A Regularized Couple Stress Theory and its Implications on Nucleation and Kinetics of Phase Transformations in Anti-Plane Shear

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Abstract

Reversible martensitic transformations occur in a variety of alloys such as AgCd, CuAlNi, NiTi, CuSn and CuZn, which are generally termed Shape Memory Alloys (SMA). Such solid to solid phase transformations can be induced by the application of traction or a change in temperature. While there have been many experimental and some theoretical investigations of the response of these materials, most theoretical studies have been restricted to one-dimensional circumstances. The goal of this thesis is to develop a higher-dimensional mathematical model and to then use it to solve several problems pertaining to the pseudoeLASTIC behavior of SMAs.

The approach involves regularizing the classical continuum theory of sharp interfaces by developing a related, thermodynamically consistent, theory involving couple stresses; this introduces an additional material length-scale into the problem and accordingly the sharp interfaces are now replaced by narrow zones of transition. We show how the sharp interface theory is recovered from the couple stress theory in an appropriate limit, and how the couple stress theory implies an effective kinetic relation. Couple stress effects are introduced here solely for purposes of mathematical regularization, and are done in a way that has minimal influence on the bulk response of the material.

The specific problems which are studied involve the stress-induced transformation of both homogeneous and inhomogeneous domains. In the former case, the results are compared with analytical solutions; they also shed light on the structure and dissipative character of a phase boundary. The transformation of a domain containing either rigid inclusions or cavities of different shapes is also studied. Such problems are of interest, since experimental data suggests that the propagation and nucleation of phase boundaries is influenced by inhomogeneities. The nucleation, development and propagation of martensitic domains are studied in detail and the dissipative character of the various stages is quantified. The results focus on both the macroscopic response of the specimen and the local behavior of the material, and they shed light on how the local evolution of the martensitic and austenitic domains affect the global mechanical response.

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Chapter 1

Introduction

Reversible martensitic transformations, (or \textit{thermoelastic martensitic transformations}), occur in a variety of alloys such as AgCd, CuAlNi, NiTi, CuSn and CuZn, which are generally termed \textit{Shape Memory Alloys} (SMA). Such transformations can be induced by the application of traction or a change in temperature. While there have been many experimental and theoretical investigations of this phenomenon, most theoretical studies have been restricted to one-dimensional circumstances. The goal of this thesis is to develop a higher-dimensional mathematical model and to use it to solve several problems in anti-plane shear.

One of the main reasons why there have been essentially no multi-dimensional problems solved in the past is because of numerical difficulties associated with the tracking of a large number of moving surfaces. The classical continuum theory of phase transformations represents the interfaces between different phases by surfaces of strain discontinuity, and in order to analyze the process of phase transformation one must track every one of these moving boundaries, and a typical problem can involve a large number of them. Our approach involves regularizing the classical continuum theory by developing a related, thermodynamically consistent, theory involving \textit{couple stresses}; this introduces an additional material length-scale into the problem and accordingly the sharp interfaces are now replaced by narrow zones of transition. We show how the sharp interface theory is recovered from the couple stress theory in an appropriate limit. We emphasize that couple stress effects are introduced here solely for purposes of analytical regularization; we will always choose small values for the
material length-scale, and therefore we view our study as in fact pertaining to the sharp interface theory.

The specific problems which we will solve involve either rigid inclusions or cavities. Such problems are of interest, since experimental data suggests that the propagation of phase boundaries is influenced by the presence of such inhomogeneities. For example, in uni-axial tension tests one observes that the force displacement curve is serrated (see, for example, NAKANISHI's [70] observations in CuSn and LIN ET AL.'s [60] observations in NiTi). It is natural to speculate that this oscillatory variation of the applied stress is a macroscopic manifestation of a microscale process of entrapment and release of interfaces at inhomogeneities. We envision a process similar to that in plasticity, where the trapping of a dislocation line is one basic mechanism of strain hardening. Secondly, even if one did not want to study the effect of each individual particle in an SMA with inhomogeneities, one would be interested in examining the effective mechanical properties of the material by effectively smearing out the influence of the inclusions or cavities.

It should be noted that inhomogeneities play two distinct roles: on one hand, the stress concentration effect causes them to serve as nucleation sites, and on the other hand, they serve as obstacles to the propagation of pre-existing interfaces. The problems that we will study will consider both of these effects.

The specific anti-plane shear problems we examine include the following, which (when appropriate) are analyzed over a range of loading rates and inhomogeneity volume fractions:

1. a domain containing a single particle, void or crack which serves to elucidate the interdependency between nucleation, loading and the geometric shape of the inclusion;
2. periodic arrangements of particles or voids which serve to examine the effective properties of an inhomogeneous medium; and
3. a periodic arrangement of inhomogeneities which is used to study the influence of obstacles on a pre-existing phase boundary.
1.1. SHAPE MEMORY ALLOYS

Solutions to a number of axisymmetric anti-plane shear problems, which are governed by a single ordinary differential equation, have been reported in the literature. One of the few truly two-dimensional problems which has been solved is the Mode-III crack problem studied numerically by Silling [74] and analytically by Abeyaratne [1]. Silling modeled the crack as a slender ellipse and found that the crack-tip is the nucleation site for a complicated microstructure: near the tip, martensite nucleates and extends itself in a narrow band ahead of which is a microstructure of alternating layers of martensite and austenite. He then showed analytically, that in a different but analogous problem, an austenite-martensite laminate of circularly aligned rays is an energy minimizer for a phase transforming material. Abeyaratne's study relied on the hodograph transformation but his analytical solution did not exhibit the laminated microstructure; instead, his solution involved a region which contained the intermediate unstable material and he has speculated that this was a homogenized manifestation of Silling's laminated microstructure. Luskin [62] has performed some three-dimensional dynamical calculations on two-phase configurations that minimize the total energy of the system. Klouček & Luskin [50] calculate the development of twinned martensite microstructure and the propagation of austenite-martensite interfaces. Their problems involve multi-well energy minimizations to attain the optimal configuration of the microstructure. The problems, while intellectually challenging, involve the very simple physical circumstance of an infinite medium under homogeneous boundary conditions.

1.1 Shape memory alloys

The first SMA was developed over 40 years ago, but it is only after the family of NiTi shape memory alloys was discovered that extensive theoretical studies began. There is currently much work aimed at developing new shape-memory alloys, particularly ones that are both SMA and magnetostrictive. Concurrently, there are many efforts aimed at understanding and improving existing SMA's. An ongoing effort is being made to improve the experimental data and the necessary continuum level modeling.
Most of the available experimental data on SMAs are from tests on wires. A notable exception are the on-going bi-axial experiments on CuAlNi currently being carried out by CHU [23], CHU & JAMES [22]; they have up to now only examined the properties of the martensite phase but expect to study the austenite-martensite transformation soon. Recently, SHAW & KYRIAKIDES (1995) documented in [76] some experimental data of remarkable quality. They analyzed a wide variety of thermomechanical loadings at different loading rates and environmental conditions. Over a decade ago MIYAZAKI studied in [65] the properties of NiTi under similar conditions. In 1993 LEO, SHIELD & BRUNO [57] extended the results of MUKHERJEE [68], in which measured temperature changes were related to loading rate and environmental conditions. Some other notable studies on the thermomechanical properties of NiTi have been performed by BUEHLER [19], WASILEWSKI [87], JACKSON [46] and LING & KAPLOW [61].

Continuum scale modeling has been of two types. One set of models (e.g. BRINSON & LAMMERING [17] and GRAESSER & COZZARELLI [37]) have been developed by extending the ideas of plasticity theory. The emphasis here has been on developing models which describe macroscopic experimental measurements without an effort to capture the underlying micromechanisms; in some cases these models have proven to be thermodynamically inconsistent. An alternative approach (e.g. ABEYARATNE & KNOWLES [7], JAMES [45] and ACHENBACH & MÜLLER [9]) has been to construct continuum models by using explicitly the multiple energy-well character of the lattice; this leads to models which, at least qualitatively, are able to capture a wide variety of different phenomena. This will be described more fully below.

SMA's can undergo a phase transformation under either stress or temperature or both. In addition, they exhibit two distinct phenomena, viz. pseudoelasticity and the shape-memory effect, both of which are independently of interest.
1.1.1 Temperature-induced transformation

A temperature-induced transformation can be caused by heating and cooling of a freely suspended specimen. At low temperatures, the material is in its low-symmetry martensitic phase. On raising the temperature of the specimen, the material nucleates its high-symmetry phase austenite, forming a coherent phase boundary with the parent phase martensite. In the case of NiTi the crystallographic structure of austenite is body centered cubic and martensite is face centered cubic. The temperature at which this initial nucleation occurs is called the austenite-start temperature $A_s$. The austenite phase will grow continuously as the temperature is raised, until the entire specimen has been transformed at the austenite-finish temperature $A_f$, ($A_f \geq A_s$). By cooling the specimen, the transformation can be reversed, with martensite nucleating at the martensite-start temperature $M_s$, and with the interface having fully traversed the specimen at the martensite-finish temperature $M_f$, ($M_s \geq M_f$). The original martensite structure of the material has now been recovered and so the transformation is reversible.

1.1.2 Pseudoelasticity

If the material is subjected to an isothermal tensile test at a fixed temperature above $A_f$, one obtains the mechanical analog of the temperature-induced transformation described above. This is the stress-induced transformation more commonly called pseudoelasticity. To make the explanation more transparent, consider a typical uniaxial tension test under displacement control (see schematic Figure 1.1): As the specimen is elongated, the stress begins to increase. The austenitic parent phase is elastically strained until a critical stress level $\sigma_{ms}$ is reached at (b) at which point martensite is nucleated. As the bar is stretched further, the martensite grows by the propagation of the phase boundary into the austenitic material. A stress plateau (b-c) develops. Eventually, the stress reaches the value $\sigma_{mf}(\geq \sigma_{ms})$ at (c) at which point the specimen has fully transformed to martensite. After point (c) the fully martensitic bar will respond elastically to an increase in the loading (c-d). If the bar is now unloaded, the reverse
Figure 1.1: (a) Applied force versus displacement for a uniaxial one dimensional hard device experiment of a shape transforming polycrystalline material. (b) The inferred qualitative stress-strain relation.

transformation begins at $\sigma_{as}$ corresponding to point (e), and is concluded at $\sigma_{af}(\leq \sigma_{as})$ corresponding to (f). From Figure 1.1(a) it is then obvious that during a complete loading-unloading cycle some of the mechanical work has not been recovered (area bcef), even though the original state has been recovered. This type of hysteresis is known as pseudoelasticity and is an example of a reversible thermoelastic transformation. A stress-strain relation for such a material is sketched in Figure 1.1(b). The primed indices on the stress-strain graph correspond to the unprimed indices on the force-deformation graph. Both phases can co-exist in mutual equilibrium, where the austenitic phase is characterized by (f'-b') and the martensitic phase by (e'-c').

Several engineering applications involving the dynamic response of structures like composite beams and plates (e.g. [72, 59]) exploit the phenomenon of internal damping associated with this reversible transformation and also the load-dependent nature of the elastic modulus.

### 1.1.3 Shape memory effect

At a temperature lower than $A_s$, the two previous processes can be combined to form the thermomechanical cycle associated with the so-called shape memory effect. In Figure 1.2
an idealized cycle of a uniaxial test is shown. The specimen is assumed to be a polycrystal-
talline material with twin planes of different orientation. Initially, the specimen is in a
twinned martensitic state (a) since the temperature is lower than $A_s$. Twin boundaries
are of low-energy and can be easily moved by externally applied stress. Detwinning is a
local stress-induced mechanism of deformation, that allows the material to undergo a nearly
volume preserving deformation of relatively large amount without plastic deformation. First

![Idealized graph of an applied force versus displacement for a temperature treated specimen of polycrystalline SMA, exhibiting the shape memory effect.](image)

Figure 1.2: Idealized graph of an applied force versus displacement for a temperature treated specimen of polycrystalline SMA, exhibiting the shape memory effect.

the most favorably aligned twins detwin along (abd), causing a microscopic response of
small resistance to the applied force. The less favorably aligned twins resist the deformation
more severely, effectively increasing the instantaneous modulus in the range (d-e) of the
graph. Under ideal conditions the martensite is fully detwinned at point (d). By unloading
the specimen the stored elastic strain is recovered and an apparently permanent deformation
associated with point (f) is obtained. This permanent deformation is generally smaller than
the one observed in pseudoelasticity. The undistorted martensite lattice can now be trans-
formed into austenite by heating the specimen above $A_f$. Because of self accomodation, the
final austenitic specimen and the initial twinned martensitic specimen have the same macro-
scopic geometrical features, and so it appears that the specimen has recovered its original
state. For a more detailed description of the microscopic aspects of the transformation see
for example Perkins [71].
1.2 Continuum-scale modeling

In addition to the three principal phenomena described above, SMA's also exhibit a rather wide variation in their mechanical response with temperature, loading rate, stress range, specimen geometry, thermomechanical preconditioning and ambient environment, primarily because of the nonlinear coupling between these parameters. Consequently, constitutive models which are purely phenomenological have had little success in describing all of these phenomena.

The key study which has led to today's understanding of martensitic phase transformations is that of ERICKSEN [27]. In 1975 he studied energy minimizing deformations for two-phase materials within the setting of an isothermal process for a one-dimensional bar. He showed that a stable configuration might involve co-existent phases and he elucidated the role of multiple energy-wells and the distinction between local and global energy minimizers.

The three-dimensional theory is somewhat more complicated because material symmetry considerations indicate that the energy must have many energy-wells corresponding to the low-symmetry phase martensite. These correspond to the variants of martensite associated with the physical phenomenon of twinning. In three-dimensions, the formation of an interface between austenite and a single variant of martensite is not usually possible, and usually the martensitic side of the interface involves a fine mixture of two different martensitic variants. These observations motivated, in the late 80's, the development of a three-dimensional continuum theory for the equilibria of martensitic crystals by ERICKSEN [28], BALL & JAMES [13, 14], and JAMES & KINDERLEHRER [47].

These continuum theories of thermoelasticity are well suited for describing the energy minimizing equilibrium states of two-phase materials. They do not however suffice to characterize the dynamic process of phase transformation between different phases, irrespective of whether the process is quasi-static or whether inertia is important. The existence of multiple solutions to certain dynamic initial-boundary-value problems has been demonstrated,
and this establishes the inadequacy of the static theory. This lack of uniqueness is due to the incompleteness of the classical continuum theory of thermoelasticity as far as dynamic problems are concerned, and requires that certain supplementary information be added to the theory. Physically, this information pertains to the phenomenon of nucleation, where a new phase is nucleated within the parent phase, and the phenomenon of growth, where the new phase that has been nucleated grows according to some kinetic law.

Adding nucleation and kinetic criteria to the classical theory leads to a well-posed theory which is able to describe the dynamic process of phase transformation. The reader is referred to Abeyaratne & Knowles [3, 4, 6, 7] for a description of these ideas and for examples of specific descriptions of these various constitutive ingredients. Another set of kinetic laws developed for modeling pseudoelasticity is that of Achenbach & Müller [9] and Müller & Xu [69].

The higher-dimensional problems that we wish to solve must necessarily be solved numerically. Because of the presence of moving phase boundaries (which are described by sharp interfaces of strain discontinuity) it is necessary to track each boundary, and there can be a large number of them. An example of a tracking algorithm is the one developed by Kim as described in Kim & Abeyaratne [49]. An alternative approach would be to introduce a small amount of some regularizing phenomenon which would replace the sharp interfaces by narrow zones of transition. If the magnitude of the regularizing quantity is kept small, one can often show that the regularized theory and the sharp interface theory coincide away from the transition zone. The classical mathematical example of this is in fluid mechanics, where the inclusion of viscosity and capillarity regularizes the inviscid theory of compressible fluids, and replaces shock waves by narrow zones of transition. There are two-alternative ways in which to regularize the sharp interface theory of phase transformations, one based on an order parameter theory and the other based on introducing higher gradients of the deformation gradient into the theory in some consistent way; we now describe these ideas further and in particular will distinguish between two versions of the latter approach which
we shall call strain-gradient theory and couple stress theory.

1.2.1 Sharp interface theory

First, let us briefly review the sharp interface theory of solid to solid phase transformations. This dynamic theory has been developed principally by Abeyaratne & Knowles [4, 6, 7]. Following Ericksen [27], they allow the gradient of the displacement \( u \) to suffer jump discontinuities across surfaces in the body which represent the interfaces between distinct phases of the material. The underlying free-energy of the material must have multiple energy-wells and different energy-wells are relevant on different sides of such an interface. The theory is based on the well-known concepts of nonlinear field theory outlined in [80]. The field equations and associated jump conditions are derived from the standard balance principles of linear momentum, angular momentum, energy, and the dissipation inequality. Since the dynamic process of phase transformation is generally a non-equilibrium process, the entropy production rate is non-zero. By calculating the entropy production rate, one is able to identify the thermodynamic driving force \( f \) which is conjugate to the mass flux across the phase boundary. To model the dynamics of the non-equilibrium process one must provide a description of the rate of dissipation associated with the moving interface, usually in the form of a kinetic relation involving the driving force and the mass flux (or normal velocity of propagation). The detailed structure of the kinetic relation depends on the microscale processes which are not apparent at the continuum scale. Explicit forms of the kinetic relation must either be laid down phenomenologically, or determined experimentally, or determined from a study of microscopic processes at the lattice level. Such models have led to several studies of interfacial motion in SMA (e.g. [7]). The greatest advantages of this theory is its straightforward application of well-known concepts and the flexibility it allows in choosing the constitutive ingredients; in particular, properties of the interface and of the individual bulk phases can be specified independently, thereby adapting the model to a wide range of problems. In Chapter 2 the mathematical and physical aspects of the theory will
be reviewed.

An alternative formalism of the above sharp interface theory has been presented by Gurtin & Struthers [40], though the resulting theory itself is identical. In this formalism the phases are modeled as different nonlinear hyperelastic materials that are separated by nonmaterial surfaces suffering a jump in the gradient of the deformation. These surfaces are then endowed with an additional system of forces (configurational forces) and energies intrinsic to it. In order to accommodate this idea an additional force balance known as the configurational force balance is introduced. The work done by those configurational forces is accounted for in the dissipation inequality. The configurational forces are then determined by specifying an additional constitutive relation for the surface energy. In this approach, one must introduce in addition to an independent constitutive relation an additional balance law for configurational forces with direct consequences on the dissipation inequality. The kinetic relation follows as a consequence of the new balance principle. The physical interpretation of the configurational forces and their associated stress tensor and momenta are not fully understood. In any case, the end result is the same as the preceding theory.

1.2.2 Order-parameter based theory

Order-parameters have been used extensively in the description of various problems by physicists, and recently Gurtin [41] and co-workers have developed the continuum theory of order parameters. In particular, Fried & Gurtin developed in [33] an order-parameter based theory, which serves as the regularization of the sharp interface theory of Gurtin & Struthers. The motion $y$ and the scalar field of the order parameter $\phi$ are assumed to be sufficiently smooth. In order to accommodate the order parameter, new conjugate forces have to be introduced in the energy dissipation inequality. These so-called microforces are needed in order to be able to satisfy the independent microforce balance. The conservation statements of linear momentum and angular momentum remain unchanged, and now direct coupling with the microforce balance is implied. The coupling between variables of global
deformation and of the order parameter can be introduced through nonlinear terms in the
specified energy density function $W$, which depends on the deformation gradient $\mathbf{F} = \text{Grad} \mathbf{y}$,
the order parameter $\phi$, and the gradient of the order parameter. When dissipative interfaces
are modeled, the theory requires an additional constitutive assumption that is also a function
of the order-parameter rate $\dot{\phi}$. Thus the interface is endowed with structure and damping.
It has been shown by Fried & Grach [35] that microforces and configurational forces are
related, and that the order-parameter based theory is a first order approximation to Gurtin
& Struthers' sharp interface theory. The order-parameter based theory requires one to
solve second order boundary-value problems, that might either be coupled or uncoupled,
depending on the nature of $W$. The advantages of the theory are its well-defined limit in
the sharp interface theory, and the computational simplicity. Unfortunately, no physically
meaningful interpretation of the order parameter and its conjugate microstresses have been
found (in general) up to date.

1.2.3 Strain-gradient theory

An intuitively appealing method in which to regularize propagating phase boundaries dates
back to 1901 with Korteweg's [51] models of fluid capillarity effects. His constitutive
relation for an elastic fluid generalizes the classical one by allowing the free-energy to depend
on several higher-order spatial gradients of the mass density. The classical form of the
equation of motion and the symmetry of the Cauchy stress tensor are retained.

These ideas were initially applied to liquid-vapor phase transitions of the Van der Waals
fluid. Subsequently Slemrod [75] and others noted its similarity to phase transitions in
elastic solids, with the stress-strain relation generalized to include a dependency on higher-
order strain gradients together with a viscous term to model the dissipation at the inter-
face. Several authors like Abeyaratne & Knowles [5], Rosakis [73], Truskinovsky &
Zanzotto [81], and Truskinovsky [82] have used this kind of strain-gradient model. The
manner in which the strain-gradient terms and the viscous terms are introduced into the
1.2. CONTINUUM-SCALE MODELING

constitutive description distinguishes one of these models from another. When these terms are introduced appropriately, the augmented theory can be made compatible to the sharp interface theory in the limit.

In 1985, Dunn & Serrin [26] noted difficulties that arise in such augmentations due to thermodynamic inconsistency. Their insight was based on a result proven by Coleman & Noll (e.g. [80]) who showed that for any admissible process, the second law of thermodynamics excludes any dependency of the Cauchy stress tensor on higher-order gradients of the deformation. To accommodate those gradients, the energy equation and dissipation inequality have to be modified in some way. Dunn & Serrin propose an additional mechanical energy, the so-called interstitial work flux, which accounts for the supply of mechanical energy of longer range than those reflected in the supply due to the traction. The balance of linear momentum and angular momentum remain unchanged, implying the symmetry of the Cauchy stress tensor and the validity of the classical form of the equation of motion. The general conclusion here is that one cannot introduce strain-gradient terms into a continuum theory without also considering corresponding force-like and/or energy-like entities. This leads us naturally to consider couple-stress type theories.

1.2.4 Couple stress theory and related topics

In this subsection we shall review couple stress theory, its historical origins, and some related nonlocal theories with material length scale dependency. We will distinguish between several different forms of such theories, all of which are, in a broad sense, referred to as couple stress theories. The particular theory that we use will be developed in detail in Chapter 3.

