was studied as $\tilde{\nu}$, \tilde{E} , and γ_0 were varied. In Figure 5.11, a plot of the settling time versus $\tilde{\nu}$ is presented. Here, the settling time is defined as the nondimensional time necessary for the amplitude of $\tilde{u}_1(L,t)$ to become less than 10^{-4} . As the settling time decreases, it is said that the damping of the bar increases. As expected, as $\tilde{\nu}$ decreases, the damping of the bar increases. This is primarily a result of the fact that for a given amount of strain at the interface, the nominal phase boundary velocity increases as $\tilde{\nu}$ decreases. Consequently, as $\tilde{\nu}$ decreases, there is more motion of the phase boundary in a given interval of time, which results in more energy being dissipated in that interval of time. This increase in damping as $\tilde{\nu}$ decreases is also displayed in Figures 5.2–5.7. From Figure 5.11, it appears that the "frequency" of oscillation does not significantly depend on $\tilde{\nu}$. In particular, it can be

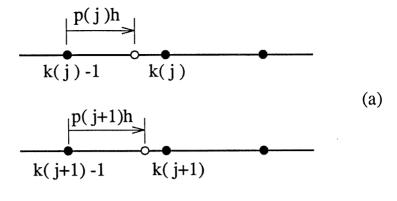
⁸ In Figure 5.10, \tilde{u} vs. \tilde{t} is plotted for $0 \le \tilde{x} \le \tilde{s}(\tilde{t})$ and \tilde{u}_1 vs. \tilde{t} is plotted for $\tilde{s}(\tilde{t}) \le \tilde{x} \le 1$. The shape deformation for phase 2 is not plotted.

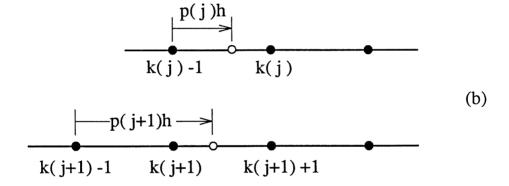
In this figure, the settling time versus $\tilde{\nu}$ is not presented for $0 < \tilde{\nu} < 0.09$ because the numerical routine is unstable for these values of $\tilde{\nu}$ when $\tilde{E} = 1.15$, $\gamma_0 = 0.1$, T = 0.01, and h = 0.02. This will be discussed further in the next section. Also, in this figure and in Figures 5.12 and 5.13, the initial conditions that were used are $\epsilon_0 = 0.001$, $v_0 = 0.001$, and $s_0 = 0.5$.

than $|\gamma_0| \approx 0.06$ would be considered infinitesimal, and a transformation strain with a magnitude greater than $|\gamma_0| \approx 0.06$ would be considered finite. These "transition" values $\gamma_0 \approx -0.06$ and $\gamma_0 \approx 0.06$ separating the infinitesimal transformation strains from the finite transformation strains are probably much smaller than most might have guessed beforehand. This also underlines the importance of treating a transformation strain that is not truly infinitesimal as a finite strain, at least for vibration problems.

5.6.2 Instabilities of the Numerical Routine

As mentioned previously, there are some instability problems with the numerical routine for values of $\tilde{\nu}$, \tilde{E} , and γ_0 outside a certain region of the parameter space. In some cases, these instabilities resemble those of highly damped systems, which are sometimes referred to as stiff systems in the numerical-methods literature [3]. In the remaining cases, the loss of stability of the numerical routine resembles that of a standard centered-difference numerical routine for a wave equation, when the coefficient multiplying the term representing the spatial derivative becomes greater than one. In both cases, however, the values of $\tilde{\nu},~\tilde{E},~$ and $\gamma_0,~$ where the numerical routine loses stability, depends on the values of T and h that are used. For example, for $h=0.02, \ \tilde{E}=1.15$ and $\gamma_0=0.1$, the numerical routine loses stability as $\tilde{\nu}$ is decreased at $\tilde{\nu} \approx 0.22$, when T=0.018, and at $\tilde{\nu} \approx 0.09$, when T=0.01. The loss of stability in both of these cases resembles that of stiff systems. In fact, for the latter case, the displacements reach their settling time in almost one half of one "cycle" of oscillation. One should note, however, that as $\tilde{\nu}$ gets close to zero, the assumption that ν is such that the magnitude of \dot{s}^2 is negligible in comparison to the magnitudes of the first-order terms in Equation (5.1.9) becomes less valid. For $h=0.02,\ \tilde{\nu}=0.5,\ {\rm and}\ \gamma_0=0.1,$ the value of \tilde{E} beyond which the numerical routine is unstable is $\tilde{E} \approx 1.23$, when T=0.018, and $\tilde{E} \approx 4.01$, when T=0.01. Both of these values of \tilde{E} correspond to $\tilde{E}(T/h)^2\approx 1$ (recall that this term appears in the finite-difference approximation of the forced wave equation for phase 2 given by (5.5.12)). For $T=0.018,\ h=0.02,\ \tilde{E}'=1.265,\ \text{and}\ \tilde{\nu}'=0.05,\ \text{the numerical}$ routing is stable for $0.021<\gamma_0<0.152.$ The loss of stability at $\gamma_0\approx 0.021$ corresponds to $\tilde{E}(T/h)^2\approx 1$, and the loss of stability at $\gamma_0\approx 0.152$ resembles that of a stiff system. For $T=0.01,\ h=0.02,\ \tilde{E}'=1.265,\ \text{and}\ \tilde{\nu}'=0.05,\ \text{the numerical}$ routing is stable for $-0.232<\gamma_0<0.256.$ For this case, the losses of stability at both $\gamma_0\approx 0.256$ and $\gamma_0\approx -0.232$ resemble that of stiff systems.





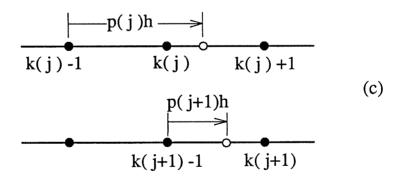


Figure 5.1. The nodes near the interface after being updated for the case where: (a) 0.5 < p(j+1) < 1.5; (b) p(j+1) < 0.5; (c) p(j+1) > 1.5, before being updated.

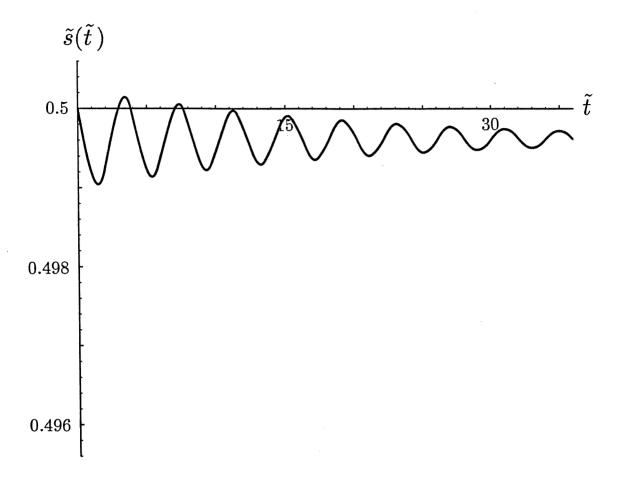


Figure 5.2. The position of the interface vs. time; $\tilde{E}=1.15,~\gamma_0=0.1,~\tilde{\nu}=1,$ $\varepsilon_0=0.001,~v_0=0.001,~s_0=0.5.$

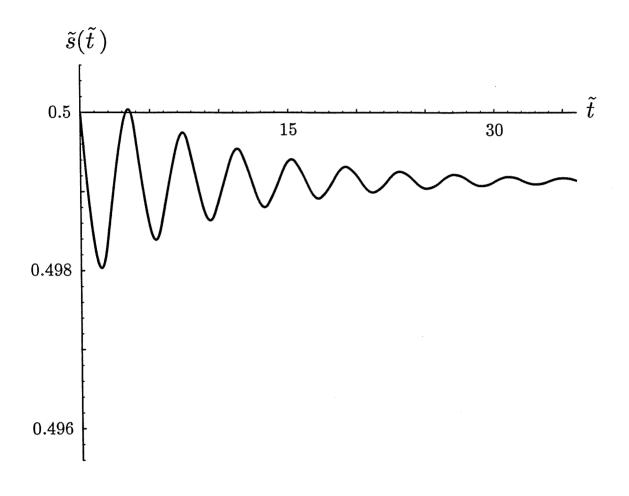


Figure 5.3. The position of the interface vs. time; $\tilde{E}=1.15,\ \gamma_0=0.1,\ \tilde{\nu}=0.5,$ $\varepsilon_0=0.001,\ v_0=0.001,\ s_0=0.5.$