The theory of couple stresses traces its origins to a wide variety of general theories of rods, shells, and theoretical studies on the elastic properties of crystals by Voigt [85]. In 1909 this led the Cosserat brothers, E. & F. Cosserat [21], to develop a three-dimensional theory in which the interaction between one part of the body upon another due to contact is represented by a traction vector $\tau$ and a couple vector $\mathbf{m}$. The couple
vectors are considered to be the result of a more refined description of the kinematics. A material point of the continuum is now endowed with six degrees of freedoms (like a rigid body). Each material particle is now considered to be a rigid subdomain of small but finite extent. The orientation of each point is then given by three perpendicular directors, forming a so-called triad. In the case of a Cosserat medium, or in Eringen's terminology a micropolar medium, this triad is allowed to translate and rotate rigidly. To describe the state of a material point one must therefore specify vectors of translation and rotation. This newly found richness gives rise to a Cauchy stress tensor which is not necessarily symmetric. A completely posed boundary-value problem (in a purely mechanical theory) consists of the field equations of linear momentum and angular momentum, together with boundary conditions for the traction \( t \) and the couple vector \( m \) or their respective conjugate velocities. Due to this complexity, and related computational difficulties, most of these couple stress theories did not find extensive application until the end of this century.

Subsequent to the Cosserat's pioneering work, several authors generalized the theory and solved several boundary-value problems. The most significant contributions to the basic development of the theory occurred in the 1960's. A good review of the state of this subject (at the time that article was written) is given by Toupin [78]. He constructed the constitutive equations for finite deformations of a Cosserat medium. Two years later he derived in [79] the underlying balance laws by using Hamilton's principle. In 1962 Mindlin & Tierstein [63] revisited the Cosserat equations and proposed a constitutive model for the linearized theory. Their results were able to reconcile differences between the previously published results of Grioli's [38] constitutive model and that of Aero & Kuvshinski [10], which until then had been a source of considerable argument. Most of our work will be based on the insight of Mindlin & Tierstein.

Around this same time, workers like Ericksen & Truesdell began to relax the idea of a rigid material element and allowed the directors to stretch and rotate relatively to each other. An all encompassing description of such micromorphic media can be found
in Eringen [29]. In [64], Mindlin formulates a linear theory, which incorporates some properties of a crystal lattice and is related to the theory of deformable directors.

In 1973 Germain [36] published a paper on materials with microstructure. His development starts from the Principle of Virtual Work and the necessary kinematics of micromorphic materials. Up to this point, we neglected to mention the existence of media of “different degrees of order”. These degrees can be considered as the order of a Taylor expansion of the velocity field in the neighborhood of a material point. Thus, for example, a material with a first-order Taylor expansion is called a micromorphic material of degree 1. In the special case where the Jacobian Matrix is restricted to being skewsymmetric, the material element is carrying out a rigid motion, and the Cosserat equations are recovered. Higher degree materials are derived by introducing higher order approximations of the velocity field in the neighborhood of the point. In this thesis only materials of degree-1 are considered.

In order to be thermodynamically consistent, one must introduce higher-order derivatives of the deformation into the couple stress theory. The exact nature of the terms introduced depends on the precise nature of the couple stresses. They must be consistent. In comparison to the previously described strain-gradient theory, all conservation laws can now be consistently satisfied including the energy balance. This firm mathematical foundation of couple stress theory makes it attractive for our purposes. Balance laws, as well as indirect methods such as Hamilton’s Principle and other variational methods can be sufficiently enriched to yield the equations of the couple stress theory.

In recent years there have been many studies of micromechanical phenomena in which a material length scale is important. Several theories have been brought forward (related to a wide range of physical applications). Some specific examples are the Cosserat-type plasticity theory of Fleck & Hutchinson [30], the nonlocal plasticity theory of Dai & Parks [24], and work of Aifantis [11], Vardoulakis [86], Xia & Hutchinson [89], and Mühlhaus & Aifantis [66]. Fleck & Hutchinson use the couple stress theory to directly incorporate the micromechanical effects previously observed in several experiments by Fleck [31]
and others. They argue that the creation of geometrically necessitated dislocations leads to a material length scale \( l_m \). This length scale will be rigorously developed in Chapter 3. For a linear isotropic material this necessitates that an additional elastic modulus exist whose dimension is force; this modulus, in conjunction with the Young's modulus, gives rise to a material dependent length scale \( l_m \). In the novel approach proposed by Dai & Parks, they introduce a material length scale into the internal evolution equations of the variable representing strength in plasticity. Thus the classical balance laws and the symmetry of the Cauchy stress are preserved, and it is sufficient to solve the customary boundary-value problems, simplifying the computational effort considerably. They were able to reproduce several scale dependent phenomena of plastic deformation. Aifantis and co-workers analyze the influence of strain gradients on the localization of plastic flow, the formation and propagation of deformation bands, and the determination of the structure of the crack tip. The introduced higher-order gradients stabilize these mechanisms and made it possible to describe the material's response beyond the pre-localization regime. A collection of other applications is listed in [67]. Generally, couple stress theories try to adequately describe the effect of microstructure on a macroscale level.

1.3 Outline of thesis

The main body of this thesis can be divided into three parts: the development of the theoretical framework, a discussion of the numerical method, and a description of the problems solved and the results.

In Chapter 2 the sharp interface theory is reviewed. We begin our discussion with the classical conservation laws of continuum thermomechanics and develop from there the concept of driving traction, kinetic relation and nucleation criterion. The theory is then specialized to anti-plane shear motions.

In Chapter 3 we proceed to develop a thermodynamically consistent regularization of the preceding sharp interface theory. The kinematics and balance laws pertaining to couple
stress theory are discussed. We then linearize the kinematics but retain nonlinearity in the constitutive relations. Necessary restrictions on the constitutive structure are then examined if the material is to be able to undergo anti-plane shear motions; this requires that the energy potential satisfy certain compatibility conditions stemming from the requirement that the three equations of motion only involve a single unknown, the out-of-plane displacement. The final form of energy depends on both the strain and the strain gradient, and as a function of strain, the energy has multiple energy-wells. The model is completed by adding, to the stress, a term proportional to the strain rate; this captures the dissipative nature of a propagating interface.

In Chapter 4 we relate the preceding sharp interface and couple stress theories. Since dissipation in the sharp interface theory is modeled by a kinetic relation, whereas in the couple stress theory it is achieved by the bulk viscosity, it is necessary to understand the relation between these two mechanisms. We examine this by studying a traveling wave of a uniformly propagating planar phase boundary. The traveling wave problem can be solved explicitly, and in the limit of vanishing strain-gradient parameter and viscosity parameter, we show that the solution converges to a solution of the sharp interface theory which is propagating according to a certain kinetic law. We calculate explicitly this "effective kinetic relation" of the couple stress model. Linearizing it for small values of propagation velocity allow us to calculate the mobility of the interface. Thus, in this chapter, we show that using the couple stress theory is equivalent to using the sharp interface theory together with a particular kinetic relation. If we want to model other kinetic relations, the viscous term must simply be introduced differently, e.g. as a cubic instead of linearly.

With both formulations in place and their equivalence established, we introduce the numerical methods for implementing the couple stress theory in Chapter 5. The Finite Element Method is shown to be applicable to the couple stress theory if elements have the required continuity. We introduce the predictor-corrector scheme that we use and illustrate some of the solved verification problems.
In Chapter 6 we describe the specific anti-plane shear problems that we solve. The problems include those motivated by engineered composites and their effective properties at different volume fractions of fibers, the implication of particles and holes as nucleation sites for interfaces, the role of particles and voids as obstacles to propagating phase boundaries, and the effective kinetic relation of an SMA with voids and particles.

The results are presented and discussed in Chapter 7.

In summary, the goal of this thesis was to construct a consistent couple stress theory which regularizes sharp interfaces, and to use it to solve some higher-dimensional problems. The theory was chosen to be as simple as the framework allowed. The material length scale $l_m$ of the couple stress theory provides a measure of the thickness of the transition layer between the austenite and martensite phases. This length scale plays an important role in problems involving phase transformation. As expected however, the sensitivity of the results on the material length scale $l_m$ is almost nonexistent when only one phase exists, because the theory has been designed so that couple stress effects are significant only near a phase boundary. In order to achieve this, the length scale $l_m$ is chosen to be several times smaller than has been used in past studies of couple stress theories designed for examining bulk effects. Even so, we find that nucleation and kinetics is strongly influenced by $l_m$. A concluding discussion is found in Chapter 8.
Chapter 2

Sharp interface theory

Introduction

In recent years several physical mechanisms encountered in materials have been mathematically modeled by the sharp interface theory of nonlinear elasticity. Some commonly, investigated problems are the formation of shear bands in plasticity and several types of solid state phase transformations occurring in alloys. We will concentrate on alloys that undergo a reversible phase transformation and form solid to solid interfaces. Those transformations are characterized by deformations with discontinuous first gradients and cause a breakdown of the strong ellipticity criterion in the governing field equations of nonlinear elastostatics. They require the specification of additional constitutive assumptions to yield unique solutions for the displacement field.

In this chapter we will review in (Section 2.1) the basic balance laws, field equations, and jump conditions associated with such discontinuous displacement fields. In the next section we introduce the concept of a driving traction. In Section 2.3 the preceding is specialized to isothermal quasi-static processes, and several issues associated with the loss of strong ellipticity are addressed, viz. the additional constitutive assumptions of a kinetic relation and a nucleation criterion. In Section 2.4 we specialize the field equations and jump conditions to anti-plane shear motions and discuss two separate issues. First, we study necessary and sufficient conditions for a material to be able to undergo an anti-plane shear
deformation; secondly, we take into account the additional implications on the material due to the presence of sharp interfaces.

2.1 Balance laws, field equations, jump condition

Consider a continuous body $B$ that occupies the three dimensional region $R$ on a time interval $\mathcal{T} = (t_0, t_1)$. The motion of the body is characterized by a one-parameter family of invertible and continuous mappings $y(x, t) : R \rightarrow R_t$, so that the position vector $y$ in $R_t$ is given by

$$y = y(x, t) = x + u(x, t) \quad \forall x \in R, \ t \in \mathcal{T}. \quad (2.1)$$

Each material point $x \in R$ is mapped from its reference configuration $R$ to its deformed configuration $R_t$ by the displacement vector $u$. It is assumed that the deformation $y$ is at least twice continuously differentiable on $R \times \mathcal{T}$, except on a collection of piecewise smooth surfaces $\Sigma$ contained in $R$. On $\Sigma$ the gradient of the motion $y$ may suffer a finite jump discontinuity. Deformations of this kind are called multiphase deformations, since it allows the material on opposite sides of $\Sigma$ to belong to different phases. In our setting, this surface $\Sigma$ of discontinuity is referred to as the phase boundary or the interface associated with the phase transformation of body $B$, and its position may vary with time. We note that the $\Sigma$ is really the Lagrangian image in the reference configuration of the "real" phase boundary in the current configuration. The deformation gradient tensor $F = \text{Grad} y(x, t)$ represents the map of $dx \in R$ to $dy \in R_t$ at a given time $t \in \mathcal{T}$ and is defined by

$$F_{ij} = \frac{\partial y_i}{\partial x_j} = \delta_{ij} + \frac{\partial u_i}{\partial x_j} \quad \forall x \in R \setminus \Sigma, \quad (2.2)$$

where $\delta_{ij}$ is the Kronecker delta. The latin subscripts have the range \{1, 2, 3\}, and summation is implied by a repeated subscript. Since the map $y(x, t)$ is one-to-one the Jacobian determinant, $J = \det F > 0$, is positive. An objective measure of distortion in the theory of large deformation is the right Cauchy-Green tensor

$$C = F^T F. \quad (2.3)$$
The particle velocity \( \mathbf{v} \) is denoted at points \((\mathbf{x}, t)\), wherever it exists, by
\[
\mathbf{v} = \mathbf{v}(\mathbf{x}, t) = \frac{\partial \mathbf{u}(\mathbf{x}, t)}{\partial t} \quad \forall \mathbf{x} \in R \setminus \Sigma.
\] (2.4)

We now consider an arbitrary subregion \( D \subset R \) of the reference configuration \( R \) with boundary \( \partial D \). The nominal stress tensor, or the so called Piola-Kirchhoff stress tensor, is denoted by \( \sigma(\mathbf{x}, t) \). The mass density \( \rho(\mathbf{x}) \) is required to be continuous on \( R \), while the stress tensor \( \sigma(\mathbf{x}, t) \) and its gradient are piecewise continuous on \( R \). We disregard effects due to body forces and internal heat generation. A complete treatment, incorporating those physical effects is given by ABEYARATNE & KNOWLES [4]. The global balance laws of linear momentum and angular momentum require for every regular subregion \( D \) at any time \( t \in \mathcal{T} \) that
\[
\int_{\partial D} \sigma \mathbf{n} \ dA = \frac{d}{dt} \int_D \rho \mathbf{v} \ dV,
\] (2.5)
\[
\int_{\partial D} \mathbf{y} \times \sigma \mathbf{n} \ dA = \frac{d}{dt} \int_D \mathbf{y} \times \rho \mathbf{v} \ dV,
\] (2.6)
with \( \mathbf{n} \) being the outward unit normal to \( \partial D \). Next, the internal energy \( \varepsilon(\mathbf{x}, t) \) per unit mass and the entropy \( \eta(\mathbf{x}, t) \) per unit mass are assumed to be at least piecewise continuous with piecewise continuous first gradients on \( R \times \mathcal{T} \). The temperature \( \theta(\mathbf{x}, t) \) is continuous with piecewise continuous first derivatives. Then the first and second laws of thermodynamics require, respectively, that for every regular region \( D \subset R \) at each instant of time \( t \in \mathcal{T} \),
\[
\int_{\partial D} \sigma \mathbf{n} \cdot \mathbf{v} \ dA + \int_{\partial D} \mathbf{q} \cdot \mathbf{n} \ dA = \frac{d}{dt} \int_D \rho \varepsilon \ dV + \frac{d}{dt} \int_D \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} \ dV,
\] (2.7)
\[
\Gamma(D, t) \equiv \frac{d}{dt} \int_D \rho \eta \ dV - \int_{\partial D} \mathbf{q} \cdot \mathbf{n} \ dA \geq 0.
\] (2.8)
Inequality (2.8) is often referred to as the entropy production rate inequality or the Clausius-Duhem version of the second law of thermodynamics with entropy production \( \Gamma(D, t) \). Localization of the global balance laws (2.5-2.8) yields at a point in \( D \setminus \Sigma \) at a fixed time instant \( t \in \mathcal{T} \) the usual local field equations:
\[
\text{Div } \sigma = \rho \dot{\mathbf{v}},
\] (2.9)
\[ \sigma F^T = F \sigma^T, \]  
\[ \sigma \cdot \dot{F} + \text{Div} \, q = \rho \dot{\epsilon}, \]  
\[ \text{Div} \left( \frac{q}{\theta} \right) \geq \rho \dot{\eta}. \]

On the other hand at points on \( \Sigma(t) \) where the deformation gradient \( F \) suffers jump discontinuities, localization of (2.5), (2.7-2.8) yields at \( t \in \mathcal{T} \) the following jump conditions:

\[ \left[ [\sigma n_\Sigma] \right] + \rho [v] V_n = 0, \]  
\[ \left[ [\sigma n_\Sigma \cdot v] \right] + \left[ [\rho \left( \varepsilon + \frac{1}{2} v \cdot v \right)] \right] V_n + \left[ [q \cdot n_\Sigma] \right] = 0, \]  
\[ \left[ [\rho \eta] \right] V_n + \left[ \left[ \frac{q \cdot n_\Sigma}{\theta} \right] \right] \leq 0. \]

In addition to the jump conditions (2.13-2.15), the continuity assumptions imposed on the deformation have the immediate consequence that

\[ \left[ [F] \right] l = 0, \quad \forall \, x \in \Sigma, \, t \in \mathcal{T}, \]  
\[ \left[ [v] \right] = -V_n \left[ [F] \right] n_\Sigma, \quad \forall \, x \in \Sigma, \, t \in \mathcal{T}, \]

where \( l \) is any vector tangent to the surface \( \Sigma(t) \). The scalar normal velocity \( V_n \) denotes the velocity of the moving surface \( \Sigma(t) \). The unit normal vector \( n_\Sigma \) on the singular surface \( \Sigma(t) \) is chosen such that \( V_n \geq 0 \), if \( V \) points into the positive region \( \overset{\circ}{D} \). The positive region \( \overset{\circ}{D} \) and the negative region \( \overset{\circ}{D} \) of the body \( D \) are separated by \( \Sigma(t) \). The notation \( \left[ [g(x, t)] \right] \) of a generic function \( g(x, t) \) stands for

\[ \left[ [g(x, t)] \right] = \overset{\circ}{g}(x, t) - \overset{\circ}{g}(x, t), \]

of the limiting values across the discontinuity \( \Sigma(t) \).

### 2.2 The driving traction for isothermal processes

In the previous section an account of the necessary field equations and jump conditions was made. A useful alternative for the modeling of materials with interfaces has been given by
2.2. THE DRIVING TRACTION FOR ISOTHERMAL PROCESSES

Abeyaratne & Knowles [4]. They express the jump condition of entropy (2.15) by the inequality

\[ fV_n \geq 0 \quad \forall \, \mathbf{x} \in \Sigma, \, t \in \mathcal{T}. \]  \hspace{1cm} (2.19)

The driving traction \( f(\mathbf{x}, t) \) is defined on the singular surface \( \Sigma(t) \) by

\[ f(\mathbf{x}, t) = \rho(\mathbf{x}) \left[ \psi(\mathbf{x}, t) \right] - \frac{1}{2} \left\{ \mathbf{\sigma}(\mathbf{x}, t) + \mathbf{\sigma}(\mathbf{x}, t) \cdot [\mathbf{F}(\mathbf{x}, t)] \right\} \quad \forall \, \mathbf{x} \in \Sigma, \, t \in \mathcal{T}, \]  \hspace{1cm} (2.20)

after introducing the Helmholtz free energy \( \psi(\mathbf{x}, t) \) as

\[ \psi(\mathbf{x}, t) = \varepsilon(\mathbf{x}, t) - \theta \eta(\mathbf{x}, t) \quad \forall \, \mathbf{x} \in \mathcal{R}, \, t \in \mathcal{T}, \]  \hspace{1cm} (2.21)

which inherits the smoothness assumptions of \( \varepsilon(\mathbf{x}, t) \). The inequality (2.19) provides a restriction upon the possible direction of motion of a moving phase boundary, and (2.20) is a thermodynamical force exerted on the discontinuity \( \Sigma(t) \).

Their results can be attained by making use of the rate of entropy production (2.8), the local field equation of energy (2.11), and the associated jump conditions of linear momentum (2.13), of energy (2.14), and of the kinematics (2.17). After some algebra the total rate of entropy production \( \Gamma(D, t) \) can be decomposed into physically meaningful contributions. We assume from now on that all processes occur isothermally at a constant temperature

\[ \theta(\mathbf{x}, t) = \theta_0 \quad \forall \, \mathbf{x} \in \mathcal{R}, \, t \in \mathcal{T}. \]  \hspace{1cm} (2.22)

Thus the entropy production due to heat conduction vanishes and \( \Gamma(D, t) \) simplifies to:

\[ \Gamma = \Gamma_{Mat} + \Gamma_f, \]  \hspace{1cm} (2.23)

\[ \Gamma_{Mat} = \frac{1}{\delta} \int_D (\rho \dot{\theta} \theta + \mathbf{\sigma} \cdot \mathbf{\bar{F}} - \rho \dot{\varepsilon}) \, dV, \]  \hspace{1cm} (2.24)

\[ \Gamma_f = \frac{1}{\delta} \int_{\Sigma(t) \cap D} f V_n \, dA. \]

The contribution \( \Gamma_{Mat} \) arises due to the local dissipation of the material away from the singular surface, and the rate of entropy \( \Gamma_f \) is associated with the motion of the singular surface \( \Sigma(t) \). By localizing the modified rate of entropy production (2.23-2.24) one gets for isothermal processes at a point \( \mathbf{x} \) away from the singular surface \( \Sigma(t) \) that

\[ \rho \delta \geq 0 \quad \forall \, \mathbf{x} \in \mathcal{R} \setminus \Sigma, \, t \in \mathcal{T}, \]  \hspace{1cm} (2.25)
where $\delta(x, t)$ is the internal dissipation:
\[
\delta \equiv \theta \dot{\gamma} + \frac{1}{\rho} \sigma \cdot \dot{F} - \dot{\varepsilon},
\]
which was taken from Truesdell [80]. The corresponding jump condition is defined by inequality (2.19). Up to now no use was made of a constitutive relation. In the next section we will consider a nondissipative thermoelastic material undergoing slowly evolving deformations with respect to time.

### 2.3 Slow isothermal processes and thermoelastic materials

We will from now on focus our attention on materials that are thermoelastic and undergo a quasi-static process. A quasi-static motion is a one parameter family of equilibrated deformations that approximate a motion of extremely slow velocity, so that inertia is ignorable. In the global mechanical balance laws (2.5-2.6) the momentum $\rho \mathbf{v}$ is set equal to zero, and upon localization those field equations and jump conditions become:

\[
\begin{align*}
\text{Div} \sigma &= 0, \\
\sigma F^T &= F^T \sigma^T, \\
[[\sigma n_\Sigma]] &= 0, \\
[[F]] l &= 0,
\end{align*}
\tag{2.27}
\]

\[
\forall x \in R \setminus \Sigma, \ t \in T,
\]

Now suppose that the body $D$ is composed of a homogeneous, compressible and hyperelastic material with elastic potential or stored energy $W = W(F, \theta)$ per unit undeformed volume. Thus by choosing a thermoelastic material with stored energy
\[
W = \rho \psi(F, \theta),
\tag{2.29}
\]

the contribution $\Gamma_{Mat}$ of the rate of entropy production in (2.23) vanishes and the total rate of entropy production is due to the motion of the interface $\Sigma(t)$. This defines the work energy relation for an isothermal, quasi-static, and elastic process as
\[
\mathcal{P}(D, t) = \theta_0 \Gamma_f = \int_{\partial D} \sigma \cdot n \cdot v \, dA - \frac{d}{dt} \int_D W \, dV,
\tag{2.30}
\]
2.3. SLOW ISOTHERMAL PROCESSES AND THERMOELASTIC MATERIALS

with \( \mathcal{P}(D, t) \) being the rate of energy dissipation. This suggests that \( f(\mathbf{x}, t) \) of (2.20) can be thought of as a traction that is applied on the surface \( \Sigma(t) \) by the body \( D \).

For a thermoelastic material the nominal stress \( \mathbf{\sigma} \) is determined by

\[
\mathbf{\sigma}(\mathbf{x}, t) = \frac{\partial W(\mathbf{F}(\mathbf{x}, t))}{\partial \mathbf{F}} \quad \forall \mathbf{x} \in \mathbb{R} \setminus \Sigma, \; t \in \mathcal{T}. \tag{2.31}
\]

It is necessary that the energy (and the stress) be frame indifferent, and consequently that the function \( W \) depend on \( \mathbf{F} \) through the objective right Cauchy-Green tensor \( \mathbf{C} = \mathbf{F}^T \mathbf{F} \),

\[
W(\mathbf{F}) = W(\mathbf{C}). \tag{2.32}
\]

By the chain rule and (2.32) the constitutive relation (2.31) becomes

\[
\mathbf{\sigma}(\mathbf{x}, t) = 2\mathbf{F} \frac{\partial W(\mathbf{C}(\mathbf{x}, t))}{\partial \mathbf{C}}, \quad \sigma_{ij} = 2F_{ik} \frac{\partial W}{\partial C_{kj}}. \tag{2.33}
\]

The stored energy function \( W \) is said to be strongly elliptic, if for every admissible deformation gradient \( \mathbf{F} \) and for all nonzero vectors \( \mathbf{a} \) and \( \mathbf{b} \) the following holds

\[
\frac{\partial W}{\partial F_{ij} \partial F_{kl}} a_i b_j a_k b_l > 0. \tag{2.34}
\]

Knowles & Sternberg demonstrated in [55] that this classical result ceases to be valid for equilibrated multiphase deformations. They showed that such deformations are sustainable only if \( W \) ceases to be strongly elliptic at some value of \( \mathbf{F} \). Hence, in order to model a solid to solid phase transformation a non-convex energy potential \( W \) is required. On the other hand, an equilibrated deformation for which the strong ellipticity condition fails will be unstable at some part of the body as shown by James [44] and Gurtin [39]. Equations (2.27-2.28), (2.33) are the usual equations of elastostatics. Even in this purely mechanical setting the entropy production rate has to be satisfied, such that the inequality (2.19) continues to hold

\[
fV_n \geq 0 \quad \forall \mathbf{x} \in \Sigma, \; t \in \mathcal{T}. \tag{2.35}
\]

Under the assumption of a quasi-static process formula (2.20) of the driving traction can now be written with the aid of (2.29) as

\[
f(\mathbf{x}, t) = [\lbrack W \rbrack] - \mathbf{\overline{\sigma}} \cdot [\mathbf{F}(\mathbf{x}, t)] \quad \forall \mathbf{x} \in \Sigma, \; t \in \mathcal{T}, \tag{2.36}
\]
where the nominal stress \( \hat{\sigma} \) and \( \bar{\sigma} \) are respectively the stresses on \( \hat{D} \) and \( \bar{D} \).

Let us now introduce the potential energy \( G \) per unit reference volume as

\[
G = G(F, \theta, \sigma) = W(F) - \sigma \cdot F. \tag{2.37}
\]

It is then obvious that (2.36) can be written as

\[
f(x, t) = [[G]] \quad \forall x \in \Sigma, \ t \in T. \tag{2.38}
\]

A material that can undergo a thermoelastic phase transition should have a potential energy \( G \) with at least two local minima or so called energy wells. The corresponding stored energy \( W \) will be non-convex, and the stress-strain relation will be non-monotonic. Each energy well of \( G \) is then identified with a different phase of the material, and each of these phases corresponds in the sharp interface theory to positive sloped branches of the stress-strain relation. Thus the potential energy has two energy wells at \( F = \hat{F} \) and \( F \), which are separated by a local maximum corresponding to an energy barier between the two phases. The phase with the smaller value of \( G \) is the more stable phase. In our isothermal case the energy wells can only shift from one energetic level to the other by the application of a stress field. The energy well with the lowest potential energy is the local minimizer and the preferred phase for a material point \( x \). The difference in potential energy between those two phases determines the strength of the driving traction \( f \). Thermodynamically equilibrated phases have the same potential energy \( G \) and by (2.38) the driving traction \( f = 0 \), one speaks of those states \( (\hat{F}, \theta) \) and \( (\bar{F}, \theta) \) as being in phase equilibrium. No motion of the interface is observed if \( G(\hat{F}, \theta, \sigma) = G(\bar{F}, \theta, \sigma) \). On the other hand if \( G(\hat{F}, \theta, \sigma) > G(\bar{F}, \theta, \sigma) \) the driving traction \( f \) is positive and according to (2.35) the normal velocity \( V_n \) is positive and the phase propagates into the positive region \( \hat{D} \), transforming material from a state \( (\hat{F}, \theta) \) to a state \( (\bar{F}, \theta) \). The direction of propagation is reversed if \( G(\bar{F}, \theta, \sigma) > G(\hat{F}, \theta, \sigma) \).

As particles cross the interface \( \Sigma(t) \) they transform from one phase to the other at a rate that is determined by the kinetics of the transformation. If one assumes that this phase
transformation depends only on the respective states \((\hat{F}, \theta)\) and \((\overline{F}, \theta)\) found on either side of the interface the propagation of the phase boundary is governed by a relation of the form

\[ V_n = \phi(\hat{F}, \overline{F}, \theta). \quad (2.39) \]

By inverting for each phase the constitutive relation (2.31) the deformation gradient \(\hat{F}\) and \(\overline{F}\) can be expressed in terms of \(\theta\) and \(\sigma = W_F\). As a special case, kinetic law can with the help of (2.36) be taken as a function of the driving traction \(f\) and the temperature \(\theta\),

\[ V_n(x, t) = V_n(f(x, t)), \theta). \quad (2.40) \]

The kinetic relation \(V_n(f, \theta)\) or its inverse \(f(V_n, \theta)\) describe the evolution of existing interfaces, and do not specify the needed stress level and temperature, to observe the nucleation of a phase boundary. This initial transition of the domain from a single-phase configuration to a two-phase configuration is controlled by a nucleation criterion. The kinetic relation and nucleation criterion are necessary additional constitutive assumptions, in order to obtain well-posed boundary value problems in the sharp interface theory.

### 2.4 Anti-plane shear

The preceding will now be specialized to an anti-plane shear motion \(y(x, t)\) along the \(e_3\) direction in a fixed orthonormal basis \(\{e_1, e_2, e_3\}\) associated with the reference configuration \(R\). Consider a cylindrical body with cross section \(\Pi\) and generators parallel to \(e_3\) which is mapped from its reference configuration \(R\) to its deformed configuration \(R_t\) by the motion

\[ y = y(x, t) = x + u(x_1, x_2, t)e_3 \quad \forall x \in R, \ t \in \mathcal{T}. \quad (2.41) \]

The out-of-plane displacement field \(u\) depends at each time instant \(t \in \mathcal{T}\) on the material points \(x_\alpha = x \cdot e_\alpha\), and is for now continuous with at least continuous first gradients on \(R \times \mathcal{T}\). The plane \(\Pi\) is spanned by the unit vectors \(e_1\) and \(e_2\), and greek subscripts have the reduced range \(\{1, 2\}\). The deformation gradient tensor \(F\) associated with the anti-plane
shear deformation (2.41) is

\[ F = I + u_\alpha e_3 \otimes e_\alpha = I + e_3 \otimes k, \]  

(2.42)

with the shear vector \( k = k_\alpha e_\alpha \). The components of the two dimensional vector \( k \) are the shear strains. They are constants in simple shear. The determinant of \( F \) is equal to 1 and therefore the anti-plane shear deformation given by (2.41) is locally volume preserving. The right Cauchy-Green tensor takes on the form

\[ C = C(k_1, k_2) = I + k \otimes e_3 + e_3 \otimes k + k \otimes k. \]  

(2.43)

Deformations of this kind are commonly studied to unveil qualitative features in different areas of the mechanics of materials, like the effect of nonlinearities on crack singularities. The popularity of anti-plane shear stems from its simplicity of formulation. If the energy potential is chosen accordingly, it is sufficient to solve a single partial differential equation on \( \Pi \).

It is not necessary that a general material will sustain nontrivial states of anti plane shear in the absence of body forces. This can be illustrated by considering a homogeneous compressible material undergoing an anti-plane shear deformation. Following Tsai & Rosakis [83] the constitutive relation (2.33) can now be expressed by

\[ \sigma_{\alpha j} = 2 \frac{\partial W(C)}{\partial C_{\alpha j}}, \quad \sigma_{33} = 2 \left( k_\alpha \frac{\partial W(C)}{\partial C_{\alpha 3}} + \frac{\partial W(C)}{\partial C_{33}} \right), \]  

(2.44)

\[ \sigma_{3\alpha} = 2F_{ik} \frac{\partial W_0(k_1, k_2)}{\partial k_\alpha}, \]  

(2.45)

where the elastic anti-plane shear potential \( W_0 \) is defined by

\[ W_0(k_1, k_2) = W(C(k_1, k_2)). \]  

(2.46)

The stress components \( \sigma_{3\alpha} \) are the shear stresses and correspond to the shear strains \( k_\alpha \). We recall that the deformation \( u = ue_3 \) only depends on the \( x_1 \) – and \( x_2 \) coordinates. Therefore the equation of equilibrium Div \( \sigma = 0 \) can now be specialized to two in-plane equations

\[ \left( \frac{\partial W(C)}{\partial C_{\alpha \beta}} \right)_{,\beta} = 0 \quad \forall \mathbf{x} \in \Pi \setminus \Sigma, \ t \in \mathcal{T}, \]  

(2.47)
and the \textit{out-of-plane equation}

\[
\frac{\partial^2 W_0(k)}{\partial k_\alpha \partial k_\beta} u_{\alpha\beta} = 0 \quad \forall \mathbf{x} \in \Pi \setminus \Sigma, \ t \in \mathcal{T}.
\] (2.48)

For an arbitrary stored energy \(W\), equations (2.47) and (2.48) constitute an overdetermined system, and one should expect only very special solutions of \(u\) to be compatible with all three partial differential equations. On the other hand one can view the in-plane equations (2.47) as conditions on the strain energy which allow the material to admit non-trivial states of anti-plane shear. Then the solution to a suitably posed boundary value problem governed by (2.48) is unique provided the elastic potential satisfies the condition of strong ellipticity and the material is such that (2.47) holds automatically. KNOWLES rigorously derives those necessary and sufficient condition on the strain energy density for homogeneous, isotropic, incompressible materials in [52] and for compressible materials in [53]. A special class of compressible stored energy functions conforming to those conditions have been given by \textsc{Jiang \& Knowles} [48]. The topic has also been revisited by authors like \textsc{Abeyaratne, Hill} and \textsc{Sternberg}. We postpone a more detailed discussion of this issue until Chapter 3. From now on we will assume that all materials of interest are solely governed by (2.48), and automatically satisfy (2.47) for any anti-plane shear deformation.

Next we turn back to fields that allow the deformation gradient \(F\) and consequently the shear vector \(k\) to be discontinuous on \(\Sigma(t)\), with the interface \(\Sigma(t)\) now denoting a collection of curves on \(\Pi\). This curves propagate in the reference configuration with velocity \(\mathbf{V} = \mathbf{V}(x_1, x_2, t) = V_n n_\Sigma\) such that \(\mathbf{V} \cdot e_3 = 0\). The governing equation of equilibrium specializes for a quasi-static and isothermal process undergoing an anti-plane shear deformation to

\[
\frac{\partial^2 W_0(k)}{\partial k_\alpha \partial k_\beta} u_{\alpha\beta} = 0 \quad \forall \mathbf{x} \in \Pi \setminus \Sigma,
\] (2.49)

and the corresponding mechanical jump conditions (2.28) reduce to

\[
\begin{align*}
[[\sigma_{3\alpha}]] n_\alpha &= 0, \\
[[u_{\alpha}]] l_\alpha &= 0,
\end{align*}
\quad \forall \mathbf{x} \in \Sigma.
\] (2.50)
with \( n_\alpha \) being the components of the normal vector of the curve \( \Sigma(t) \). The driving traction of (2.36) acting on \( \Sigma(t) \) during an anti-plane shear motion takes on the form

\[
f(\mathbf{x}, t) = [[W_0]] - \frac{1}{2} \delta_{3\alpha} [[k_\alpha]] \quad \forall \mathbf{x} \in \Sigma, \ t \in \mathcal{T},
\]

(2.51)

with inequality (2.35) now restricting the motion of \( \Sigma(t) \) in the plane \( \Pi \).

As was already noted in previous sections materials that allow such displacement fields are not anymore strongly elliptic, and thus solutions of the governing equation (2.49) are not unique. We speak in the case of anti-plane shear of strong ellipticity if the matrix \( \frac{\partial^2 W_0(\mathbf{k})}{\partial k_\alpha \partial k_\beta} \) is positive definite. This loss of ellipticity requires the specification of additional constitutive assumptions: the kinetic relation for the propagation of existing phases and the nucleation criterion for the initiation of a phase transformation. Nevertheless, it is possible to circumvent the specification of such relations by other means. We will in the next chapter perform a systematic regularization that allows us to disregard the jump condition and the explicit specification of a kinetic law and nucleation criterion by introducing an augmented constitutive theory that makes the displacement field sufficiently smooth.
Chapter 3

Couple stress theory

Introduction

In the previous chapter the basics of the sharp interface theory was reviewed. Another option to mathematically model solid to solid phase transformations is to regularize those fields. Then the displacement fields will be sufficiently smooth to replace the sharp interface by a thin transition layer with steep deformation gradients. It is said that the interface is given structure. One gains the mathematical simplification of solving a single boundary value problem governed throughout the whole body by partial differential equations and appropriate boundary conditions on the boundary. Once the merits of both approaches are clear, we will reflect on the computational advantages and disadvantages of both theories in Chapter 5.

The core idea to regularize propagating phase boundaries dates back to VAN DER WAAL and KORTWEG and originated from problems where capillarity was significant and could not be modeled by the standard equations of fluid mechanics. Nevertheless, in most cases regularization was of a purely mathematical nature and often inconsistent with thermodynamical considerations, as was shown for example by DUNN & SERRIN [26]. In this chapter a so called couple stress theory or first-order gradient theory is presented which has the capability to regularize sharp interfaces and is thermodynamically consistent. This theory traces its origins to a wide variety of general theories of rods, shells, and theoretical studies on the elastic properties of crystals by VOIGT [85]. In 1909, E. & F. COSSERAT [21] developed a
three-dimensional theory that unified those concepts. Subsequent to the Cosserat's pioneering work several authors generalized the theory. The most significant contributions to the basic development of the theory were made by Toupin [78, 79], Mindlin & Tierstein [63], Mindlin [64], and Eringen [29]. Clearly, such theories have a much wider scope and has found recent application in different areas of the mechanics of materials (Fleck [31], Fleck & Hutchinson [30], Aifantis [11], Vardoulakis [86], Mühlhaus & Aifantis [66] and Dai & Parks [24]).

The version of couple stress theory illustrated in this chapter is one of the simplest formulations found in the literature. Its main features are the introduction of a couple vector $\mathbf{m}$ and its kinematic conjugate $\omega$. These couples still fit our common notion of a moment vector, whereas for more general theories this is not anymore the case, giving rise to stress tensors of order greater than two. Thus the stored energy function depends on two strain measures that are derivable from a single displacement field, where the additional measure of deformation is a function of the gradient of the deformation gradient.

In the theory discussed in Section 3.4 this augmentation of the stored energy function introduces at least one new material parameter when compared to standard continuum models. This material length scale $l_m$ is formed by the square root of the ratio of the bending-twisting modulus to the commonly used shear modulus, and contains the essential difference to the classical theory of elasticity. If $l_m$ is large, more significant changes are observed in the bulk fields of the body. In more physical terms couple stress effects could be important if the loading's wave length or area of contact become comparable to the material length scale $l_m$, or if the material has a microstructure with a comparable length scale, such that the axioms of locality fail. This lends the couple stress theory to be applied in the field of micromechanics. Some specific examples are the strain gradient plasticity of Fleck & Hutchinson, where size effects and its influence on the distribution of geometrically necessitated dislocations are absorbed by the material length scale $l_m$. Aifantis and co-workers use the constitutive models dependency on $l_m$ to model the size effect encountered in laminates, and to stabilize
the regime found in physical phenomenas like the localization of plastic flow, the formation and propagation of deformation bands, and the buckling of fibers in composites. Generally, couple stress theories try to adequately describe the effect of microstructure on a macroscale level. The goal of this thesis is to scale the thickness of the transition layer with \( l_m \). Since we wish to model very sharp interfaces and alter the fields away from those discontinuities as little as possible the material length scale \( l_m \) is made as small as possible.

The following is structured such that in Section 3.1 we briefly review the necessary kinematics. In the next section the global balance laws are established and localized, and in Section 3.3 we introduce the stored energy potential and derive the constitutive relations. A significant portion of this chapter is dedicated to Section 3.4, in which we linearize the kinematics and derive the equations of the associated theory. We specify a strain energy per unit undeformed volume, which contains additively the nonlinear elastic contribution and the isotropic energy contribution of higher order. In Section 3.5 all previous results are specialized to an anti-plane shear deformation. In Section 3.6 a variational statement of the governing equation of anti-plane shear is given and the appropriate boundary conditions are derived. In Section 3.7 a summary of the anti-plane shear deformation is discussed, in which the results of Section 3.5 and 3.6 are modified to include dissipative effects due to the motion of an interface. This final version of the constitutive theory will be referred to as the augmented theory.

### 3.1 Kinematics

Let us consider a continuous body \( B \) that occupies a three dimensional space on a time interval \( \mathcal{T} = (t_0, t_1) \). As in Chapter 2, this body undergoes a motion \( y(\mathbf{x}, t) \), which is characterized by a one-parameter family of invertible and continuous mappings \( y(\mathbf{x}, t) : \mathbb{R} \rightarrow R_t \), so that the position vector \( y \) in \( R_t \) is given by

\[
y = y(\mathbf{x}, t) = \mathbf{x} + \mathbf{u}(\mathbf{x}, t) \quad \forall \mathbf{x} \in \mathbb{R}, \ t \in \mathcal{T}.
\]  

(3.1)
The motion \( y(x, t) \) is now assumed to be smooth and each material point \( x \in R \) is mapped from its reference configuration \( R \) to its deformed configuration \( R_t \) by the displacement vector \( u \). The deformation gradient tensor \( F = \text{Grad } y(x, t) \) represents the map of \( dx \in R \) to \( dy \in R_t \) at a given time \( t \in T \) and is defined by

\[
F_{ij} = \frac{\partial y_i}{\partial x_j} = \delta_{ij} + \frac{\partial u_i}{\partial x_j} \quad \forall x \in R, \ t \in T. \tag{3.2}
\]

Since the map \( y(x, t) \) is one-to-one the Jacobian determinant, \( J = \det F > 0 \), is positive. The map \( y(x, t) \) is unique and invertible, since no two distinct particles \( x \) occupy the same position \( y \) at time \( t \in T \), and no two distinct positions \( y \) can be of the same particle \( x \in R \). The inverse function is defined by

\[
x = \hat{x}(y, t), \quad \forall y \in R_t, \ t \in T. \tag{3.3}
\]

By using (3.1) we focus our attention on the motion of a particle, whereas equation (3.3) allows us to study the motion \( y \) at a given point in space. The former is traditionally referred to as the Lagrangian description and the later as the Eulerian description. We emphasize this point since in solids mechanics, generally, the Lagrangian description is preferred, whereas in the theory of couple stress it is advantageous to work in the deformed configuration \( R_t \) in terms of the spatial variables \((y, t)\). Consider the velocity vector

\[
v = v(x, t) = \frac{\partial u(x, t)}{\partial t}, \quad \forall x \in R, \ t \in T, \tag{3.4}
\]

by replacing \( x \) with the inverse map (3.3) the spatial velocity field \( v(y, t) \) depends now on the position \( y \) at time \( t \). The additional kinematic variable \( \omega(y, t) \) will be useful to us and it is a rigid rotation about an axis through the spatial position \( y \) with angular velocity

\[
\omega(y, t) = \frac{1}{2} \text{curl } v(y, t), \quad \omega_i = \frac{1}{2} \epsilon_{ijk} \frac{\partial v_k}{\partial y_j}, \quad \forall y \in R_t, \ t \in T, \tag{3.5}
\]

where \( \epsilon_{ijk} \) is the alternator. This concludes the discussion of the necessary kinematics, to formulate the balance laws of this simplest theory of couple stresses.
3.2 Balance laws

In order to study the laws of conservation of linear momentum, angular momentum, and energy we consider an arbitrary subregion \( D_t \subset R_t \) with simply closed boundary \( \partial D_t \). Due to the more general kinematic description of body \( D_t \) we can now characterize the physical interactions on the boundary by a traction vector \( t(y, n, t) \) and a couple vector \( m(y, n, t) \), and in the interior by the body force vector \( b(y, t) \) and the body couple vector \( c(y, t) \). These forces and couples generate a resultant force \( f \), a resultant moment \( m_o \) about the origin, and expend power \( p \) during an isothermal process:

\[
\mathbf{f} = \int_{\partial D_t} \mathbf{t} \, dA + \int_{D_t} \mathbf{b} \, dV, \tag{3.6}
\]

\[
\mathbf{m}_o = \int_{\partial D_t} \mathbf{y} \times \mathbf{t} \, dA + \int_{D_t} \mathbf{y} \times \mathbf{b} \, dV + \int_{\partial D_t} \mathbf{m} \, dA + \int_{D_t} \mathbf{c} \, dV, \tag{3.7}
\]

\[
p = \int_{\partial D_t} \mathbf{t} \cdot \mathbf{v} \, dA + \int_{D_t} \mathbf{b} \cdot \mathbf{v} \, dV + \int_{\partial D_t} \mathbf{m} \cdot \mathbf{\omega} \, dA + \int_{D_t} \mathbf{c} \cdot \mathbf{\omega} \, dV. \tag{3.8}
\]

For a quasi-static deformation the resultant force \( \mathbf{f} \) and the resultant moment \( \mathbf{m}_o \) are at each instant of time set equal to zero:

\[
\mathbf{f} = 0, \quad \mathbf{m}_o = 0. \tag{3.9}
\]