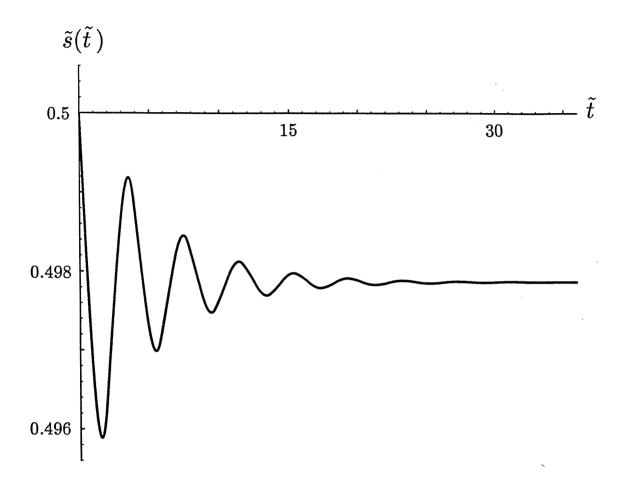


Figure 5.4. The position of the interface vs. time; $\tilde{E}=1.15,~\gamma_0=0.1,~\tilde{\nu}=0.25,$ $\varepsilon_0=0.001,~v_0=0.001,~s_0=0.5.$

observed from this figure that as $\tilde{\nu}$ is varied, the settling time remains constant over an interval of $\tilde{\nu}$, and when the settling time changes, it does so discontinuously. This is a reflection of the fact that as $\tilde{\nu}$ decreases, the amplitude of oscillation decreases, but the "frequency" of oscillation does not.

In Figure 5.12, the settling time versus \tilde{E} is presented. From this figure it can be concluded that as \tilde{E} goes to zero, the damping goes to zero (i.e., the settling time goes to infinity), and as \tilde{E} increases, the damping increases. Additionally, for the values of $\tilde{\nu}$ and γ_0 considered, and as \tilde{E} increases, the amount of damping begins to level off at $\tilde{E}\approx 0.3$. The damping beyond this value of \tilde{E} is relatively high.

For the plots of the settling time versus the transformation strain γ_0 , we do not vary γ_0 and keep \tilde{E} and $\tilde{\nu}$ constant. This is because \tilde{E} and $\tilde{\nu}$ can remain constant as γ_0 is varied only if E_1/E and $\nu/\sqrt{\rho E}$ also change values. We instead let $\tilde{E}'=E_1/E$ and $\tilde{\nu}'=\nu/\sqrt{\rho E}$ and substitute $\tilde{E}=\tilde{E}'/(1+\gamma_0)$ and $\tilde{\nu}=\tilde{\nu}'/\gamma_0$ into the difference equations of the finite-difference program. We then plot the settling time versus γ_0 , while keeping \tilde{E}' and $\tilde{\nu}'$ constant. An example of such a plot is shown in Figure 5.13. From this figure we can conclude that as γ_0 goes to zero, the damping goes to zero, and as the magnitude of γ_0 increases, the damping increases. We can also observe from this figure that as the magnitude of γ_0 becomes greater than $|\gamma_0| \approx 0.06$, the damping becomes appreciable, and for $|\gamma_0|$ less than this value, the damping is relatively small. It is interesting to note that if one were to define an infinitesimal transformation strain as one producing a vibration response that is qualitatively like that produced as $\gamma_0 \rightarrow 0$, and if one were to define a finite transformation strain as one producing a vibration response that is qualitatively like that produced by a γ_0 that is close to or less than -0.5 or is close to or greater than 1, for the values of \tilde{E}' and $\tilde{\nu}'$ considered, a transformation strain with a magnitude less