Thus effects associated with the inertia of a material particle \( \mathbf{x} \) are considered negligible, and only slowly varying forces and couples with respect to time are admissible. Suppose now without lose of generality that the region \( D_t \) is a tetrahedron of side length \( \delta \). Then the balance of forces (3.6) and moments (3.7) will yield in the limit \( \delta \to 0 \) the relations

\[
t_i(y, n, t) = T_{ij}(y, t)n_j, \quad m_i(y, n, t) = M_{ij}(y, t)n_j \text{ on } \partial D_t, \tag{3.10}
\]

implying the existence of the spatial stress tensor field \( T \) and the spatial couple stress tensor field \( M \). These two fields satisfy the local field equations

\[
\frac{\partial T_{ij}}{\partial y_j} + b_i = 0 \text{ on } D_t, \tag{3.11}
\]
\[
\frac{\partial M_{ij}}{\partial y_j} + \epsilon_{ijk} T_{kj} + c_i = 0 \quad \text{on } D_t, \tag{3.12}
\]

which follow from (3.6), (3.7), (3.9), (3.10). Clearly, the stress tensor field \( T \) is not necessarily symmetric except for spatially constant \( M \) and no body couple \( c \). By decomposing \( T \) into its symmetric part \( T^s \) and antisymmetric part \( T^a \):

\[
T_{ij} = T^s_{ij} + T^a_{ij} \tag{3.13}
\]

\[
\begin{align*}
T^s_{ij} & = \frac{1}{2} (T_{ij} + T_{ji}), \\
T^a_{ij} & = \frac{1}{2} (T_{ij} - T_{ji}).
\end{align*} \tag{3.14}
\]

The field equation (3.12) stemming from the balance of moments can be written as

\[
T^a_{ij} = \frac{1}{2} \epsilon_{ijk} \left( \frac{\partial M_{kl}}{\partial y_l} + c_k \right), \tag{3.15}
\]

expressing the nonsymmetric nature of \( T \) explicitly. In the absence of body couples \( c \) and surface couples \( m \) the usual requirement that \( T \) must be symmetric is recovered. Further, it is convenient to decompose the couple stress tensor \( M \) into its spherical part and deviatoric part \( M^d \) as

\[
M_{ij} = M^d_{ij} + \frac{1}{3} M_{kk} \delta_{ij}, \tag{3.16}
\]

where \( \delta_{ij} \) is the Kronecker delta. We note that substitution of (3.16) into (3.15) will not lead to immediate simplifications

\[
T^a_{ij} = \frac{1}{2} \epsilon_{ijk} \left( \frac{\partial M^d_{kl}}{\partial y_l} + \frac{1}{3} \frac{\partial M_{qq}}{\partial y_k} + c_k \right), \tag{3.17}
\]

but can be used to eliminate the antisymmetric stress tensor \( T^a \) from the differential equation (3.11), to form the combined differential equation

\[
\frac{\partial}{\partial y_j} T^s_{ij} + \frac{1}{2} \epsilon_{pij} \frac{\partial^2 M^d_{pq}}{\partial y_j \partial y_q} + \frac{1}{2} \epsilon_{pij} \frac{\partial c_p}{\partial y_j} + b_i = 0. \tag{3.18}
\]

This single governing equation (3.18) involves the deviatoric couple stress tensor \( M^d \) and the symmetric stress tensor \( T^s \), suggesting that it might be sufficient to find a constitutive theory for those two quantities.
This becomes more obvious when considering the rate of working. Assume the material is elastic and the rate of working $p$ is equal to the rate of increase of stored energy, then

$$p = \frac{d}{dt} \int_D \rho \psi \ dV,$$

(3.19)

where $\psi$ is the stored energy density per unit mass and $\rho(y, t)$ the density of mass in the current configuration. The local form of (3.8) and (3.19) becomes

$$\rho \dot{\psi} = T_{ij}^s \frac{\partial v_i}{\partial y_j} + M_{ij}^d \frac{\partial \omega_i}{\partial y_j},$$

(3.20)

by making use of the decomposition (3.16) and writing $\dot{\psi}$ for the material time derivative of $\psi$. Thus work is only done by the symmetric stress tensor $T^s$ and the deviatoric couple stress tensor $M^d$. All necessary quantities to solve the governing equation (3.18) can be determined by the local balance of energy (3.20).

3.3 Constitutive relation

The final form of the constitutive relation for $M^d$ and $T^s$ strongly depend on the arguments chosen for the stored energy density $\psi$. In the absence of couple stress effects the lagrangian strain tensor $E$ is commonly used as a deformation measure. Since we would like to recover the well known constitutive theory it is a reasonable assumption to take $E$ as one of the arguments of $\psi$. The richer description of the kinematics and the general forces suggest an additional dependency on the third order tensor Grad $E$ or Grad $F$. It can be shown that this later assumption leads to additional compatibility equations on the potential $\psi$, which restrain the deformation of the body $D_t$ unnecessarily. TOUPIN [78] and MINDLIN & TIERSTEIN [63] propose that the energy $\psi$ depend on the lagrangian strain $E$ and the tensor $K = (\text{Curl} \ E)^T$ as:

$$\psi = \psi(E, K),$$

(3.21)

with the components of the objective second order tensors $E$ and $K$ given by

$$E_{ij} = \frac{1}{2} \ (F_{ik} F_{jk} - \delta_{ij}), \quad K_{ij} = \epsilon_{jqp} \frac{\partial E_{ip}}{\partial x_q},$$

(3.22)
and therefore guaranteeing an objective energy $\psi$. We also note that the tensor $E$ and $K$ have the property
\[ E = E^T, \quad \text{tr} \; K = 0. \] (3.23)
Consequently we may assume that $\psi(E, K)$ has been arranged to satisfy the relations
\[ \frac{\partial \psi}{\partial E} = \frac{\partial \psi}{\partial E^T}, \quad \frac{\partial \psi}{\partial (\text{tr} \; K)} = 0. \] (3.24)
We now are in the position to derive the constitutive relations by explicitly calculating the material time derivative $\dot{\psi}$ of the balance of energy and work given by (3.20) as
\[ T_{ij} D_{ij} + M_{ij}^d \frac{\partial \omega_i}{\partial y_j} = \rho \frac{\partial \psi}{\partial E_{ij}} \dot{E}_{ij} + \rho \frac{\partial \psi}{\partial K_{ij}} \dot{K}_{ij}, \] (3.25)
by noting that $T^s \cdot \text{grad} \; v = T^s \cdot D$. The symmetric stretching tensor $D(y, t)$ is defined in the usual manner by
\[ D(y, t) = \frac{1}{2} \left( L(y, t) + L^T(y, t) \right), \quad D_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial y_j} + \frac{\partial v_j}{\partial y_i} \right). \] (3.26)
Next we express $\dot{E}$ and $\dot{K}$ as functions of the tensors $D_{ij}$ and $\frac{\partial \omega_i}{\partial y_j}$, in order to relate the stress tensor $T^s$ and the deviatoric couple stress tensor $M_{ij}^d$ to $\frac{\partial \psi}{\partial E_{ij}}$ and $\frac{\partial \psi}{\partial K_{ij}}$. A direct calculation of the material time derivative of $E(x, t)$ and $K(x, t)$ shows that
\[ \dot{E}_{ij} = F_{ki} D_{kl} F_{lj}, \] (3.27)
\[ \dot{K}_{ij} = - \epsilon_{pqj} (H_{aq} F_{bp} + H_{bp} F_{aq}) D_{ab} - \epsilon_{pqj} F_{ai} F_{bp} \frac{\partial D_{ab}}{\partial x_q}, \] (3.28)
where $H = \text{Grad} \; F$ is the material gradient of the deformation gradient $F$ with components
\[ H_{ijk} = \frac{\partial F_{ij}}{\partial x_k}. \] (3.29)
The expression for $\dot{K}$ requires further manipulation, since no measure $\frac{\partial D_{ab}}{\partial x_q}$ exists in (3.25). Using the chain rule, $\frac{\partial D_{ab}}{\partial x_q} = \frac{\partial D_{aiq}}{\partial y_i} F_{lj}$, multiplying the second term of (3.28) by $F_{kj}$, and recalling the identity
\[ J \epsilon_{blk} = \epsilon_{pqj} F_{bp} F_{lq} F_{kj}, \] (3.30)
one can relate $\frac{\partial D_{ab}}{\partial x_q}$ to the kinematic variable $\frac{\partial \omega_k}{\partial y_j}$ by

$$-\epsilon_{pqj}F_{ai}F_{bp}\frac{\partial D_{ab}}{\partial x_q}F_{kj} = JF_{ai}\frac{\partial \omega_k}{\partial y_a},$$

(3.31)

where $J = \det \mathbf{F}$. Finally, by using equation (3.28) and (3.31) we derive the components of $\dot{K}$ to be

$$\dot{K}_{ij} = -\epsilon_{pqj}(H_{aiq}F_{bp} + H_{bpq}F_{ai})D_{ab} + JF_{bi}F_{ja}^{-1}\frac{\partial \omega_a}{\partial y_b}.$$  

(3.32)

The final step is to substitute (3.27) for $\dot{E}$ and (3.32) for $\dot{K}$ into the work energy equation (3.25), and order the terms with respect to the independent tensors $D_{ab}$ and $\frac{\partial \omega_a}{\partial y_b}$, to attain for all isothermal and quasi-static processes

$$[T_{ab}^s - \rho \frac{\partial \psi}{\partial E_{ij}}F_{ai}F_{bj} + \rho \frac{\partial \psi}{\partial K_{ij}} - \epsilon_{pqj}(H_{aiq}F_{bp} + H_{bpq}F_{ai})]D_{ab} +$$

$$[M_{ab}^d - \rho J \frac{\partial \psi}{\partial K_{ij}}F_{bi}F_{ja}^{-1}\frac{\partial \omega_a}{\partial y_b}] = 0.$$  

(3.33)

Since $D$ is symmetric and $\frac{\partial \omega_a}{\partial y_b}$ is traceless, it follows that the term multiplying $D$ can be at most antisymmetric and the term multiplying $\frac{\partial \omega_a}{\partial y_b}$ is equal to zero. Thus the constitutive relations for the symmetric stress tensor $T^s$ and the deviatoric couple stress tensor $M^d$ become:

$$T_{ij}^s = \frac{1}{2} \rho \frac{\partial \psi}{\partial E_{ab}}F_{ia}F_{jb}$$

$$- \frac{1}{2} \rho \frac{\partial \psi}{\partial K_{ab}}\epsilon_{pqb}(H_{iaq}F_{jp} + H_{jpa}F_{ia} + H_{jaq}F_{ip} + H_{ipa}F_{ja}),$$

$$M_{ij}^d = \rho J \frac{\partial \psi}{\partial K_{pq}}F_{jp}F_{qi}^{-1}. $$

(3.34)

(3.35)

It may be observed that the mean normal couple stress is a workless quantity and no restrictions are imposed on it by the work energy relations (3.20) or (3.33). Consequently, the antisymmetric stress tensor $T^a$ does only work through $M^d$. Nevertheless, the governing equation (3.18) only requires the constitutive relation for $T^s$ and $M^d$, to ultimately solve for the displacement vector $u$. This peculiarity of the theory does not impede the solution of properly posed boundary value problems, but never allows the explicit evaluation of the stress $T^a$ without additional assumptions on the trace of $M$. 


3.4 Linearization

Let us remind ourselves that the goal of this work is to solve some higher dimensional problems, where the material is able to sustain solid to solid interfaces of strain discontinuities. We are not interested in the direct implication of couple stress theory, but wish to use it as a vehicle to consistently regularize those strain discontinuities. We also prefer not to introduce further complexity by analyzing the problem under the regime of large deformations. Consequently, we will specialize the foregoing theory to circumstances in which the kinematics can be linearized and the nonlinearity of the constitutive theory, which facilitate the occurrence of phase boundaries, is retained. This is for example a common approach in small-strain plasticity.

The standard procedure to linearize the kinematics in continuum mechanics is to assume that the components of the displacement gradient to be much smaller than unity

$$|\text{Grad } u| \ll 1.$$  \hspace{1cm} (3.36)

Then the two measures of deformation $E$ and $K$ have the linearized equivalents $\gamma$ and $\kappa$, respectively:

$$\gamma = \frac{1}{2} (\text{Grad } u + \text{Grad } u^T), \quad \gamma_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right),$$ \hspace{1cm} (3.37)

$$\kappa = \frac{1}{2} (\text{Curl Grad } u^T)^T, \quad \kappa_{ij} = \frac{1}{2} \varepsilon_{jqp} \frac{\partial^2 u_p}{\partial x_q \partial x_i},$$ \hspace{1cm} (3.38)

where $\gamma(x, t)$ is the small strain tensor and $\kappa(x, t)$ the curvature-twist tensor. Both tensors preserve the properties of $E$ and $K$ as

$$\gamma = \gamma^T, \quad \text{tr } \kappa = 0.$$ \hspace{1cm} (3.39)

The interpretation of $\kappa$ becomes clear when one considers the antisymmetric tensor $W(x, t)$ of small rotations and its dual vector $w(x, t)$:

$$W = \frac{1}{2} (\text{Grad } u - \text{Grad } u^T), \quad W_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right),$$ \hspace{1cm} (3.40)
\[
\mathbf{w} = \frac{1}{2} \text{Curl } \mathbf{u}, \quad w_i = \frac{1}{2} \varepsilon_{ijk} \frac{\partial u_k}{\partial x_j}. \tag{3.41}
\]

The vector \( \mathbf{w} \) describes the local rotation at each material point and defines \( \kappa \) as the material gradient of the rotation \( \mathbf{w} \),

\[
\kappa = \text{Grad } \mathbf{w}^T, \quad \kappa_{ij} = \frac{\partial w_j}{\partial x_i}, \tag{3.42}
\]

measuring the rate of twist and curvature of an arc of material. By substituting (3.41) into (3.42) the original definition (3.38) is recovered. It should be noted that \( \gamma \) is dimensionless and \( \kappa \) has the dimension of reciprocal length. Let us recall that linearization also implies that a nondimensional stored energy \( \hat{\psi} \) satisfy

\[
|\hat{\psi}(\gamma, \kappa) - \hat{\psi}(0, 0)| \ll 1. \tag{3.43}
\]

This condition is in the linearization of the couple stress theory not automatically satisfied by solely imposing (3.36). It requires the additional condition

\[
|l_m \text{ Grad Grad } \mathbf{u}| \ll 1, \tag{3.44}
\]

where \( l_m \) is the material length scale associated with the contribution of \( \kappa \) to the stored energy \( \psi \). This can be illustrated by the following example:

\[
\psi = \frac{\mu}{2} \mathbf{E} \cdot \mathbf{E} + \frac{\lambda}{2} \mathbf{K} \cdot \mathbf{K}, \tag{3.45}
\]

where the material lengthscale \( l_m \) is defined by

\[
l_m = \sqrt{\frac{\lambda}{\mu}}. \tag{3.46}
\]

By dividing the stored energy (3.45) with \( \mu \) we get

\[
\frac{2\psi}{\mu} = \mathbf{E} \cdot \mathbf{E} + l_m^2 \mathbf{K} \cdot \mathbf{K}. \tag{3.47}
\]

It is seen that the first term is small if and only if (3.36) holds and the second term is by comparison small, if and only if (3.44) holds additionally. When both contribution are
sufficiently small we replace $E$ and $K$ of the stored energy (3.45) with the linearized measures $\gamma$ and $\kappa$.

In its linearized form the law of conservation of mass $\rho = \rho_0 \det F$ is such that the density $\rho$ is equal to the mass density $\rho_0$ in the reference configuration, and the stored energy per unit volume $\phi(\gamma, \kappa)$ is introduced by

$$\phi = \rho_0 \psi.$$  \hspace{1cm} (3.48)

The constitutive relations (3.34-3.35) of the theory of large deformations now simplify to the form

$$T_{ij}^s = \frac{\partial \phi}{\partial \gamma_{ij}},$$  \hspace{1cm} (3.49)

$$M_{ij}^d = \frac{\partial \phi}{\partial \kappa_{ji}}.$$  \hspace{1cm} (3.50)

In our further discussion the body force $\mathbf{b}$ and the body couple $\mathbf{c}$ are not of interest and are taken as

$$\mathbf{b} = 0, \quad \mathbf{c} = 0,$$  \hspace{1cm} (3.51)

simplifying the governing equation (3.18) to

$$T_{ij,j}^s + \frac{1}{2} \epsilon_{piz} M_{pq,ij}^d = 0,$$  \hspace{1cm} (3.52)

where subscripts preceded by a comma denote partial differentiation with respect to the corresponding $x$-coordinates. More generally, the linearization of the kinematics allow us to consider all previously derived field equations (3.11, 3.12, 3.15, 3.18), containing a partial differentiation with respect to $y$-coordinates to be field equations valid in the reference configuration, by simply taking $\frac{\partial}{\partial y_i} = \frac{\partial}{\partial x_i}$.

To complete the formulation of the linearized theory a specific material has to be considered. In this work we take $\phi$ to have the following characteristics:
i) the energy $\phi(\gamma, \kappa)$ is additively decomposed into a function which depends only on the strain $\gamma$ and a second function which depends on the strain gradient $\kappa$, thus

$$\phi(\gamma, \kappa) = \phi_e(\gamma) + \phi_h(\kappa);$$  \hspace{1cm} (3.53)

ii) the contribution $\phi_e$ only depends on two of the three possible strain invariants of $\gamma$:

$$\phi_e(\gamma) = \phi_e(I, \Delta),$$  \hspace{1cm} (3.54)

with the two invariants $I$ and $\Delta$ given as

$$I = 2\gamma_{ij}\gamma_{ij}, \quad \Delta = \gamma_{ii};$$  \hspace{1cm} (3.55)

iii) the higher order strain gradient term is assumed to be quadratic in $\kappa$:

$$\phi_h(\kappa) = \frac{1}{2} N_{ijkl} \kappa_{ij} \kappa_{kl},$$  \hspace{1cm} (3.56)

and the 4th order tensor $N$ with material coefficients $A, B, C$ is taken to be isotropic

$$N_{ijkl} = A \delta_{ik} \delta_{jl} + B \delta_{il} \delta_{jk} + C \delta_{ij} \delta_{kl}.$$  \hspace{1cm} (3.57)

This leads to

$$\phi_h(\kappa) = \frac{A}{2} \kappa_{ij} \kappa_{ij} + \frac{B}{2} \kappa_{ij} \kappa_{ji},$$  \hspace{1cm} (3.58)

when recalling that $\kappa$ has the property $\kappa_{ii} = 0$.

Now $\phi$ hast the form

$$\phi = \phi_e(I, \Delta) + \frac{A}{2} \kappa_{ij} \kappa_{ij} + \frac{B}{2} \kappa_{ij} \kappa_{ji}.$$  \hspace{1cm} (3.59)

Finally $\phi$ is assumed to be equal to zero if no external forces are applied on the body, thus we must have by (3.49-3.50) that

$$\phi_e = \frac{\partial \phi_e}{\partial I} = \frac{\partial \phi_e}{\partial \Delta} = 0 \quad \text{for} \quad I = \Delta = 0,$$  \hspace{1cm} (3.60)
and that $\phi_h = 0$ for $\kappa = 0$, which is trivially satisfied for the quadratic energy potential $\phi_h$. Substituting the energy given by (3.59) into our linearized constitutive relations (3.49-3.50) one obtains the symmetric stress $T^s$ and the deviatoric couple stress $M^d$ as

$$T^s_{ij} = 4 \frac{\partial \phi_e}{\partial I} \gamma_{ij} + \frac{\partial \phi_e}{\partial \Delta} \delta_{ij}, \quad \text{(3.61)}$$

$$M^d_{ij} = A \kappa_{ij} + B \kappa_{ij}. \quad \text{(3.62)}$$

After utilizing the constitutive relations (3.61-3.62) and the equilibrium equation (3.52), the governing equilibrium equation with respect to the strain $\gamma$ and the curvature-twist tensor $\kappa$ is derived as

$$4 \left( \frac{\partial \phi_e}{\partial I} \gamma_{ij} \right)_j + \frac{\partial \phi_e}{\partial \Delta} \gamma_{bb,i} + \frac{1}{2} \epsilon_{pij} (A \kappa_{qp,qj} + B \kappa_{pq,qj}) = 0, \quad \text{(3.63)}$$

If one assumes the tr $M$ to be at most constant the antisymmetric stress $T^a$ can be determined as

$$T^a_{ij} = \frac{1}{2} \epsilon_{pij} (A \kappa_{kp,k} + B \kappa_{pk,k}). \quad \text{(3.64)}$$

Alternatively, equation (3.63) can now be derived by the equation of conservation of linear momentum $T^s_{ij,j} + T^a_{ij,j} = 0$, since the complete statement of angular momentum has been implied by the compatible specification of $M$ and $T^a$ in (3.64).

### 3.5 Anti-plane shear

We once again consider the anti-plane shear motion $y$, along the $e_3$ direction in a fixed orthonormal basis $\{e_1, e_2, e_3\}$, that is associated with the cylindrical reference configuration $R$, with cross section $\Pi$ in the $e_1$-$e_2$ plane. The anti-plane shear motion is characterized by

$$y = y(x, t) = x + u(x_1, x_2, t)e_3 \quad \forall x \in R. \quad \text{(3.65)}$$

In anti-plane shear the strain $\gamma$ and the curvature-twist tensor $\kappa$ simplify to

$$\gamma = \frac{1}{2} \begin{bmatrix} 0 & 0 & u_{11} \\ 0 & 0 & u_{22} \\ u_{11} & u_{22} & 0 \end{bmatrix}, \quad \kappa = \frac{1}{2} \begin{bmatrix} u_{12} & -u_{11} & 0 \\ u_{22} & -u_{12} & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \text{(3.66)}$$
with the invariants of $\gamma$ given by

$$I = |k|^2 = k_\alpha k_\alpha, \quad \Delta = 0. \quad (3.67)$$

Thus the components of the symmetric stress tensor $T^s$ of (3.61) take on the form

$$T^{s}_{3\alpha} = \frac{\partial \phi_e}{\partial I} u_{,\alpha}, \quad T^{s}_{\alpha\beta} = \frac{\partial \phi_e}{\partial \Delta} \delta_{\alpha\beta}, \quad T^{s}_{33} = \frac{\partial \phi_e}{\partial \Delta}, \quad (3.68)$$

where the partial derivatives of $\phi_e$ are evaluated at $I = |k|^2$ and $\Delta = 0$. The components of the deviatoric couple stress tensor $M^d$ of (3.62) are given by

$$M^{d}_{3i} = 0, \quad M^{d}_{11} = -M^{d}_{22} = \frac{A+B}{2} u_{,12}, \quad M^{d}_{12} = \frac{A}{2} u_{,22} - \frac{B}{2} u_{,11}, \quad M^{d}_{21} = -\frac{A}{2} u_{,11} + \frac{B}{2} u_{,22}. \quad (3.69)$$

Both stress tensors $T^s$ and $M^d$ are now required to satisfy the governing equation (3.52) of equilibrium, which simplifies in light of (3.68-3.69) and (3.65) to

$$T^{s}_{i\gamma,\gamma} + \frac{1}{2} \varepsilon_{\alpha i\gamma} M^{d}_{\alpha\beta,\beta\gamma} = 0 \quad \text{on } \Pi. \quad (3.70)$$

By substituting the constitutive relations (3.68-3.69) of $T^s$ and $M^d$ into the first two equilibrium equations of (3.70), $(i = 1, 2)$ one finds that

$$\frac{\partial}{\partial x_\alpha} \left( \frac{\partial \phi_e}{\partial \Delta} \right) = 0 \quad \text{on } \Pi. \quad (3.71)$$

Upon integrating each term with respect to its corresponding $x$-variable one concludes that $\frac{\partial \phi_e}{\partial \Delta}$ is at most constant for all admissible displacement fields on $\Pi$. Moreover, when recalling the material's restriction (3.60), an anti-plane shear motion is only sustainable if the elastic part $\phi_e$ of the stored energy function is such that

$$\frac{\partial \phi_e}{\partial \Delta} = 0 \quad \text{for } I \geq 0, \Delta = 0. \quad (3.72)$$

This reflects the well-known fact that an arbitrary nonlinearly elastic material can not sustain an anti-plane shear deformation in the absence of body forces. Only a particular class of such materials can do so, and in the present setting a necessary and sufficient condition is that
(3.72) holds. Under this circumstances, the symmetric stress tensor $T^s$ of (3.68) simplifies to

$$T_{33}^s = T_{33}^s = \mathcal{M}(k) u_{\alpha},$$

(3.73)

and the remaining equation of equilibrium ($i = 3$) yields

$$(\mathcal{M}(k) u_{\alpha})_\alpha - \frac{A}{4} \nabla^2 \nabla^2 u = 0 \quad \text{on } \Pi,$$

(3.74)

where we have set

$$\mathcal{M}(k) = 2 \left. \frac{\partial \phi_e}{\partial I} \right|_{I = k^2, \Delta = 0} \quad \text{for } -\infty < k < \infty.$$  

(3.75)

The secant modulus of shear $\mathcal{M}(k)$ can be determined by the elastic response of a material in simple shear

$$u = k x_2,$$

(3.76)

for which the elastic anti-plane shear response is characterized by the constitutive function

$$W(k) = \phi(k^2, 0).$$

(3.77)

The shear stress $T_{32}^s$ of (3.73) associated with the simple shear deformation (3.76) is then

$$T_{32}^s = 2 \frac{\partial \phi_e}{\partial I} k = W'(k), \quad I = k^2,$$

(3.78)

and equal to the stress-strain relation

$$\hat{\tau}(k) = W'(k).$$

(3.79)

Thus the secant modulus $\mathcal{M}$ can be written as

$$\mathcal{M}(k) = \frac{\hat{\tau}(k)}{k} = \frac{W'(k)}{k},$$

(3.80)

and the infinitesimal shear modulus $\mu$ is

$$\mu = \mathcal{M}(0) = \hat{\tau}'(0).$$

(3.81)
3.6. VARIATIONAL FORMULATION OF ANTI-PLANE SHEAR

In this setting one of the material length scales introduced by the overall constitutive assumptions with material parameters $\mu$, $A$ and $B$ becomes

$$l_m = \sqrt{\frac{A}{4\mu}}. \quad (3.82)$$

The governing equation (3.74) has a contribution due to the elastic response in anti-plane shear, and a second biharmonic term reminiscent to Kirchhoff’s plate theory. Thus the material parameters $A$ and $B$ are equivalent to the well-known plate stiffness $D$ and twice the Poisson’s ratio times the plate stiffness, respectively. The term of the energy associated with $B$ in (3.59) is due to anti-elastic curvature and in most cases small in comparison to the term $\frac{A}{2} \kappa_{ij} \kappa_{ij}$. Hence, to further reduce the number of needed material parameters we restrict ourselves in the analyzes to materials with $B = 0$, which is in the theory of thin plates equivalent to an isotropic material with no Poisson effect. As previously discussed the governing equation (3.74) could also have been derived by the equation of equilibrium $T_{ij,j,j}^s + T_{ij,j,j}^a = 0$, and by assuming that the mean couple stress tensor of $M$ is at most constant. Nevertheless, it is preferable to approach the problem as outlined in our discussion, because no additional assumptions have to be made. We will in the next section show that the trace of $M$ can be eliminated from the boundary conditions, making the constitutive relations (3.69) and (3.73) the only ones necessary to formulate boundary value problems in anti-plane shear.

3.6 Variational formulation of anti-plane shear

In this section we concern ourselves with two questions pertaining to anti-plane shear deformations in the framework of the couple stress theory. First, we would like to examine the type of boundary conditions which have to be prescriberd with the governing equation (3.74). Second, we seek a variational formulation to establish the weak form of (3.74) so as to be able to numerically solve later on some specific boundary value problems.

We consider once again the anti-plane shear deformation of a cylindrical body $R$ with cross section $\Pi$. The smooth and simple boundary $\partial \Pi$ is comprised of four segments $\partial \Pi_i$,
with \( i = \{1, 2, 3, 4\} \), such that

\[
\partial \Pi_1 \cup \partial \Pi_2 = \partial \Pi_3 \cup \partial \Pi_4 = \partial \Pi. \tag{3.83}
\]

Thus each set is comprised of two segments that are allowed to overlap each other and cover the whole boundary of \( \Pi \). A kinematically admissible displacement field \( u = u e_3 \) is a three-times continuously differentiable function \( u : \Pi \rightarrow \mathbb{R} \), with the non-zero components of the strain tensor \( \gamma \) and the curvature-twist tensor \( \kappa \) given by

\[
\gamma_{3a} = \gamma_{a3} = \frac{1}{2} u_{,a}, \quad \kappa_{ab} = -\frac{1}{2} \epsilon_{3a} u_{,ab}. \tag{3.84}
\]

Consider the functional \( \Psi \) associated with such an admissible deformation \( u \) to be of the form

\[
\Psi = \int_{\Pi} \phi \, dA - \int_{\partial \Pi_2} \hat{t}_u \, ds - \int_{\partial \Pi_4} \hat{m} \frac{\partial u}{\partial n} \, ds, \tag{3.85}
\]

which depends on the energy potential \( \phi(\gamma, \kappa) \) given by (3.59), and the traction \( \hat{t} \) and the surface couple \( \hat{m} \). On the boundary segments \( \partial \Pi_1 \) and \( \partial \Pi_3 \) the kinematic boundary conditions or the so called essential boundary conditions are prescribed:

\[
\begin{align*}
  u & \quad \text{given on } \partial \Pi_1, \\
  \frac{\partial u}{\partial n} & \quad \text{given on } \Pi_3.
\end{align*} \tag{3.86}
\]

A necessary and sufficient condition for an equilibrated displacement field is that the functional \( \Psi \) is extremized. Following standard procedures of the calculus of variation this is ensured if the first variation \( \delta \Psi \) of (3.85) vanishes, giving rise to

\[
\int_{\Pi} \left\{ \frac{\partial \phi}{\partial I} \delta I + \frac{\partial \phi}{\partial \Delta} \delta \Delta + \frac{\partial \phi}{\partial \kappa_{ab}} \delta \kappa_{ab} \right\} \, dA - \int_{\partial \Pi_2} \hat{t}_u \delta u \, ds - \int_{\partial \Pi_4} \hat{m} \, \delta \left( \frac{\partial u}{\partial n} \right) \, ds = 0. \tag{3.87}
\]

When carrying out the indicated variations \( \delta I, \delta \Delta, \) and \( \delta \kappa_{ab} \), we encounter terms of the form \( \delta \left( \frac{\partial u}{\partial x_a} \right) \) and its higher derivatives with respect to \( x \). It can be shown that the operation of variations commutes with the spatial differentiation, so that the variations \( \delta I, \delta \Delta, \) and \( \delta \kappa_{ab} \) can be replaced by derivatives of the variation of the displacement, that are then eliminated.
by integration by parts. In this way we transform (3.87) into

\[ 0 = - \int_{\Omega} \left\{ T_{3a,a}^s + T_{3a,a}^{ad} \right\} \delta u \, dA \]
\[ + \int_{\partial \Omega} \left\{ T_{3a}^s + T_{3a}^{ad} \right\} n_\alpha \, \delta u \, ds - \int_{\partial \Omega} \frac{1}{2} \epsilon_{3\alpha\beta} M_{\beta\gamma}^d n_\gamma \, \delta u,_{\alpha} \, ds \]
\[ - \int_{\partial \Omega_2} \hat{\iota} \delta u \, ds - \int_{\partial \Omega_4} \hat{m} \, \delta \left( \frac{\partial u}{\partial n} \right) \, ds, \]  

(3.88)

where the non-zero stresses are defined by

\[ T_{3a}^s = 4 \frac{\partial \phi}{\partial I} \gamma_{3a}, \quad M_{\alpha\beta}^d = \frac{\partial \phi}{\partial \kappa_{\beta\alpha}}, \quad T_{3a}^{ad} = \frac{1}{2} \epsilon_{3\alpha\beta} M_{\beta\gamma}^d, \]  

(3.89)

with \( T_{3a}^{ad} \) being some additional antisymmetric stress that depends only on the specified components of \( M_{\alpha\beta}^d \). An intermediate result is that the components \( T_{3a}^s \) of the symmetric stress tensor are independent of \( \Delta \), and that the only components expected to be given by a constitutive relation are \( T_{3a}^s \) and \( M_{\alpha\beta}^d \). Before proceeding further one must recall that essential boundary conditions have been predescribed on the boundary segments \( \partial \Pi_1 \) and \( \partial \Pi_3 \), which require the variations \( \delta u \) and \( \delta \left( \frac{\partial u}{\partial n} \right) \) to vanish:

\[ \begin{align*}
\delta u &= 0 \quad \text{on } \partial \Pi_1, \\
\delta \left( \frac{\partial u}{\partial n} \right) &= 0 \quad \text{on } \partial \Pi_3.
\end{align*} \]

(3.90)

Further on one has now to access the independence of the variation \( \delta u,_{\alpha} \) in (3.88). If we decompose the variation of the gradient of \( u \) into a component along the outward unit normal \( n \) and the tangent \( s \), the variation \( \delta u,_{\alpha} \) becomes

\[ \delta u,_{\alpha} = \delta \left( \frac{\partial u}{\partial n} \right) n_\alpha + \delta \left( \frac{\partial u}{\partial s} \right) s_\alpha. \]  

(3.91)

The variation of the tangential component is not independent of \( \delta u \) for a prescribed displacement \( u \) along the segment \( \partial \Pi_1 \). Therefore, we use (3.91) for the second line integral of (3.88) and perform an integration by parts along the boundary arc \( ds \). We eliminate one term by using the identity

\[ \int_{\Gamma} \frac{\partial f}{\partial s} \, ds = 0, \]  

(3.92)

which holds for all simple closed boundaries \( \Gamma \) and smooth functions \( f(s) \). Thus, we first transform the integrand with variation \( \delta u,_{\alpha} \) into two terms with independent variations \( \delta u \)
and $\delta \left( \frac{\partial u}{\partial n} \right)$. We then relate the tangential vector $s$ to the unit normal $n$ ($s_\alpha = -\epsilon_{\alpha\beta\gamma}n_\beta$), and take the restriction (3.90) on the variations on $\partial \Pi_1$ and $\partial \Pi_3$ into account. Then we obtain the following useful variational statement:

$$
0 = -\int_{\Pi} \left( T_{3\alpha}^s + T_{3\alpha}^{ad} \right) \delta u \, dA
+ \int_{\partial \Pi_2} \left\{ \left( T_{3\alpha}^s + T_{3\alpha}^{ad} \right) n_\alpha - \frac{\partial}{\partial s} \left( \frac{1}{2} M_{\alpha\beta}^d n_\alpha n_\beta \right) - \hat{t} \right\} \delta u \, ds
- \int_{\partial \Pi_4} \left\{ \frac{1}{2} M_{\alpha\beta}^d s_\alpha n_\beta + \hat{m} \right\} \delta \left( \frac{\partial u}{\partial n} \right) \, ds.
$$

(3.93)

The arbitrariness of the variation $\delta u$ in $\Pi$ now leads to the governing field equation

$$
\left( T_{3\alpha}^s + T_{3\alpha}^{ad} \right)_{,\alpha} = 0 \quad \text{on } \Pi,
$$

(3.94)

whereas the arbitrariness of $\delta u$ on $\partial \Pi_2$ and that of $\delta \left( \frac{\partial u}{\partial n} \right)$ on $\partial \Pi_4$ lead to the natural boundary conditions

$$
\begin{align*}
\left( T_{3\alpha}^s + T_{3\alpha}^{ad} \right) n_\alpha - \frac{\partial}{\partial s} \left( \frac{1}{2} M_{\alpha\beta}^d n_\alpha n_\beta \right) &= \hat{t} \quad \text{on } \partial \Pi_2, \\
\frac{1}{2} M_{\alpha\beta}^d s_\alpha n_\beta &= -\hat{m} \quad \text{on } \partial \Pi_4.
\end{align*}
$$

(3.95)

The boundary value problems to be solved consists of the governing differential equation (3.94), the natural boundary conditions (3.95), and the essential boundary conditions for $u$ on $\partial \Pi_1$ and $\frac{\partial u}{\partial n}$ on $\partial \Pi_3$. After the substitution of (3.89) into (3.94) the attained governing equation is the same as (3.74). Thus the governing equation and the natural boundary conditions given by (3.95) are independent of the trace of $M$. It also has been shown that the functional (3.85) is an appropriate weak formulation of (3.74) and hence useful for the finite element method.

### 3.7 Summary of the augmented theory in anti-plane shear

In the previous we have discussed to considerable detail the direct implication of introducing a non-standard continuum theory. Nevertheless, we never have addressed the question if this generalized theory is in its present form truly capable of modeling solid to solid interfaces. From the discussion in chapter 2 it is clear that sharp interfaces dissipate energy proportionately to the interface's speed of propagation. In the detailed couple stress theory no such
effects are presently captured. We thus propose to introduce an additional constitutive assumption. It is assumed that the dissipation can be modeled by adding a newtonian viscosity to the symmetric stress tensor \( T^a \). In the future we will refer to it as the augmented constitutive relation. In the case of an anti-plane shear deformation the non-zero contributions of the symmetric stress components listed in (3.73) take on the augmented form

\[
T_{3\alpha}^g = \mathcal{M}(k)u_{,\alpha} + \nu \dot{u}_{,\alpha}, \quad (3.96)
\]

with \( \nu \) as the positive coefficient of viscosity. The couple stress tensor \( M^d \) given by (3.69) remains unchanged and its non-zero components allow for \( B = 0 \) the alternative representation

\[
M_{\alpha\beta}^d = -2 \lambda \varepsilon_{3\gamma\alpha} u_{,\beta\gamma} \quad (3.97)
\]

where \( \lambda \) is commonly called the capillarity and here defined by

\[
\lambda = \frac{A}{4} \quad (3.98)
\]

The material length scale \( l_m \) of (3.82) can now be written as

\[
l_m = \sqrt{\frac{\lambda}{\mu}}. \quad (3.99)
\]

Consequently, the out-of-plane equation governing the anti-plane shear deformation can be written in its augmented form as

\[
(M(k)u_{,\alpha})_{,\alpha} + \nu \nabla^2 \dot{u} - \lambda \nabla^2 \nabla^2 u = 0 \quad \text{on } \Pi. \quad (3.100)
\]

Further discussions become less cumbersome if we take \( \text{tr} M = 0 \), in which case the couple stress tensor \( M \) and \( M^d \) coincide. It is possible, from a mathematical point of view, to take this for granted because, as mentioned previously, the trace of the couple stress tensor remains indetemined in the present theory and plays no role in either the governing equation (3.100) or the natural boundary conditions (3.95). It only allows us to explicitly specify an antisymmetric stress tensor \( T^a \) as

\[
T_{3\alpha}^a = -\lambda \nabla^2 u_{,\alpha}, \quad T_{\alpha3}^a = \lambda \nabla^2 u_{,\alpha}. \quad (3.101)
\]
Thus the non-zero components of the stress tensor $T = T^s + T^a$ corresponding to an anti-plane shear deformation are given by

$$
\begin{align*}
T_{3\alpha} &= \mathcal{M}(k)u_{,\alpha} + \nu \dot{u}_{,\alpha} - \lambda \nabla^2 u_{,\alpha}, \\
T_{\alpha 3} &= \mathcal{M}(k)u_{,\alpha} + \nu \dot{u}_{,\alpha} + \lambda \nabla^2 u_{,\alpha}.
\end{align*}
$$

The traction has only an $x_3$-component and is given by $t = T_{3\beta} n_\beta$, and the surface couple vector is given by $m_\alpha = M_{\alpha\beta} n_\beta$. The boundary conditions associated with an anti-plane shear equilibrium problem are

$$
\begin{align*}
u &= \dot{u} & \text{on } \partial\Pi_1, \\
\frac{\partial u}{\partial n} &= \dot{\Theta} & \text{on } \partial\Pi_3, \\
t - \frac{\partial}{\partial s} \left( \frac{1}{2} \mathbf{m} \cdot \mathbf{n} \right) &= \dot{t} & \text{on } \partial\Pi_2, \\
\frac{1}{2} \mathbf{m} \cdot \mathbf{s} &= -\dot{m} & \text{on } \partial\Pi_4,
\end{align*}
$$

where the quantities $\dot{u}$, $\dot{\Theta}$, $\dot{t}$, and $\dot{m}$ are prescribed on the corresponding boundaries such that $\partial\Pi_1 \cup \partial\Pi_2 = \partial\Pi_3 \cup \partial\Pi_4 = \partial\Pi$. 
Chapter 4

The traveling wave problem in anti-plane shear

Introduction

In the previous chapters two distinct theories to mathematically model solid to solid phase transformations were described. The theories can be compared by considering the problem of a traveling wave in anti-plane shear. We recall that one of the major differences of the two theories is their respective constitutive assumptions. In the sharp interface theory we gave, in addition to a non-monotonic stress-strain relation, a kinetic relation, which described the evolution of the interface. On the other hand, as we now show, when we use the couple stress theory this kinetic relation is implied by the augmentation and scaled by the two new material parameters $\lambda$ and $\nu$. Clearly, both theories will generally yield independent results for the same physical process, if arbitrary kinetic relations and arbitrary material parameters $\lambda$ and $\nu$ are given. However by choosing the kinetic relation and $\lambda, \nu$ consistently, the results of both theories can be made to correspond. Thus, the following question arises: what kinetic relation in a sharp interface theory gives a physically identical solution to the couple stress theory? For an identical body and loading we interpreted this as observing similar dissipative properties of the interface, similar kinematic evolution of the interface, and the same stress and strain fields sufficiently far away from the interface. The kinetic relation satisfying these conditions is termed the effective kinetic relation of the augmented material.
In this chapter the effective kinetic relation will be analytically calculated by closely following the work of Abeyaratne & Knowles [5]. We consider a traveling wave which propagates through an infinite body described by a trilinear stress-strain relation and an augmentation with material parameters $\lambda$ and $\nu$. We then calculate the associated dissipation of the traveling wave with respect to the interface’s speed, to determine the equivalent kinetic relation. The work is organized as follows, in Section 4.1 and 4.2 the sharp interface theory of Chapter 2 and the couple stress theory of Chapter 3 is specialized to the motion of a traveling wave along the $x_1$-direction. In the remainder the boundary value problems are set up and the strain field and driving traction $f$ are explicitly calculated.

### 4.1 Basic equations of the sharp interface theory

Consider a cylindrical body $D$ whose cross section $\Pi$ lies in the $x_1, x_2$-plane of the reference configuration $R$. The cross section occupies the entire $(x_1, x_2)$-plane. The anti-plane shear motion (2.41) described in Chapter 2 is specialized to a case in which the $y_3$ component of the motion $y(x, t)$ along the $x_3$-axis is characterized by

$$y_3 = y = x_3 + u(x, t). \quad (4.1)$$

The displacement $u$ only depends on the position $x = x_1$ of a material point along the $x_1$-direction at time $t$, and is at least continuous with piecewise continuous first and second derivatives in space and time. Thus the general anti-plane shear deformation (2.41) with shear strains $k_\alpha$ has been simplified to a state with linear shear strain $\gamma(x, t) = k_1(x_1, t)$ and $k_2 = 0$. The linear strain $\gamma$ and the velocity $v(x, t)$ are given by

$$\gamma = u_x, \quad v = \dot{u}. \quad (4.2)$$

The curve of discontinuity $\Sigma(t)$ on $\Pi$ now is a line $x_1 = s(t)$. To ensure the invertibility of the map $x \rightarrow x_3 + u(x, t)$, the strain $\gamma$ is restricted to the range $(-1, +\infty)$. Suppose, that we are interested in such strain fields, then in the quasi-static theory of sharp interfaces
the balance of linear momentum yields for the nominal shear stress $\sigma_{31} = \tau$ the differential equation

$$\tau_x = 0,$$

(4.3)

and that the shear stress $\tau$ be continuous throughout the body at all time $t$

$$[[\tau]] = 0 \quad \text{on } x = s(t),$$

(4.4)

as shown in (2.501). Kinematic compatibility requires in the continuous regions that

$$v_x = \dot{\gamma},$$

(4.5)

and at the discontinuity $x = s(t)$ the jump condition (2.502) takes at all time $t$ on the form:

$$[[v]] = \dot{s}\gamma \quad \text{on } x = s(t).$$

(4.6)

The discontinuity of the strain field propagates with the normal velocity $V_n = \dot{s}(t)$. We use the notation $[[g]]$ for the limiting values of $g(x, t)$ on either side of the discontinuity,

$$[[g]] = g(s(t)+, t) - g(s(t)-, t).$$

The trilinear stress-strain relation $\hat{\tau}(\gamma)$.

Figure 4.1: The used trilinear stress-strain relation $\hat{\tau}(\gamma)$.