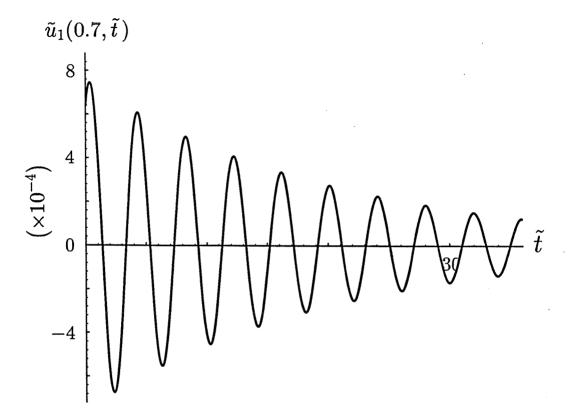


Figure 5.5. The displacement at $\tilde{x}=0.7$ vs. time; $\tilde{E}=1.15,\ \gamma_0=0.1,$ $\tilde{\nu}=1,\ \varepsilon_0=0.001,\ v_0=0.001,\ s_0=0.5.$

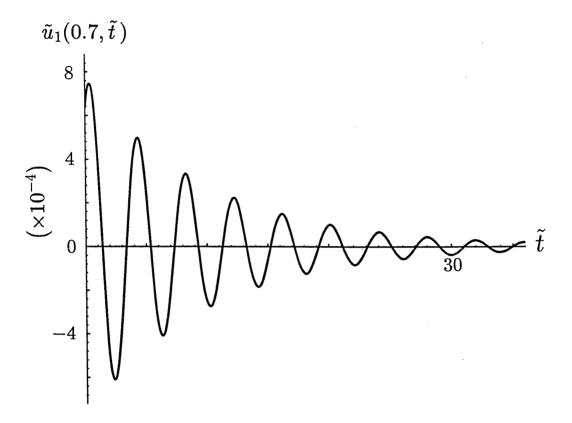


Figure 5.6. The displacement at $\tilde{x}=0.7$ vs. time; $\tilde{E}=1.15,~\gamma_0=0.1,$ $\tilde{\nu}=0.5,~\varepsilon_0=0.001,~v_0=0.001,~s_0=0.5.$

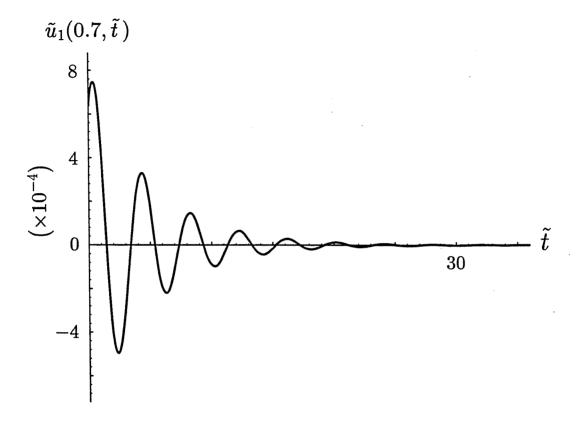


Figure 5.7. The displacement at $\tilde{x}=0.7$ vs. time; $\tilde{E}=1.15,\ \gamma_0=0.1,$ $\tilde{\nu}=0.25,\ \varepsilon_0=0.001,\ v_0=0.001,\ s_0=0.5.$

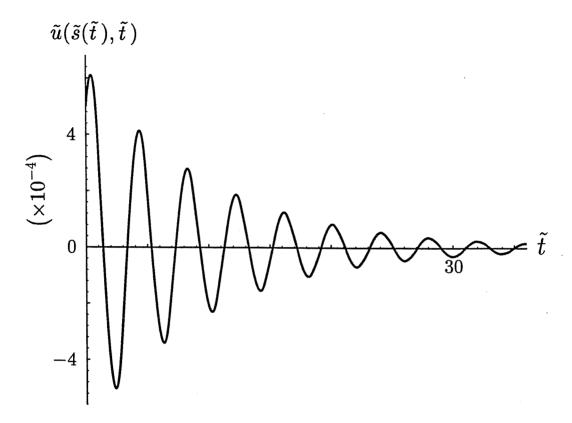


Figure 5.8. The displacement at the interface vs. time; $\tilde{E}=1.15,~\gamma_0=0.1,$ $\tilde{\nu}=0.5,~\varepsilon_0=0.001,~v_0=0.001,~s_0=0.5.$

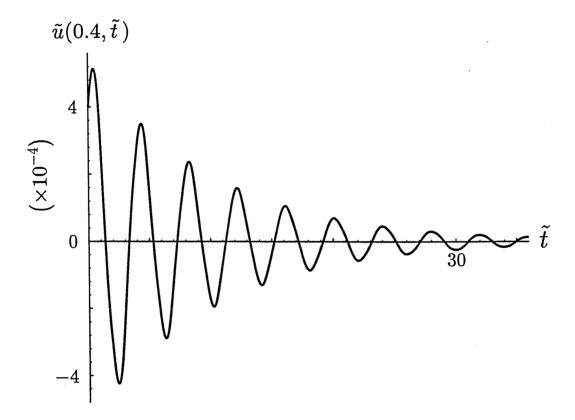


Figure 5.9. The displacement at $\tilde{x}=0.4$ vs. time; $\tilde{E}=1.15,~\gamma_0=0.1,$ $\tilde{\nu}=0.5,~\varepsilon_0=0.001,~v_0=0.001,~s_0=0.5.$

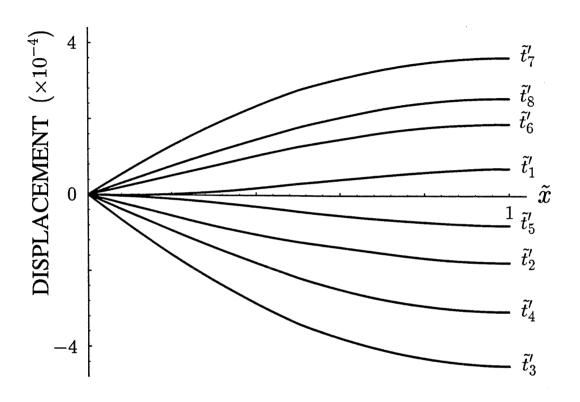


Figure 5.10. The mode shape at times $\tilde{t}_1'<\tilde{t}_2'<\cdots<\tilde{t}_8'$, representing one "cycle" of oscillation; $\tilde{E}=1.15,\ \gamma_0=0.1,\ \tilde{\nu}=0.5,\ \varepsilon_0=0.001,\ v_0=0.001,$ $s_0=0.5.$

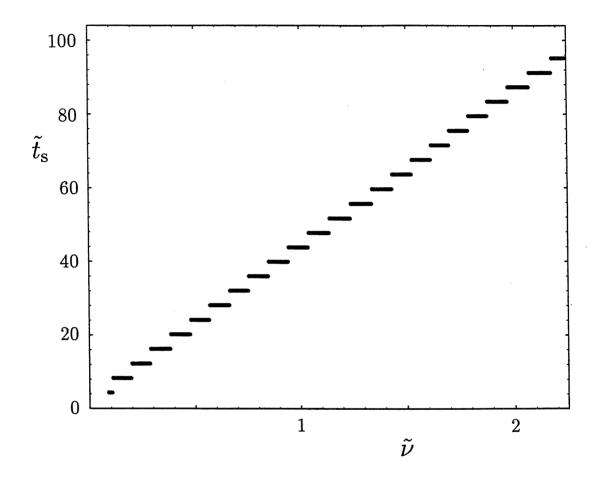


Figure 5.11. The settling time $\tilde{t}_{\rm s}$ vs. the kinetic coefficient $\tilde{\nu}$; $\tilde{E}=1.15,\,\gamma_0=0.1.$

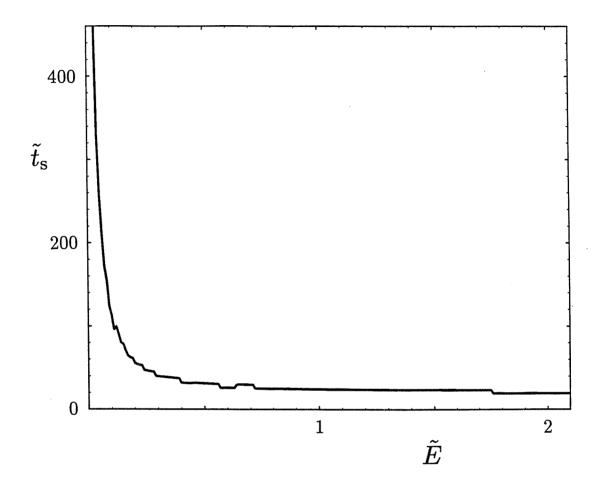


Figure 5.12. The settling time $\tilde{t}_{\rm s}$ vs. the moduli ratio $\tilde{E};~\gamma_0=0.1,~\tilde{\nu}=0.5.$