The nonmonotonic stress-strain relation $\hat{\tau}(\gamma)$ shown in Figure 4.1 is related to the shear stress $\tau(x, t)$ by

$$\tau = \hat{\tau}(\gamma).$$

(4.7)
This constitutive relation allows a material point to be either in phase 1 (austenite), 2, or 3 (martensite), if the the shear strain $\gamma(x, t)$ is in the intervals $(-1, \gamma_M]$, $(\gamma_M, \gamma_m)$ or $[\gamma_m, \infty)$, respectively. This specific material is piecewise linear and fully determined by

$$\hat{\tau}(\gamma) = \begin{cases} 
\mu \gamma & -1 \leq \gamma \leq \gamma_M, \\
-\mu_2 \gamma + \tau_2 & \gamma_M \leq \gamma < \gamma_m, \\
\mu(\gamma - \gamma_T) & \gamma_m \leq \gamma \leq \infty,
\end{cases}$$

(4.8)

where the stress $\tau_2$ can be expressed by $\tau_2 = (\mu + \mu_2)\gamma_M$. Of the possible material constants, $\gamma_M$, $\gamma_m$, $\gamma_T$, $\tau_M = \hat{\tau}(\gamma_M)$, $\tau_m = \hat{\tau}(\gamma_m)$, $\tau_0$, $\mu$, and $\mu_2$, to describe the material only four constants can be chosen independently, where the constants $\mu$ and $\gamma_T$ represent the shear modulus and the transformation strain. The level of stress at which the two enclosed areas below and above the stress-strain relation $\hat{\tau}(\gamma)$ are equal is referred to as the Maxwell stress $\tau_0$ and is in this particular case

$$\tau_0 = \frac{\tau_M + \tau_m}{2}.$$  

(4.9)

### 4.2 Local theory of phase boundaries

The kinetic relation

$$f = \hat{f}(\dot{\gamma}),$$  

(4.10)

relates the velocity of propagation $\dot{\gamma}(t)$ to the driving traction $f(t)$, and provides a continuum description of the microscale processes of phase transformation. In the following we define the driving traction $f$ for the one-dimensional problem of a propagating interface in simple shear. Let us consider a slice of the body $D$ occupying the interval $(a, b]$ in the reference configuration $R$, containing a single moving jump in strain at $x = s(t)$. Then in the local theory of phase boundaries the rate of work done by external forces is not necessarily equal to the rate of change of stored strain energy, since the moving interface may dissipate energy as described by equation (2.30). The stored strain energy per unit volume is now

$$W(\gamma) = \int_0^\gamma \hat{\tau}(\gamma^*) \, d\gamma^*,$$

(4.11)
4.2. LOCAL THEORY OF PHASE BOUNDARIES

Figure 4.2: A graphical depiction of the interrelation between the applied stress and the driving traction \( f \) to propagate a straight interface.

and the local balance of energy yields at the interface the rate of dissipation as

\[
\tau(b, t)v(b, t) - \tau(a, t)v(a, t) - \dot{W}(\gamma) = f(t)s, \tag{4.12}
\]

which is set equal to the product of the driving traction \( f(t) \) and the speed \( s(t) \). This result is attained by specializing (2.51) to the motion (4.1), or equivalently by a direct calculation using (4.11) and (4.3-4.6). Equations (4.11) and (4.12) define the driving traction \( f \) acting on the strain discontinuity as

\[
f = \hat{f}(\gamma, \dot{\gamma}) \equiv \int_{\gamma}^{\dot{\gamma}} \tau(\gamma) \, d\gamma - \tau(\dot{\gamma} - \gamma). \tag{4.13}
\]

Equation (4.13) can be specialized to the trilinear material (4.8) by assuming a sharp interface as shown in Figure 4.2. Then the driving traction \( f \) is computed to be

\[
f = \gamma_T(\tau - \tau_0). \tag{4.14}
\]

If the material is thermoelastic and the transformation occur isothermally the second law of thermodynamics will require that the entropy of a particle crossing the front must increase:

\[
f(t)s(t) \geq 0. \tag{4.15}
\]
Abeyaratne & Knowles refer in [4, 5] to it as the entropy inequality which ought to hold at all strain discontinuities under isothermal conditions. Then the entropy inequality (4.15) and the driving traction (4.14) imply:

- If \( \tau > \tau_0 \) the domain undergoes a transformation from austenite to martensite. The interfacial driving traction \( f \) and velocity \( \dot{s} \) are positive.

- If \( \tau < \tau_0 \) the domain undergoes a transformation from martensite to austenite. The interfacial driving traction \( f \) and velocity \( \dot{s} \) are negative.

### 4.3 The augmented theory

#### 4.3.1 Theory of couple-stresses

From Chapter 3 one recalls equation (3.102) with the non-zero stresses

\[
\begin{align*}
T_{3\alpha} &= \mathcal{M}(k)u_{,\alpha} + \nu \dot{u}_{,\alpha} - \lambda \nabla^2 u_{,\alpha}, \\
T_{a3} &= \mathcal{M}(k)u_{,\alpha} + \nu \dot{u}_{,\alpha} + \lambda \nabla^2 u_{,\alpha}.
\end{align*}
\]

The terms proportional to the strain-rate model the dissipative nature of propagating interfaces. In case the motion \( y(x, t) \) and the shear strain \( \gamma(x, t) \) given by (4.1) and (4.2) are substituted into the constitutive relation (4.16) and by using \( \dot{\gamma}(\gamma) = \mathcal{M}(\gamma) \gamma \) the augmented constitutive relation simplifies to

\[
\tau = \dot{\gamma} + \nu \gamma - \lambda \gamma_{xx}.
\]

The positive material parameters \( \nu \) and \( \lambda \) are the viscosity and the strain-gradient coefficient, respectively. They lend themselves to form the lengthscale \( l_m \), the timescale \( t_m \), and the velocity \( u_m \):

\[
l_m = \sqrt{\frac{\lambda}{\mu}}, \quad t_m = \frac{\nu}{\mu}, \quad u_m = \frac{l_m}{t_m}.
\]

Observe that \( l_m, t_m, \) and \( u_m \) are material parameters. Since an infinite medium does not provide an additional geometrical lengthsble, it is convenient to define the following nondimensional variables:

\[
\bar{x} = \frac{x}{l_m}, \quad \bar{t} = \frac{av}{t_m}, \quad \bar{u} = \frac{u}{\gamma T l_m}.
\]
\[ \bar{s} = \frac{s}{l_m}, \quad \bar{\tau} = \frac{\tau}{\mu \gamma_T}, \quad \bar{f} = \frac{f}{\mu \gamma_T^2}. \] (4.20)

Also, consider the strain ratios given by
\[ \bar{\gamma} = \frac{\gamma}{\gamma_T}, \quad \bar{\gamma}_M = \frac{\gamma_M}{\gamma_T}, \quad \bar{\gamma}_m = \frac{\gamma_m}{\gamma_T}. \] (4.21)

To simplify our notation the overbar will be dropped on all further nondimensional equations.

The constitutive relation (4.17) now becomes
\[ \tau = \hat{\tau}(\gamma) + \dot{\gamma} - \gamma_{xx}, \] (4.22)

with the stress-strain relation (4.8) transformed to
\[ \hat{\tau}(\gamma) = \begin{cases} 
\gamma & \frac{-1}{\gamma_T} \leq \gamma \leq \gamma_M, \\
\gamma + \gamma_M & \gamma_M < \gamma < \gamma_m, \\
\gamma - \gamma_m & \gamma_m \leq \gamma \leq \infty,
\end{cases} \] (4.23)

where the parameter \( m \) represents the ratio
\[ m = \frac{\mu_2}{\mu}. \] (4.24)

The governing differential equation for the shear strain \( \gamma(x, t) \) on II can now be written as
\[ \hat{\tau}'(\gamma)\gamma_x + \dot{\gamma}_x - \gamma_{xxx} = 0. \] (4.25)

The presence of higher order derivatives in space and time of the material described by (4.22) and (4.23) allow piecewise continuous third derivatives of the strain \( \gamma(x, t) \), requiring, in light of the jump condition (4.4), \( \gamma_{xx} \) to be continuous.

### 4.3.2 Solution of the traveling wave

Since our final goal is to examine the kinetic relation implied by the augmented theory in an elastic medium, we consider a traveling wave
\[ u(x, t) = u(\xi), \quad \xi = x - \dot{s}t, \] (4.26)

with propagation speed \( \dot{s} \), and strain
\[ \gamma(\xi) = u'(\xi). \] (4.27)
Let us assume that at infinity the strain $\gamma$ approaches the values

$$\gamma(\xi) \to \overline{\gamma} \quad \text{as} \quad \xi \to \pm \infty, \quad (4.28)$$

smoothly connecting the strains $\overline{\gamma}$ and $\overline{\dot{\gamma}}$. Once we have solved for $\gamma(\xi)$ the necessary stress to sustain the motion of the interface for a given speed $\dot{s}$ is known to us, and hence the effective kinetic relation implied by the augmented constitutive relation can be found. Under the change of coordinate given by (4.26) the nondimensional constitutive relation (4.22) becomes

$$\tau = \hat{\tau}(\gamma) + \dot{s} \gamma' - \gamma'', \quad (4.29)$$

and the traveling wave satisfies the governing differential equation

$$\gamma''' + \dot{s} \gamma'' - \hat{\tau}'(\gamma) \gamma' = 0, \quad (4.30)$$

at all points $-\infty < \xi < +\infty$, where $\gamma''(\xi)$ exists. By integrating equation (4.30) we attain the second order differential equation

$$\gamma'' + \dot{s} \gamma' - \hat{\tau}(\gamma) = B \quad \text{for} \quad -\infty < \xi < +\infty, \quad (4.31)$$

with constant $B$ being

$$B = \hat{\tau}(\overline{\gamma}) = \hat{\tau}(\overline{\dot{\gamma}}). \quad (4.32)$$

Due to the piecewise linear nature of the constitutive relation (4.22), the solution $\gamma(\xi)$ to equations (4.28), (4.31-4.32) can be constructed by solving three linear problems, for which $\gamma(\xi)$ is in the parent phase for $-\infty < \xi \leq 0$, in the transition layer for $0 < \xi < b$ and in the transformed phase for $b \leq \xi < +\infty$. The thickness $b$ of the transition layer will be determined later on. Consistently with the smoothness assumptions the following additional conditions hold at the interface at $\xi = 0$ and $\xi = b$:

$$\gamma(0-) = \gamma_M, \quad \gamma(0+) = \gamma_M, \quad \gamma'(0-) = \gamma'(0+), \quad (4.33)$$

$$\gamma(b-) = \gamma_m, \quad \gamma(b+) = \gamma_m, \quad \gamma'(b-) = \gamma'(b+), \quad (4.34)$$
4.3. THE AUGMENTED THEORY

thus in connection with the differential equation (4.31), \( \gamma''(\xi) \) is automatically continuous at points \( \xi = 0 \) and \( \xi = b \). The first problem, a boundary-value problem is valid in the range \(-\infty < \xi \leq 0\), whereas the second and third problems are initial-value problems in the ranges \( 0 < \xi < b \) and \( b \leq \xi < +\infty \), respectively. The three problems are given as:

**Problem 1:**

\[
\gamma'' + \dot{\gamma} - \gamma = B \quad \text{on} \ (-\infty, 0],
\]
\[
\gamma(-\infty) = \bar{\gamma}, \quad \gamma(0-) = \gamma_M,
\]

**Problem 2:**

\[
\gamma'' + \dot{\gamma} + m \gamma = B + (1 + m)\gamma_M \quad \text{on} \ [0, b],
\]
\[
\gamma(0+) = \gamma_M, \quad \gamma'(0+) = \gamma'(0-),
\]

**Problem 3:**

\[
\gamma'' + \dot{\gamma} - \gamma = B - 1 \quad \text{on} \ [b, \infty),
\]
\[
\gamma(\infty) = \gamma^+, \quad \gamma(b+) = \gamma_m.
\]

By formulating the problem for \( \gamma(\xi) \) on \((-\infty, \infty)\) as outlined, we utilize all three interface conditions of (4.33) at \( \xi = 0 \), and one of three interface conditions (4.34) at \( \xi = b \). The non-prescribed boundary conditions at \( \xi = \pm\infty \) will be enforced such that the solution satisfies the remaining requirements

\[
-1 \leq \gamma \leq \gamma_M \quad \text{for} \ -\infty < \xi \leq 0,
\]
\[
\gamma \geq \gamma_m \quad \text{for} \ \xi \geq b.
\]

In summary a total of eight conditions are given to determine the six constants of integration, the thickness \( b \) of phase 2, and the constant stress \( B \). We will now focus on the detailed solution of each problem. For Problem 1 we set \( B \) equal to the stress \( \tilde{\tau}(\bar{\gamma}) \), and find the solution of \( \gamma(\xi) \) in the interval \([-\infty, 0]\) to be

\[
\gamma(\xi) = (\gamma_M - \bar{\gamma})e^{\pi \xi} + \bar{\gamma}, \quad -\infty < \xi \leq 0.
\]
The positive root \( p_1 \) and the negative root \( p_2 \) of the characteristic equation are calculated as
\[
p_1 = -\frac{1}{2}(\dot{s} - P), \quad p_2 = -\frac{1}{2}(P + \dot{s}),
\]
with the function \( P = P(\dot{s}) \) as
\[
P = \sqrt{\dot{s}^2 + 4}.
\]
We will utilize root \( p_2 \) for the second and third problem. The general solution of Problem 2 is
\[
\gamma(\xi) = D_1 e^{q_1 \xi} + D_2 e^{q_2 \xi} + \gamma_0, \quad 0 < \xi < b,
\]
with the particular solution \( \gamma_0 \) defined by
\[
\gamma_0 = \frac{B + (1 + m)\gamma_M}{m}.
\]
After we impose the two boundary conditions (4.38) and eliminate \( \gamma \) with the aid of
\[
(\gamma_M - \dot{\gamma}) = \frac{q_1 q_2}{p_1 p_2} (\gamma_M - \gamma_0),
\]
the constants of integration \( D_1 \) and \( D_2 \) become
\[
D_1 = - (\gamma_M - \gamma_0) \frac{q_2}{p_2} (p_2 - q_1), \quad D_2 = (\gamma_M - \gamma_0) \frac{q_1}{p_2} (p_2 - q_2).
\]
Because of the interrelation between the speed \( \dot{s} \) and the ratio \( m \), the roots \( q_1 \) and \( q_2 \) are possibly complex:
\[
q_1 = -\frac{1}{2}(\dot{s} - Q), \quad q_2 = -\frac{1}{2}(\dot{s} + Q),
\]
where the function \( Q = Q(\dot{s}) \) is defined by
\[
Q = \begin{cases} \sqrt{\dot{s}^2 - 4m} & \text{if } \dot{s}^2 \geq 4m, \\ i\sqrt{4m - \dot{s}^2} & \text{if } \dot{s}^2 \leq 4m. \end{cases}
\]
Finally, Problem 3 takes on the general solution
\[
\gamma(\xi) = (\gamma_M - \dot{\gamma}) e^{q_2 \xi} + \dot{\gamma}, \quad \xi \geq b.
\]
We note that the characteristic equation of Problem 1 and 3 are the same and thus the root in the exponent of (4.51) is given by (4.43). The solution \( \gamma(\xi) \) as given on \([b, \infty]\) by
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(4.51) satisfies the two boundary conditions (4.40) automatically. In order to complete the construction of the overall solution $\gamma(\xi)$ on $(-\infty, \infty)$ the remaining requirements

$$\gamma(b-) = \gamma_m, \quad \gamma'(b-) = \gamma'(b+),$$

(4.52)

are interpreted to be equations for the up to now undetermined thickness $b$ of the transition layer and the constant stress $B$. The equations given by (4.52) allow with the aid of (4.45), (4.51) the representation

$$(\gamma_m - \gamma_m) p_2 - (\gamma_m - \gamma_m) q_2 = D_1(q_1 - q_2)e^{q_1b},$$

(4.53)

$$(\gamma_m - \gamma_m) p_2 - (\gamma_m - \gamma_m) q_1 = D_2(q_2 - q_1)e^{q_2b},$$

(4.54)

where the strain $\gamma$ can be eliminated by

$$(\gamma_m - \gamma_m) = \frac{q_1 q_2}{p_1 p_2} (\gamma_m - \gamma_m),$$

(4.55)

After substituting (4.48) for $D_1$ and $D_2$ into equations (4.53-4.54) the two equations take on the form

$$e^{Qb} = \frac{(Q - P)^2}{(Q + P)^2},$$

(4.56)

$$e^{\bar{Q}b} = \frac{(\bar{Q} - P)^2}{(\bar{Q} + P)^2} \left( \frac{\gamma_m - \gamma_m}{\gamma_m - \gamma_m} \right)^2.$$

(4.57)

Thus by finding the root of the former we attain an explicit expression for the thickness $b$ as a function of the velocity $\dot{s}$ and the ratio $m$. The latter implies the restriction, that the strains have to be compatible with the constant stress $B$ throughout the domain. We will first solve for the thickness $b$ by noting that we can restrict our analyses to cases in which $Q$ of (4.50) is purely complex. It then follows from (4.56) that $b$ is given by

$$b = b_n = \frac{1}{|Q|} [2\pi(n + 1) - 4\theta_p],$$

(4.58)

and the angle $\theta_p$ obeys the relation

$$\tan \theta_p = \frac{\sqrt{4m - \dot{s}^2}}{\sqrt{4 + \dot{s}^2}}.$$

(4.59)
Next the restriction (4.57) upon the data is solved by making use of (4.23). The dependency on the strain $\gamma_0$ can be replaced with one on the stress and it becomes clear that (4.57) is a compatibility condition between the stress $\tau$ and the strain $\gamma(\xi)$ on $(-\infty, \infty)$, and is given by

$$\tau = (\tau_m + \tau_M) \frac{H}{1 + H}, \quad (4.60)$$

with the positive function

$$H = H(\dot{s}) = \frac{P - \dot{s} - \dot{s}}{\dot{s} + P} e^{-\frac{1}{2} \dot{s} b}. \quad (4.61)$$

The function $H$ has the two properties: $H(0) = 1$, which recovers the Maxwell stress, and that $H$ approaches the value 0 when increasing the speed $|\dot{s}|$. Next we substitute equation (4.60) into (4.14) (we multiply(4.14) by minus one to correct for the fact that matensite is now to the right of the interface) to attain the nondimensional kinetic relation

$$f = f(\dot{s}) = \frac{1}{2} (\tau_M - \tau_m) \frac{1 - H}{1 + H}. \quad (4.62)$$

The pointsymmetry of the kinetic relation (4.62) is a feature of the trilinear constitutive relation with equal elastic modulus $\mu$ for martensite and austenite. The material's properties can be summarized as follows:

1. The straight interface is only stationary if the applied stress is exactly the Maxwell stress $\tau_0$. This observation is not consistent with experimental observations, but inherent to the linear augmentation with respect to the strain rate $\dot{\gamma}$.

2. The applied stress differential $|\tau - \tau_0|$ necessary to propagate an interface at a given speed $|\dot{s}|$ is the same for the transformation of austenite $\rightarrow$ martensite and martensite $\rightarrow$ austenite.

3. The rate of dissipation is the same for the forward and reverse transformation.

In Figure 4.3 we plot the ratio of the nondimensional kinetic relation (4.62) with respect to the nondimensional stress differential $(\tau_M - \tau_m) (> 0)$. Thus the graphs are characteristic
Figure 4.3: Kinetic relation for the trilinear material for three different ratios of $m = 1.5, 1.0, 0.5$.

for all trilinear materials (4.23) when the parameter $m = \mu_2/\mu$ is 1.5, 1.0, 0.5. We note that the dependency of the kinetic relation (4.62) on $m$ diminishes for increasing values of $m$.

In our later work we concern ourselves with very slow moving interfaces, where the linearized kinetic relation is valid. This linear relation is given by

$$f = f(\dot{s}) = \frac{1}{4}(\tau_M - \tau_m)(1 + \frac{1}{2}b)\dot{s},$$ (4.63)

with the thickness $b$ as

$$b = \frac{\pi - 2 \arctan \sqrt{m}}{\sqrt{m}}.$$ (4.64)
Chapter 5

Numerical methods

Introduction

After having presented in Chapter 2 and 3 two theoretical frameworks in which to mathematically model solid to solid interfaces, we will now focus on the numerical implementation of the second of these frameworks, i.e. the couple stress theory with viscosity or the "augmented theory". The advantages of the augmented theory over the sharp interface theory are mostly computational. To solve a problem which is set up in the framework of the sharp interface theory, it is necessary to track the location and speed of each interface location accurately. This can become cumbersome for problems of higher dimensions, since the solution might exhibit multiple interfaces of complex geometry. For example SILLING documented in [74] a rather complex needle structure near the tip of a crack loaded in Mode-III. On the other hand the augmented couple stress theory involves a single higher-order boundary value problem that is valid over the whole body. The nucleation and evolution of interfaces is build into the governing differential equation, thus implying, for the sharp interface theory, a certain implicit nucleation criterion and kinetic relation (see Chapter 2.3). This simplification is attained by specifying higher order differential equilibrium equations that transform, in the case of anti-plane shear, the laplacian operator $\nabla^2 u$ into

$$\nabla^2 u - l_m^2 \nabla^2 \nabla^2 u, \quad (5.1)$$

where $l_m$ is a material length scale associated with the augmentation. Equation (5.1) is of
fourth order, requiring the specification of an additional set of boundary conditions.

Several numerical methods are useful for this kind of task. We choose the Finite Element Method (FEM) in our computational implementation. The FEM evolved to its present-day state from different origins. Commonly, the behavior of a continuum is approximated by discrete elements that compose the domain. The underlying procedures to attain the integral equation of FEM vary. The most common one is the displacement approach. This approach relies on the statement of virtual work, in which the external work is equal to the internal work done by the stresses. The statement is applied to each element and the integral over the volume of each element is summmed up to reflect the overall virtual work done by external forces and the internal virtual work due to the stresses at a given variation of the displacement field. Another method is the variational method. In case of conservative problems the solution is attained by extremizing a functional and solving the arising set of equations numerically. Unfortunately, not every partial differential equation and its natural boundary conditions can be represented by a functional, or so called weak form. A rather general method of deriving the integral equations of FEM dates back to GALERKIN (see [32]). It has the advantage that it is not necessary to refer to a physically tractable concept like the principle of virtual work, or to have knowledge of the functional associated with a given partial differential equation. It is sufficient to know the appropriate partial differential equations and boundary conditions. The Galerkin-weighted residual method can be made to coincide with the variational method whenever it is possible to specify a functional. Other methods like the mixed formulation where variations of other than the displacement exist have found a wide range of application, but will not be used in the present work.

The numerical issues that have to be addressed in adapting the augmented couple stress theory to the Finite Element Method are mostly related to the materials ability to undergo a stress-induced phase transformation. This nonlinearity requires the continuous updating of the stiffness matrix and is such that the stiffness matrix would cease to be positive definite without regularization, whenever phases are nucleated. Thus two numerical problems have to
be addressed. First, what is an appropriate spatial discretization, in order to include couple stress effects, and secondly, how to stably propagate the solution in time with sufficient accuracy.

Before we focus on the approach taken in this work let us recall some other common methodology in the context of Shape Memory Alloys:

- A method commonly used by Auricchio, Boyd, Lagoudas and their co-workers [56, 12] is closely related to the classical theory of plasticity. The plastic strain plays now the role of the transformation strain and the strain hardening function depends on the volume fraction of martensite. The model has been implemented in conjunction with commercial finite element codes, to simulate the response of structures.