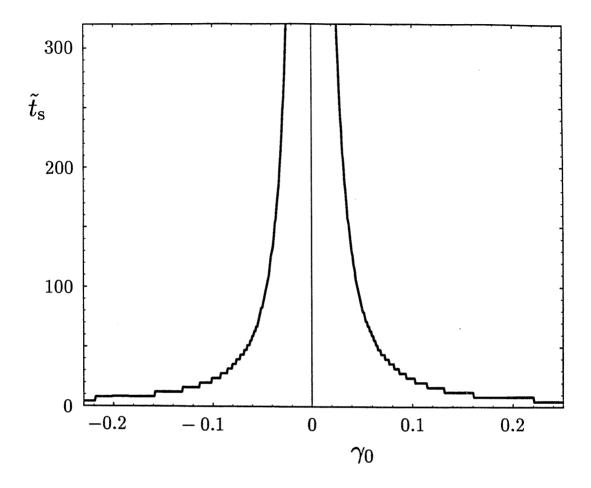


Figure 5.13. The settling time \tilde{t}_s vs. the transformation strain γ_0 ; $\tilde{E}'=1.265,$ $\tilde{\nu}'=0.05.$

CHAPTER 6 SUMMARY AND CONCLUDING REMARKS

In this thesis, a continuum model for materials that can undergo martensitic phase transformations was developed. The continuum model was then used to study several problems that deal with which phase or which variant of martensite is preferred during the application of a mechanical loading, a thermomechanical problem involving a finite, two-phase bar, and the free vibrations and damping properties of a finite, fixed-free, two-phase bar.

In the continuum model that was developed in Chapter 2, each phase has its own constitutive equations, which are defined with respect to a reference configuration that, in general, is unique to that phase. Additionally, this reference configuration is used for the expression of the field equations for that phase. A two-phase material in a purely mechanical process was considered in most of Chapter 2. The field equations and jump conditions for the two-phase material, where the reference configuration for one phase is stationary and the reference configuration for the other phase is a general function of time, were derived and discussed. It was then shown that this continuum model can be used to represent a material with phases that are elastic if the mapping representing the reference configuration for each phase is restricted to having the form given by (2.6.6). In this case, the stress power for each phase is equal to the time rate of change of the integral of the elastic potential for that phase, where the elastic potential and stress tensor for that phase are defined with respect to the reference configuration for that phase. It was also pointed out that if the reference configuration for a given phase is moving, the quantities that are defined with respect

to that reference configuration (e.g., the stress) do not have a true nominal form. This continuum model was then specialized to represent materials where each phase of the material behaves elastically and has a configuration corresponding to an unstressed, undeformed state. It was assumed that the reference configuration for each phase of these materials corresponds to the unstressed, undeformed configuration of that phase. With respect to the undeformed austenite phase, these reference configurations coincide with the shape deformations of the martensites. Because different elastic potentials are used for the different phases of the material, the material symmetry groups of the different phases can be chosen independently of each other and can be chosen to reflect any type of crystal symmetry with any orientation. Thus, the change in crystal structure that takes place during a martensitic phase transformation and the orientation relation between the crystal lattices of the different phases of the material can be accurately represented. In fact, because the elastic potential for each phase is defined with respect to the undeformed configuration of that phase, the material symmetry group for that elastic potential can be chosen to be the crystallographic point group corresponding to the crystal symmetry of that phase. The driving traction corresponding to the two-phase material was also presented and discussed. Next, the form of the boundary value problem in terms of the displacements was considered. The fact that working with displacements that are functions of points on a moving reference configuration results in the accelerations in terms of these displacements containing many inertial-type terms and results in the boundary conditions for that phase having to be expressed with respect to a moving boundary was pointed out. A coordinate transformation that eliminates most of these inertial-type terms and results in a completely Lagrangian description of the boundary value problem, while still working with field quantities that are defined with respect to the different reference configurations, was then discussed.

One of the main advantages of working with multiple reference configurations in the manner described in the latter portion of Chapter 2 is that the field equations and jump conditions are in forms that permit direct linearization, while still retaining finite shape deformations for the martensites. This is the case since the field quantities for each phase are in terms of displacements that are measured from the reference configuration corresponding to an unstressed, undeformed configuration of that phase, and consequently, for the appropriate initial and boundary conditions, the displacement gradients can be considered infinitesimal. Also, assuming that the gradients of these displacements are infinitesimal in no way restricts the magnitudes or forms of the shape deformations for the phases. The linearized field equations, jump conditions, driving traction, and kinetic relation were presented in Chapter 3. Another advantage of using multiple reference configurations in this manner is that for the linear problem, the true stress for each phase is approximately equal to the nominal stress for that phase. This is very useful for solving certain types of boundary value problems, including the linear problems that were considered in the rest of Chapter 3. All of these problems dealt with the issue of which phase or which variant of martensite is preferred during the growth process during the application of a mechanical loading. After the general problem was discussed, the special case of an applied, uniaxial, tensile traction was considered. A result that corresponds with observations made from experiments was derived. The last problem considered in this chapter involves the application of a hydrostatic pressure to a two-phase material with a martensite phase that has a finite shape deformation with an infinitesimal dilatation. The case where the two phases represent two different variants of the same martensite was then considered as a special case. It was shown that for this case, the hydrostatic pressure favors the growth of neither variant, which is what should be expected since everything else in the problem is completely symmetric. All of the problems considered in Chapter 3 demonstrate the convenience and accuracy of using the continuum model that was developed in this thesis.

In Chapter 4, a finite, two-phase, thermoelastic bar subject to different temperatures at each boundary and to a mechanical end-loading was studied. linearized problem was considered. The temperature at the interface was calculated and studied as the position of the interface, the material coefficients, the temperature boundary conditions, and the end-loading were varied. Additionally, the quasi-static motions of the phase boundary were studied for a kinetic relation with an interval of driving traction corresponding to a zero phase boundary velocity. Quasi-static thermomechanical processes in the neighborhoods of three different temperatures were considered. One of these temperatures represented the martensitic start temperature and one of them represented the austenite start temperature. The effects that varying the material coefficients, temperature boundary conditions, and end-loading have on the quasi-static processes for each of the three cases considered were studied. This problem is not only an example of a thermomechanical problem where a continuum model employing multiple reference configurations is used, it also serves as an example of solving a nontrivial boundary value problem that corresponds to such a continuum model.

The longitudinal free vibrations of a fixed-free, finite, two-phase, elastic bar were the subject of Chapter 5. The process was assumed to be purely mechanical, and the linearized problem was considered. A finite-difference numerical routine was used to obtain the displacement solutions of the initial-boundary-value problem. The main focus in this problem was the damping behavior of the two-phase bar that is due to the motions of the phase boundary during the free vibrations of the bar. It was found that the position of the phase boundary oscillates as time progresses and decays to a new

position that has a distance and direction from its initial position that is proportional to the magnitude and "direction" of its initial conditions. The displacements also have a decaying oscillatory form, and they go to zero as time goes to infinity. The damping behavior was studied as the material coefficients $\tilde{\nu},~\tilde{E},~$ and γ_0 were varied. It was found that the damping of the bar does not attain a maximum at any intermediate values of the material coefficients. Instead, the damping monotonically increases or decreases as these material coefficients vary. In particular, the damping increases as $ilde{E}$ increases or as $ilde{
u}$ decreases, and the damping goes to zero as $ilde{E}$ goes to zero or as $\tilde{\nu}$ goes to infinity. The fact that the damping increases as $\tilde{\nu}$ decreases should be expected, since for a given amount of strain at the interface, the nominal phase boundary velocity increases as $\tilde{\nu}$ decreases. Consequently, as $\tilde{\nu}$ decreases, there is more motion of the phase boundary in a given interval of time, resulting in more energy being dissipated in that interval of time. It was also found that the damping increases as the magnitude of γ_0 increases, and the damping goes to zero as γ_0 goes to zero. It was pointed out that if one were to define an infinitesimal transformation strain as one that produces a vibration response that is qualitatively like that produced as $\gamma_0 \to 0$, and a finite transformation strain as one that produces a vibration response that is qualitatively like that produced as the magnitude of γ_0 becomes larger and γ_0 approaches, say, -0.5 or 1, the negative and positive values of γ_0 that separate the infinitesimal transformation strains from the finite transformation strains are relatively small. There were also some instability problems with the numerical routine. In some cases, these instabilities resembled those of highly damped systems, which are sometimes referred to as stiff systems in the numerical-methods literature, and in the remaining cases the loss of stability resembled that of a standard centered-difference numerical routine for a wave equation, when the coefficient multiplying the term representing the spatial derivative becomes greater than one.

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