- The one-dimensional phenomenological models proposed by workers like Brinson, Tanaka & Nagaki, Liang & Rogers are thermodynamically consistent (as noted by Brinson [18]) and rely on material parameters that can be measured in uniaxial stress-strain-temperature experiments. The constitutive model relies on the volume fraction of martensite or a combination of the volume fraction of twinned and detwinned martensite. Hence, the model is not useful in the study of the kinetics of phase boundaries. Nevertheless, it has been implemented in structural analyses such as finite element procedures. Some recent developments with references to their previous work can be found in [17, 18, 58].

- Numerical simulations based on the methodology of Müller and his co-workers [9, 69] provide no information on the evolution of the microstructure. The existence of distinct phases is captured once again by the volume fraction of martensite. Nevertheless, the method is simple and flexible enough to be applied to real time control problems of SMA-wires.

We structure this chapter as follows. In Section 5.1 a brief summary of the commonly applied methodology of the FEM is given, and its usefulness to the problem at hand is
analyzed. In Section 5.2 the weak formulation of a representative boundary value problem is introduced. In the next section the implications on the choice of finite elements is addressed. In Section 5.4 the time discretization and accommodation of the materials nonlinearity are considered. At the end of this chapter several verification problems are introduced and the viability of our proposed numerical implementation is verified.

5.1 Review of the finite element concept

Before exploring the differences among several possibilities of formulation we will consider the basic idea of subdividing a physical domain into finite elements. Each finite element $e$ is defined by a series of nodes and boundary segments. The displacement $\mathbf{u}(\mathbf{x}, t)$ within an element is approximated by

$$
\mathbf{u} \approx \mathbf{\hat{u}}^e = \sum_{i=1}^{nl} N_i^e \mathbf{a}_i^e = [N_1^e, N_2^e, \ldots N_{nl}^e][\mathbf{a}_1^e, \mathbf{a}_2^e, \ldots \mathbf{a}_{nl}^e]^T = \mathbf{N}^e \mathbf{a}^e,
$$

(5.2)

where $N_i^e(\mathbf{x})$ are prescribed shape functions in position and $\mathbf{a}_i^e(t)$ is the listing of nodal values for the $i$th node of the $nl$ local nodes of the element. The list of all nodal values is $\mathbf{a} = \sum_{i=1}^{n} \mathbf{a}_i^e$, with $n$ being the global number of nodes. Applying equation (5.2) to the whole domain of $D$ defines the global interpolation $\mathbf{\hat{u}}$ as

$$
\mathbf{u}(\mathbf{x}, t) \approx \mathbf{\hat{u}}(\mathbf{x}, t) = \sum_{i=1}^{n} N_i \mathbf{a}_i = \mathbf{N}(\mathbf{x}) \mathbf{a}(t).
$$

(5.3)

The interpolation $N_i$ is defined by the local function $\mathbf{N}^e$ wherever the elements local node corresponds to the global node, and otherwise $N_i = 0$. In three-dimensional elasticity for example each displacement component of $\mathbf{u}$ requires at least the specification of the nodal vector $\mathbf{a}_i^e$ with three displacement components at the $i$th local node of each element. The necessary conditions of continuity on the shape functions of $\mathbf{N}$ and the content of the nodal vector $\mathbf{a}$ depend on the problem’s governing field equations.

Once the domain is discretized equations have to be established to ultimately solve for the nodal vector $\mathbf{a}$. Several possibilities have found application in the area of engineering and
physics. One is the direct formulation or so called displacement approach. Let us assume that the constitutive relation of the material is known to us and the measure of deformation can be expressed by the derivatives of the displacement $u$ and consequently by the derivatives of the shape function $N(x)$ given by approximation (5.3). The Piola-Kirchhoff stress $\sigma(x, t)$ is then approximated by $\hat{\sigma}(N, a)$. The statement of virtual work can be adopted to the FEM, such that external forces and their conjugates are replaced by nodal forces and the nodal variation $\delta a^c$. Nevertheless, it is not necessary to develop the FEM-equation by replacing the continuous interactions of body $D$ with nodal forces. The Principle of virtual work may be applied directly to the whole continuum. When excluding body forces, the principle of virtual work of linear elasticity becomes

$$\int_{\partial D} t \cdot \delta u \, dA = \int_D \sigma \cdot \delta \gamma \, dV, \quad (5.4)$$

where the stress $\sigma$ times the variation of the linear strain $\gamma$ is the sole contributor to the internal virtual work. In the FEM the integrals over the whole body $D$ and the boundary $\partial D$ are replaced by the sum of integrals over elements

$$\int_D (\ldots) \, dV = \sum \int_{D^e} (\ldots) \, dV, \quad \int_{\partial D} (\ldots) \, dA = \sum \int_{\partial D^e} (\ldots) \, dA. \quad (5.5)$$

The addition of contributions of individual elements implies in light of the principle of virtual work (5.4) the continuity of the displacement between adjacent elements. When boundary integrals are replaced by the sum of element integrals the contributions of adjacent elements have to cancel each other out until the traction along the boundary $\partial D$ remains. Since such integrals depend on $N$, one requires that $N$ is at least continuous which is called an element of continuity $C_0$. This approach is widely used and valid for linear, or nonlinear materials, with a possible dependency on the stress-rate of strain. It would also be applicable to the couple stress theory, if one allowed the principle of virtual work to take the generalized form

$$\int_{\partial D} t \cdot \delta u \, dA + \int_{\partial D} m \cdot \delta w \, dA = \int_D \sigma \cdot \delta \gamma \, dV + \int_D M^d \cdot \delta \kappa. \quad (5.6)$$

If the integrals of (5.6) are replaced by (5.5) similar arguments as previously prevail. In addition the boundary integral associated with the couple $m$ will depend on the normal
derivative of $\mathbf{N}$ along the boundary of each element. Thus each contribution of an adjacent element not being part of the boundary $\partial D$ has to be of equal amount, requiring that the slope of $\mathbf{N}$ is matched from one element to the next. This continuity is called $C_1$.

The principle of virtual work is a special case of a more general formalism. Let us assume the problem is mathematically described by the set of differential equations

$$
\mathbf{A}(\mathbf{u}) = 0 \quad \text{on } D, \quad (5.7)
$$

and the set of boundary conditions

$$
\mathbf{B}(\mathbf{u}) = 0 \quad \text{on } \partial D, \quad (5.8)
$$

where $\mathbf{A}$ and $\mathbf{B}$ are vector operators. As the differential equation (5.7) is satisfied at each point on $D$ it follows that

$$
\int_D \mathbf{A}(\mathbf{u}) \cdot \mathbf{v} \, dV \equiv 0, \quad (5.9)
$$

for any arbitrary set of sufficiently smooth functions $\mathbf{v}$. Conversely, if the integral (5.9) is satisfied for any $\mathbf{v}$ then the differential equations of (5.7) must be satisfied at each point. The boundary conditions (5.8) can be included by a separate integral statement and yield in connection with (5.9) the useful integral form

$$
\int_D \mathbf{A}(\mathbf{u}) \cdot \mathbf{v} \, dV + \int_{\partial D} \mathbf{B}(\mathbf{u}) \cdot \mathbf{v} \, dA = 0. \quad (5.10)
$$

The arbitrary functions $\mathbf{v}$ and $\mathbf{v}$ are restricted suitably to avoid infinite integrals. In many cases it is possible to integrate (5.10) by parts to reduce the leading order of the spatial derivatives of $\mathbf{A}(\mathbf{u})$. Thus equation (5.10) takes on the generic form

$$
\int_D \mathbf{D}(\mathbf{u}) \cdot \mathbf{C}(\mathbf{v}) \, dV + \int_{\partial D} \mathbf{F}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}) \, dA = 0, \quad (5.11)
$$

with $\mathbf{D}(\mathbf{u})$ and $\mathbf{F}(\mathbf{u})$ replacing $\mathbf{A}(\mathbf{u})$ and $\mathbf{B}(\mathbf{u})$, respectively. In case of a single governing equation of 2nd or 4th order the differential operator $\mathbf{D}(\mathbf{u})$ and $\mathbf{C}(\mathbf{v})$ is of 1st or 2nd order, respectively. This reduction of the necessary smoothness assumption of the function
5.1. REVIEW OF THE FINITE ELEMENT CONCEPT

\( \mathbf{u} \) is important for the efficient computation of integrals. Next, the unknown function \( \mathbf{u} \) is approximated by \( \tilde{\mathbf{u}} \), and the integral statement (5.11) is approximated by introducing for \( \mathbf{v} \) a finite set of prescribed functions

\[
\mathbf{v} = \tilde{\mathbf{v}} = \mathbf{w}_j \quad j = 1 \text{ to } nb, \quad (5.12)
\]

with \( nb \) being the number of unknown parameters \( \mathbf{a}_i \) \( (nb \leq n) \), and \( \mathbf{w}_j \) being compatible with the specification of essential boundary conditions. The integral equation (5.11) now yields a set of ordinary equations or ordinary differential equations with respect to the parameters \( \mathbf{a} \) of the form

\[
\int_D \mathbf{D}(\mathbf{N}\mathbf{a}) \cdot \mathbf{C}(\tilde{\mathbf{w}}_j) \, dV + \int_{\partial D} \mathbf{F}(\mathbf{N}\mathbf{a}) \cdot \mathbf{E}(\tilde{\mathbf{w}}_j) \, dA = 0 \quad j = 1 \text{ to } nb, \quad (5.13)
\]

This approximation technique is in the literature referred to as the method of weighted residuals. Certain obvious choices of the weighting function \( \mathbf{w}_j \) yield various common methods. If \( \mathbf{w}_j = \mathbf{N}_j \) one speaks of the Galerkin method. This method frequently leads to symmetric matrices and recovers the previously analyzed principal of virtual work. For example, if \( \mathbf{A}(\mathbf{u}) = 0 \) represents the equilibrium equation \( \text{Div} \ \mathbf{\sigma} = 0 \) and the arbitrary function \( \tilde{\mathbf{w}}_j = \mathbf{N}_j \) coincides with the variation \( \delta \mathbf{u} \) the integral form (5.13) is equivalent to the principle of virtual work (5.4) and the weak form of the equilibrium equation. Similarly, the principal of virtual work (5.6) for a material governed by (3.52) is equivalent to the method of Galerkin. Due to these and other reasons we adopt in our work the Galerkin method.

Another method is based on extremizing a known functional \( \psi \), which can generically be written as

\[
\delta \psi = \int_D \mathbf{A}(\mathbf{u}) \cdot \delta \mathbf{u} \, dV + \int_{\partial D} \mathbf{B}(\mathbf{u}) \cdot \delta \mathbf{u} \, dA = 0. \quad (5.14)
\]

This variational statement holds for arbitrary variations \( \delta \mathbf{u} \) and yields in the interior and boundary respectively the equations

\[
\mathbf{A}(\mathbf{u}) = 0 \quad \text{on} \ D, \quad (5.15)
\]

\[
\mathbf{B}(\mathbf{u}) = 0 \quad \text{on} \ \partial D. \quad (5.16)
\]
If the differential operator \( A(u) \) and the operator \( B(u) \) correspond precisely to the differential equation and boundary conditions, the variation is a natural variational principle and equations (5.15) is known as the Euler differential equation of the functional \( \psi \). It is possible to derive from any variational principle a corresponding set of Euler equations. On the other hand not every governing differential equation and its associated boundary conditions are Euler equations of a variational functional. In the case of the governing equation (3.94) of anti-plane shear with natural boundary conditions (3.95) and kinematic boundary conditions (3.86), the functional (3.85) could be the basis for a formulation with finite elements. The augmented theory discussed in Chapter 3.7 contains terms proportional to the rate of strain, so that the governing equation (3.100) has no natural variational principle. This problem arises rather commonly in engineering and physics. A more complete account of the finite element method can be found in [25, 77, 90, 91].

5.2 Numerical implementation of the augmented theory

The general methodology of the finite element method is now applied to the augmented theory summarized in Section 3.7 for an anti-plane shear deformation \( u(x_1, x_2, t) \) along the \( x_3 \)-axis. The displacement \( u \) is defined on the two-dimensional domain \( \Pi \) which is spanned by the unit vectors \( e_\alpha \). The combined governing differential equation is

\[
\left( T_{3\alpha}^s + \frac{1}{2} \varepsilon_{3\alpha\beta} M_{\beta\gamma\gamma}^d \right)_{,\alpha} = 0 \quad \text{on } \Pi, \tag{5.17}
\]

with boundary conditions

\[
\begin{aligned}
\begin{cases}
    u = \hat{u} & \text{on } \partial \Pi_1, \\
    \frac{\partial u}{\partial n} = \hat{\Theta} & \text{on } \partial \Pi_3, \\
    T_{\alpha\beta} n_\beta - \frac{\partial}{\partial s} \left( \frac{1}{2} M_{\alpha\beta}^d n_\alpha n_\beta \right) = \hat{t} & \text{on } \partial \Pi_2, \\
    -\frac{1}{2} M_{\alpha\beta}^d s_\alpha n_\beta = \hat{m} & \text{on } \partial \Pi_4.
\end{cases}
\end{aligned} \tag{5.18}
\]
The functions $\dot{u}$, $\dot{\Theta}$, $\dot{t}$, and $\dot{m}$ are prescribed on their respective boundary segments such that $\partial \Pi_1 \cup \partial \Pi_2 = \partial \Pi_3 \cup \partial \Pi_4 = \partial \Pi$. The essential components of the symmetric stress tensor $T^s$, the antisymmetric stress tensor $T^{ad}$, the total stress tensor $T$, and the deviatoric couple stress tensor $M^d$ are given by

$$T^s_{3\alpha} = \mathcal{M}(k) u_{,\alpha} + \nu \dot{u}_{,\alpha}, \quad T^{ad}_{3\alpha} = \frac{1}{2} \epsilon_{3\alpha\beta} M^d_{\beta \gamma, \gamma}, \quad T_{3\alpha} = T^{ad}_{3\alpha} + T^s_{3\alpha},$$

(5.19)

$$M_{\alpha \beta}^d = -2 \lambda \epsilon_{3\gamma \alpha} u_{,\beta}.$$

(5.20)

We choose to base our numerical formulation on the combined equation of motion (5.17), since it affords a nearly parallel development to the variational statement of Chapter 3.6. Nevertheless, several different possibilities are viable which will yield the same integral form of (5.17) and (5.18). To formulate the finite element method we follow the recipe outlined by equations (5.7) to (5.13) and first concern ourselves solely with the integral form of (5.17), we will later on include the integral statement of the boundary conditions (5.18). The governing equation (5.17) is multiplied by the arbitrary weighting function

$$w(x_1, x_2) = w_3(x_1, x_2),$$

(5.21)

which also can be thought of as a variation of the displacement component $u$ along the $x_3$-axis. Upon integrating this expression we attain the integral statement

$$\int_\Pi \left\{ T^s_{3\alpha, \alpha} + \frac{1}{2} \epsilon_{3\alpha\beta} M^d_{\beta \gamma, \gamma} \right\} w \ dA = 0,$$

(5.22)

that embodies the framework laid down by (5.9). Integrating the first term of (5.22) once by parts, and the second term twice by parts (followed each time by the use of the divergence theorem) yields

$$0 = -\int_\Pi T^s_{3\alpha} w_{,\alpha} \ dA + \int_\Pi \frac{1}{2} \epsilon_{3\alpha\beta} M^d_{\beta \gamma} w_{,\gamma} \ dA$$

$$+ \int_{\partial \Pi} \left\{ T^s_{3\alpha} + T^{ad}_{3\alpha} \right\} n_{\alpha} \ w \ ds - \int_{\partial \Pi} \frac{1}{2} \epsilon_{3\alpha\beta} M^d_{\beta \gamma} n_{\gamma} \ w_{,\alpha} \ ds.$$  

(5.23)

To proceed further one decomposes the derivative $w_{,\alpha}$ along the boundary $\partial \Pi$ into a component along the outward unit normal $n$ and the unit tangent $s$ by using

$$w_{,\alpha} = \left( \frac{\partial w}{\partial n} \right) n_{\alpha} + \left( \frac{\partial w}{\partial s} \right) s_{\alpha}.$$  

(5.24)
A direct calculation employing (5.24) on the last boundary integral of (5.23) transforms the weak form (5.23) into

\[
0 = -\int_{\Pi} T^s_{3a} w_{,\alpha} \, dA + \int_{\Pi} \frac{1}{2} \varepsilon_{\alpha\beta} M^{d}_{\beta\gamma} w_{,\alpha\gamma} \, dA \\
+ \int_{\partial \Pi} \left\{ \left( T^s_{3a} + T^{ad}_{3a} \right) n_{\alpha} - \frac{\partial}{\partial s} \left( \frac{1}{2} M^{d}_{\alpha\beta} n_{\alpha} n_{\beta} \right) \right\} w \, ds \\
- \int_{\partial \Pi} \left\{ \frac{1}{2} M^{d}_{\alpha\beta} s_{\alpha} n_{\beta} \right\} \frac{\partial w}{\partial n} \, ds.
\]  
(5.25)

A more detailed account of a similar calculation can be found in Chapter 3.6, where we used the decomposition to transform (3.88) into (3.93). Next the integral statement of the boundary conditions is defined by multiplying the natural boundary conditions on \( \partial \Pi_2 \) and \( \partial \Pi_4 \) of (5.18) with the weighting function \( \bar{w} \). Since \( \bar{w} \) and \( w \) are both arbitrary we can choose without any loss of generality

\[
\bar{w} = -w.
\]  
(5.26)

Integrating these two equations over their respective boundary segments and adding the results to (5.25) yields

\[
0 = -\int_{\Pi} T^s_{3a} w_{,\alpha} \, dA + \int_{\Pi} \frac{1}{2} \varepsilon_{\alpha\beta} M^{d}_{\beta\gamma} w_{,\alpha\gamma} \, dA \\
+ \int_{\partial \Pi} \left\{ \left( T^s_{3a} + T^{ad}_{3a} \right) n_{\alpha} - \frac{\partial}{\partial s} \left( \frac{1}{2} M^{d}_{\alpha\beta} n_{\alpha} n_{\beta} \right) \right\} w \, ds \\
- \int_{\partial \Pi_2} \left\{ \left( T^s_{3a} + T^{ad}_{3a} \right) n_{\alpha} - \frac{\partial}{\partial s} \left( \frac{1}{2} M^{d}_{\alpha\beta} n_{\alpha} n_{\beta} \right) - \hat{i} \right\} w \, ds \\
- \int_{\partial \Pi_2} \left\{ \frac{1}{2} M^{d}_{\alpha\beta} s_{\alpha} n_{\beta} \right\} \frac{\partial w}{\partial n} \, ds \\
- \int_{\partial \Pi_4} \left\{ \frac{1}{2} M^{d}_{\alpha\beta} s_{\alpha} n_{\beta} + \hat{m} \right\} \frac{\partial w}{\partial n} \, ds.
\]  
(5.27)

Upon collecting the common boundary terms and realizing that the essential boundary conditions on \( \partial \Pi_1 \) and \( \partial \Pi_3 \) can be automatically satisfied by the proper choice of \( u \) and \( \frac{\partial u}{\partial n} \), equation (5.27) can be written as

\[
0 = \int_{\Pi} T^s_{3a} w_{,\alpha} \, dA + \int_{\Pi} \frac{1}{2} \varepsilon_{\alpha\beta} M^{d}_{\beta\gamma} w_{,\alpha\gamma} \, dA \\
- \int_{\partial \Pi_2} \hat{i} w \, ds - \int_{\partial \Pi_4} \hat{m} \frac{\partial w}{\partial n} \, ds \\
- \int_{\partial \Pi_1} \left\{ \left( T^s_{3a} + T^{ad}_{3a} \right) n_{\alpha} - \frac{\partial}{\partial s} \left( \frac{1}{2} M^{d}_{\alpha\beta} n_{\alpha} n_{\beta} \right) \right\} w \, ds \\
- \int_{\partial \Pi_3} \left\{ \frac{1}{2} M^{d}_{\alpha\beta} s_{\alpha} n_{\beta} \right\} \frac{\partial w}{\partial n} \, ds.
\]  
(5.28)
We note that the variables $u$ and $\frac{\partial u}{\partial n}$ have disappeared along the boundary integrals taken along the segments $\partial \Pi_1$ and $\partial \Pi_3$ and that both natural boundary conditions along $\partial \Pi_2$ and $\partial \Pi_4$ are automatically satisfied. In addition if the choice of $w$ and $\frac{\partial w}{\partial n}$ is restricted such that $u = \hat{u}$ on $\partial \Pi_1$ and $\frac{\partial u}{\partial n} = \hat{\Theta}$ on $\partial \Pi_3$ we can omit the last two terms of (5.28) by restricting the choice of weighting functions which give $w = 0$ on $\partial \Pi_1$ and $\frac{\partial w}{\partial n} = 0$ on $\partial \Pi_3$. Let us now assume that $w$ is a function satisfying the cited criteria. Then by introducing the constitutive assumptions of (5.19-5.20) the integral statement (5.28) takes on the form

$$\int_\Pi \left\{ (M(k) u,_{\alpha} + \nu \hat{u},_{\alpha}) w,_{\alpha} - \lambda u,_{\alpha\beta}w,_{\alpha\beta} \right\} dA - \int_{\partial \Pi_2} \hat{t} w \, ds - \int_{\partial \Pi_4} \hat{m} \frac{\partial w}{\partial n} \, ds = 0. \tag{5.29}$$

If the approximation of (5.3) is now taken as

$$u \approx \hat{u} = N(x_1, x_2) a(t), \tag{5.30}$$

and the arbitrary weighting function $w$ as

$$w = N^T, \tag{5.31}$$

where $N$ is such that the previous conditions hold, the final form of the integral statement (5.29) can then be summarized by the matrix equation

$$b = [B + K] a + C \dot{a}. \tag{5.32}$$

The matrices $B$, $C$ and $K$ are obtained by replacing, as suggested in (5.5), all integrals on the domain $\Pi$ with the sum of element integrals

$$B = \sum B^e, \quad B^e = \int_{\Pi^e} M(k) \nabla N_i \cdot \nabla N_j \, dA, \tag{5.33}$$

$$C = \sum C^e, \quad C^e = \int_{\Pi^e} \nu \nabla N_i \cdot \nabla N_j \, dA, \tag{5.34}$$

$$K = \sum K^e, \quad K^e = \int_{\Pi^e} \lambda N_i,_{\alpha\beta} N_j,_{\alpha\beta} \, dA, \tag{5.35}$$

and on the boundary the traction $\hat{t}$ and the couple vector $\hat{m}$ are given by

$$b = \sum b_i, \quad b_i = \int_{\partial \Pi_2} \hat{t} N_i \, ds + \int_{\partial \Pi_4} \hat{m} \frac{\partial N_i}{\partial n} \, ds. \tag{5.36}$$
It is obvious that an element of $C_1$ continuity is needed to compute contributions of (5.35) and of (5.36) due to the couple $\hat{n}$. Further on, a term by term inspection shows that from a numerical point of view the integral form (5.29) imposes the same restrictions on the element as the irreducible thin plate formulation. In the next section we will specify the element that we use and take advantage of this analogy.

5.3 A $C_1$ element for an anti-plane shear deformation

The development of an element for anti-plane shear with couple stress effects is considerably simplified when exploiting the similarities with the irreducible thin plate approximation, since an extensive amount of research has been conducted in this field, and several elements exist which perform well in this kind of application. In both formulations the element has to satisfy in the interior at least continuity of the displacement and its first partial derivatives. Along the element's boundary the displacement has to be continuous and the normal derivative along the sides must be continuous among neighboring elements. This later criteria is rather difficult to satisfy, specifically with quadrilaterals as some examples in [25] illustrate. A comparison among different types of those elements under bending can be found in [91] and for three-node plate bending elements a comprehensive performance evaluation is summarized in [16]. Hence, we will consider only triangular elements with straight sides. An obvious choice that should satisfy the previous criteria is a triangle with a node at each vertex of 3 degrees of freedom and a central node with a single degree of freedom. Thus 10 independent parameters can be specified and a complete cubic polynomial be used. It was found that an element derived on this basis does not converge (see [91]).

In this work we shall consider an element of 9 degrees of freedom with 3 nodes. This element has at each node the 3 nodal variables

$$\alpha_i^e = \left[ u, \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2} \right]^T, \quad i = 1 \text{ to } 3, \quad (5.37)$$

accounting for 3 degrees of freedoms at each node. The set of three such nodes comprises
the nodal vector $\mathbf{a}^e$:

$$
\mathbf{a}^e = [a_1^e, a_2^e, a_3^e]^T.
$$

(5.38)

Following ZIENKIEWICS & TAYLOR a polynomial expression utilizing the area coordinates $L_i$ is used to define the shape functions in terms of the 9 nodal variables. The area coordinates are the ratios of the area of the three individual triangles with respect to the total triangle. The individual triangles are formed by connecting the vertices of the element to an arbitrary internal point $P$. The element depicted in Figure 5.1 would have the area coordinates

$$
L_1 = \frac{\text{area } P23}{\text{area } 123}, \quad L_2 = \frac{\text{area } P13}{\text{area } 123}, \quad L_3 = \frac{\text{area } P12}{\text{area } 123}.
$$

(5.39)

Although three coordinates are specified it is obvious that only two independent coordinates exist

$$
L_1 + L_2 + L_3 = 1.
$$

(5.40)

From the total of 10 terms of the complete cubic, the following terms were chosen to approximate the displacement function $u$ as

$$
\hat{u} = \alpha_1 L_1 + \alpha_2 L_2 + \alpha_3 L_3 + \alpha_4 L_1 L_2 + \alpha_5 L_2 L_3
+ \alpha_6 L_1 L_3 + \alpha_7 L_1^2 L_2 + \alpha_8 L_2^2 L_3 + \alpha_9 L_1 L_2^2,
$$

(5.41)

where the $\alpha$'s are free parameters to be determined. By proceeding in a standard manner
the nine \( \alpha \)'s can be related to the nodal variable \( \alpha^e \) and the approximation \( \hat{u} \) becomes

\[
\hat{u} = \sum_{i=1}^{3} N_i a_i. \tag{5.42}
\]

It is possible to add the cubic function \( L_i L_j L_k \) with zero values and slopes at all three corners to any of the nine shape functions \( N_i \):

\[
N_i^T = \begin{cases} 
N_i^1 \\
N_i^2 \\
N_i^3 
\end{cases} = \begin{cases} 
3L_i^2 - L_i^3 + 2L_iL_jL_k \\
-c_j (L_i^2 L_k + L_iL_jL_k) + c_k L_i^2 L_j \\
b_j (L_i^2 L_k + L_iL_jL_k) - b_k L_i^2 L_j 
\end{cases}, \tag{5.43}
\]

where the parameters \( b_i \) and \( c_i \) are

\[
b_i = (x_1)_j - (x_2)_k, \quad c_i = (x_1)_k - (x_2)_j, \tag{5.44}
\]

and \( i, j, k \) are the cyclic permutations of 1, 2, 3. Thus each set of nodal variables \( \alpha^e_i \) multiplies the set of three shape functions of (5.43) to yield the sum of nine terms of (5.42). The gradient of \( N \) is determined by differentiating each shape function with respect to the coordinates \( x_1 \) and \( x_2 \) by using the chain rule

\[
\frac{\partial}{\partial x_\alpha} = \frac{\partial L_j}{\partial x_\alpha} \frac{\partial}{\partial L_j}, \tag{5.45}
\]

with \( j \) having the range 1 to 3.

It was found that the integrals encountered in (5.33-5.35) can be evaluated with sufficient accuracy by using a 3-point Gaussian quadrature, with three Gauss points along the sides midway to each node. The calculated values were equivalent to those obtained by a direct integration. The element passes the test of uniform convergence for several problems with respect to an analytical solution. XIA & HUTCHINSON [88] apply the element successfully to the strain gradient theory of plasticity. Nevertheless, it is known that for problems of bending the element only satisfies the patch test fully for equilateral triangles, despite this shortcoming it is very popular and readily available from the literature. We will assess the question of accuracy and verification in a later section.
5.4 Constitutive relation and nonlinearities

We now consider the time evolution of the nonlinear set of first order differential equations given in matrix notation by (5.32). The nonlinear term is due to the elastic stress contribution $\mathcal{M}(k)u,\alpha$ of $T_{3\alpha}^s$, and by requiring a nonmonotonic stress-strain relation $\hat{\tau}(k)$ the material can sustain solid to solid interfaces. In Chapter 4 we constructed a trilinear material with an intermediate range of strain $(\gamma_M, \gamma_m)$ of negative slope. This material has discontinuous slopes at the strains $\gamma_M$ and $\gamma_m$, and leads to mathematical simplifications which make it convenient to use in analytical studies. When implemented into numerical studies however the discontinuities of $\hat{\tau}(\gamma)$ can lead to grid size oscillations. It is therefore preferable to replace the trilinear material with a response function $\hat{\tau}(k)$ with at least continuous first derivatives. This function $\hat{\tau}(k)$ contains a higher order polynomial and a linear extension at

![Figure 5.2: The used stress strain relation $\hat{\tau}(k)$](image)

an inflexion point for a strain greater than \( k_* (k_* > k_m) \):

\[
\hat{\tau}(k) = \begin{cases} 
\mu k + a k^3 + b k^5 + c k^7 & \text{for } 0 < k \leq k_*, \\
\ell_* k + a_* & \text{for } k > k_*. 
\end{cases} 
\] (5.46)

The material parameters are chosen so as to ensure that for \( k > 0 \) the function \( \hat{\tau}(k) \):

(I) the function is twice continuously differentiable,

(II) has a local maximum at some positive strain \( k = k_M \),

(III) has a local minimum at some strain \( k = k_m \in (k_M, k_*) \),

(IV) has no further extrema for \( k > 0 \).

In our numerical calculations the response function \( \hat{\tau}(k) \) is characterized by the following values for the parameters \( a = -181 \mu; b = 12,233 \mu; c = -241,875 \mu; k_* = 0.135; \mu_* = 1.1825 \mu; \) and \( a_* = -0.118575 \mu \). This leads to the depicted stress strain relation in Figure 5.2. The nonlinear nature of the problem requires an iterative scheme or Newton-Raphson method.

To attain results of sufficient accuracy the commonly employed forward and backward difference method of order \( \Delta t \) were found to be inaccurate, and a Predictor Corrector method was implemented. The predictor is based on an implicit three level Adams-Moulton method and the corrector, an accuracy controlled and slightly modified single implicit method. The modification only involves the computation of the secant modulus as given by equation (3.80) as

\[
\mathcal{M}(k) = \frac{\hat{\tau}(k)}{k}, \tag{5.47}
\]

where the strain \( k \) of (5.47) is defined as the average strain in the corresponding element.

To start the multi-level predictor corrector method a two-level method is used. It is based on a linear interpolation between weighted forward and backward steps in time

\[
a^{k+\theta} = \theta a^{k+1} + (1 - \theta) a^k, \quad 0 \leq \theta \leq 1. \tag{5.48}
\]
The time derivative $\dot{a}$ of (5.32) is replaced by the first order approximation

$$
\dot{a} = \frac{a^{k+1} - a^k}{\Delta t}.
$$

(5.49)

The set of differential equations (5.32) can now, with the aid of (5.48-5.49), be written as the set of difference equations

$$
[C + \theta \Delta t \{B + K\}] a^{k+1} = [C - (1 - \theta) \Delta t \{B + K\}] a^k + \Delta t b,
$$

(5.50)

with the nonlinear matrix $B$ being evaluated at the $k$th time level. The linearized version of this equation is considered to be implicit for $\theta = 1$ and explicit for $\theta = 0$. To improve the accuracy we choose for the two initial steps $\theta = 0.5$, which recovers for the linearized equation the trapezoidal rule of $O(\Delta t^2)$. A similar algorithm is used in the corrector step, except that $\theta = 1$ and the nonlinear term $M(k)$ is computed as

$$
M(k) = \frac{M(k_{i-1}) + 2M(k_i)}{3},
$$

(5.51)

where $k_{i-1}$ is the total shear strain of the previous corrector step and $k_i$ the total strain of the current corrector step. Thus for the first corrector step $i = 1$ one specifies $M(k) = M(k_F)$ with $k_F$ being the total strain of the last predictor step. This interpolation guarantees a stable uniform convergence for all solved problems. By reducing the back loading of $M(k)$ the rate of convergence is increased but two step gridsize oscillation in time are observed at certain loadings. The predictor that evolves the solution in time is based on the Adams-Moulton method, and takes for equation (5.32) the following form on

$$
[C + \frac{9}{24} \Delta t \{B + K\}] a^{k+1} = \left[ C - \frac{10}{24} \Delta t \{B + K\} \right] a^k \\
+ \left[ \frac{5}{24} \Delta t \{B + K\} \right] a^{k-1} \\
+ \left[ \frac{1}{24} \Delta t \{B + K\} \right] a^{k-2},
$$

(5.52)

where the terms multiplying the $a^{k-i}$ terms have to be computed at the corresponding time levels. The accuracy controlled corrector algorithm iterates on the $a^k$ solution computed by the predictor as long as the relative error on the overall domain is pointwise smaller than $10^{-6}$.
and for some problems $10^{-8}$. This rather strict criterion also includes the nodal derivatives. Several predictor corrector methods, like Heun's Method and Adams-Bashforth-Moulton were tried. None of them were able to stably propagate the solution, without accuracy control. The introduced method is easier to implement and sufficiently fast for weak nonlinearities. The rate of convergence decreases at the instant of the nucleation of an additional phase.

5.5 Verification

In this section we describe the implementation, accuracy, and verification of the numerical method of above. Since the program is not based on a commercial platform, and most contents are programmed by the author, several basic tests were carried out. The programming methodology is briefly summarized as follows. The main mathematical contents of any FEM program are the specification of the shape function and their numerical integration. All these essential ingredients were developed on the symbolic mathematics program Maple and exported into finally used code lines. These building blocks were individually checked by comparing attained results to calculations performed mostly on Maple. We checked for arbitrarily chosen single triangles the values of the shape functions and its derivatives, and compared typical matrices like $K$ and $C$ to analytical results. Each subroutine was first checked in an individual program mimicking the task and the needed interfaces. The computed results were whenever possible compared to analytical solutions. The numbering schemes of local nodes, global nodes, and equations were implemented through pretested routines of the FEM-group of Bathe.

Some verification problems testing the overall performance of the program were carried out. We will now summarize the results of some tests to evaluate the convergence. We understand under uniform convergence that the relative numerical error with respect to a known analytical solution is reduced by a power law of the form $(\Delta h)^{-p}$ with $p > 0$. The characteristic length scale $\Delta h$ is the largest side length of the triangular element. For this
purpose let us consider a rectangular domain $\Pi$ with $x_1 \in (0, 1)$ and $x_2 \in (0, 1)$. The anti-plane shear deformation $u$ along the $x_3-$ direction is assumed to satisfy the governing differential equation

$$\nabla^2 u = P(x_1, x_2) \quad \text{on } \Pi,$$

(5.53)

where the right hand side is some externally applied body force, say,

$$P(x_1, x_2) = \sin \pi x_1 \sin \pi x_2,$$

(5.54)

modeling the forced response of a linearly elastic material. We specify for Poision’s equation (5.53) the boundary condition

$$u = 0 \quad \text{on } \partial \Pi,$$

(5.55)

and found the solution to be

$$u = -\frac{1}{2 \pi^2} \sin \pi x_1 \sin \pi x_2.$$  

(5.56)

When solving this problem numerically integrals of the form

$$C^e = \int_{\Pi^e} \nabla N_i \cdot \nabla N_j \, dA,$$

$$f^e = \int_{\Pi^e} P(x_1, x_2) N_i \, dA,$$

have to be calculated. The second order partial differential equation (5.53) allows us to evaluate the performance of the nine degree of freedom element of continuity $C_1$ for problems that only require $C_0$ continuity. Thus the term associated with the higher order boundary conditions remain undetermined and $m = 0$. Several numerical experiments yield a uniform convergence with an exponent of $p = 1.74$. In addition, a problem on a circular domain with circular hole was used to verify the code.

Similarly, we evaluated the program’s capability to solve the 4th order governing equation for $u(r, \phi)$

$$\nabla^2 \nabla^2 u = 0 \quad \text{on } \Pi,$$

(5.57)
with \( \Pi \) being the circular domain with \( r \in (a, b) \). The governing equation (5.57) requires to specify the boundary conditions

\[
\begin{align*}
\begin{aligned}
    u(a, \phi) &= 0, \\
    \hat{m}(a, \phi) &= 0, \\
    u(b, \phi) &= \Delta, \\
    \hat{m}(b, \phi) &= 0,
\end{aligned}
\end{align*}
\] (5.58)

where \( \Delta \) is some constant displacement. By comparing the analytical solution to the numerical computation, for which integrals given by \( K \) have to be evaluated the error is minimal and a uniform convergence with slope \( p = 3.24 \) is found. Several other test problems commonly cited in the literature for plate elements yielded comparable results.

Next we analyze the test problem governed by the differential equation

\[
\nabla^2 u + \nabla^2 \dot{u} + D \nabla^2 \nabla^2 u = 0 \quad \text{on} \quad \Pi,
\] (5.59)

where \( \Pi \) is a square domain with side length 1 and \( x_\alpha \in (0, 1) \). Equation (5.59) models an augmented material with linear stress strain relation and an anti-plane shear deformation \( u(x_1, x_2, t) \). The associated boundary conditions were chosen as

\[
\begin{align*}
\begin{aligned}
    u(0, x_2) &= 0, \\
    \frac{\partial u(0, x_2)}{\partial n} &= 0, \\
    u(1, x_2) &= 0, \\
    \frac{\partial u(1, x_2)}{\partial n} &= \hat{\Theta}, \\
    u(x_1, 0) &= 0, \\
    \frac{\partial u(x_1, 0)}{\partial n} &= 0, \\
    u(x_1, 1) &= 0, \\
    \frac{\partial u(x_1, 1)}{\partial n} &= 0,
\end{aligned}
\end{align*}
\] (5.60)

with the forcing of the slope at \( x_1 = 1 \) given by

\[
\hat{\Theta} = -\pi e^{-(1+2\pi^2 D)t} \sin \pi x_2,
\] (5.61)
so that the general solution of (5.59), (5.60) is

\[ u = u(x_1, x_2, t) = e^{-(1+2\pi^2\tau^2)t} \sin \pi x_1 \sin \pi x_2. \]  

(5.62)

The problem has initial conditions at \( t = 0 \):

\[ u = u(x_1, x_2, 0) = \sin \pi x_1 \sin \pi x_2. \]

Based on this analytical solution the overall performance of the numerical method was studied. The 1st order discretization in time was not anymore competitive and causing for example errors of a few percentage points for \( \Delta t = 0.01 \), whereas the higher order AM-method produced errors of better than 0.02%. Clearly, this was to be expected from a linear problem, in which no corrector is necessary. The effectiveness of the corrector for slightly non-linear problems as given by the differential equation (5.17) was satisfactory. When specifying for example a power law material only a few iterations were necessary to attain physically meaningful solutions.
Chapter 6

Description of initial-boundary-value problems

Introduction

In this chapter we will describe the particular initial-boundary-value problems for SMAs that are to be studied. They can be divided into three distinct groups:

1. In the first class of problems we concentrate on the propagation of existing interfaces. They include problems where the interface propagates through a homogeneous body as well as problems where they encounter a particle or cavity as they propagate.

2. In the second set of problems, we focus on the initial nucleation of a new phase at inhomogeneities of different shapes and types. We also examine the development of the new phase soon after it has emerged.

3. Finally, we look at the complete problem of nucleation, development and propagation. From these problems we determine, in particular, the “global” response of the specimen and relate its various characteristics to “local” events.

All of the problems considered are of the anti-plane shear type and are governed by the single partial differential equation (3.100)

$$(\mathcal{M}(k)u_\alpha)_\alpha + \nu \nabla^2 \dot{u} - \lambda \nabla^2 \nabla^2 u = 0, \quad k = |\nabla u| \text{ on } \Pi.$$  \hspace{1cm} (6.1)
We also recall that the material length scale \( l_m \) of (3.99) is defined as

\[
l_m = \sqrt{\frac{\lambda}{\mu}},
\]

where \( \mu = M(0) \) is the infinitesimal shear modulus of the material and \( \lambda \) is the strain-gradient parameter.

When the cross-section of the body occupies an infinite region and it contains a single inhomogeneity, the only additional length scale admitted in the problem is the size of the void or particle. On the other hand, suppose for example that the body has a periodic distribution of inhomogeneities with a square unit cell of length \( L \) and circular inclusions of radius \( R \). It is then convenient to introduce the volume fraction \( V_f \)

\[
V_f = \frac{\pi R^2}{L^2}
\]  
(6.2)

as a parameter.

For each problem, the domain \( \Pi \) and the boundary conditions on \( \partial \Pi \) will be defined as we go along. In all cases the boundary conditions will either be purely kinematic or mixed, and in the latter event the force-type boundary condition will always be \( \hat{m} = 0 \) and/or \( \hat{t} = 0 \). Thus, roughly speaking, the loading is prescribed kinematically and the body may also have some load-free boundaries. Hence, the integral equation (5.32) simplifies to

\[
[B + K]a + C\dot{a} = 0.
\]  
(6.3)

In Chapter 6.1 we will formulate problems that we use in order to study the propagation of an existing interface and its interaction with inclusions of different types. In Chapter 6.2 we will formulate problems where nucleation (and subsequent evolution) are the focus of the study. Specifically, we consider the problem for an inclusion whose cross-section is either circular or slot-like. Then we extend those ideas to a periodic arrangement of rigid fibers as one would find in a composite. In Chapter 6.3 we propose two problems that make extensive use of the developed understanding on the nucleation and propagation of interfaces.
6.1 Propagation of an interface

In Chapter 4 we analytically studied the propagation of a planar phase boundary in an infinite *homogeneous* medium, and inferred from it the effective kinetic relation associated with couple-stress theory. We now consider a similar problem numerically but with the trilinear constitutive relation being replaced by a polynomial and with the body being either homogeneous (Sub-Section 6.1.1) or containing an inclusion (Sub-Section 6.1.2).

6.1.1 Propagation in a homogeneous medium

First, for benchmark purposes, we will consider the propagation of a phase boundary in a homogeneous body. Couple-stress effects are retained.

The domain \( \Pi \) is taken to be a rectangle, \(-w/2 < x_1 < w/2, -L/2 < x_2 < L/2 \) with \( L \) taken to be sufficiently large to model an infinite strip. The body is loaded by prescribing the displacement at \( u(x_1, L/2, t) \) and holding the opposite side fixed: \( u(x_1, -L/2, t) = 0 \).

The long sides of the domain are traction-free so that

\[
\hat{t} = 0 \quad \text{on} \quad x_1 = \pm \frac{w}{2}, \quad -L/2 < x_2 < L/2, \quad (6.4)
\]

The additional boundary conditions which must be imposed due to couple-stress effects are taken to be

\[
\frac{\partial u}{\partial n} = 0 \quad \text{on} \quad x_1 = \pm \frac{w}{2}, \quad -L/2 < x_2 < L/2, \quad (6.5)
\]

\[
\hat{m} = 0 \quad \text{on} \quad x_2 = \pm \frac{L}{2} - w/2 < x_2 < w/2. \quad (6.6)
\]

The prescribed loading on the top surface \( x_2 = L/2 \) is to be a saw-tooth loading with

\[
u(x_1, L/2, t) = \frac{\dot{a}L}{2} t + u_0 \quad \text{for} \quad 0 < t < t^* . \quad (6.7)
\]

The shearing rate \( \dot{a} \) changes sign at the instants \( t = nt^* \), \( n = 1, 2, \ldots \)

The initial conditions from which the body starts approximate a state in which there
exists a single phase boundary parallel to a short side of the domain:
\[
    u(x_1, x_2, 0) = \begin{cases} 
        \tilde{k} x_2, & -\frac{L}{2} < x_1 < \frac{L}{2}, \quad -\frac{L}{2} < x_2 < s, \\
        \frac{\tilde{k}}{k} x_2 + (\tilde{k} - \frac{\tilde{k}}{k})s, & -\frac{L}{2} < x_1 < \frac{L}{2}, \quad s < x_2 < \frac{L}{2},
    \end{cases}
\] (6.8)

where \(x_2 = s\) is the given initial location of the interface, and \(\frac{\tilde{k}}{k}\) are the shear strains on either side of it. Given the shear stress \(\tau \in (\tau_m, \tau_M)\), the corresponding martensitic shear strain \(\frac{\tilde{k}}{k}\) and austenitic shear strain \(\tilde{k}\) are calculated through the constitutive relation \(\tau = \tilde{\tau}(\frac{\tilde{k}}{k}) = \tilde{\tau}(\tilde{k})\); for our calculations we took the Maxwell stress \(\tau = \tau_0\). The initial state describes an exact equilibrium configuration within the sharp interface theory but it does not precisely describe an equilibrium state in the couple-stress theory. The field given by (6.8) is therefore numerically annealed to attain a field that satisfies the governing equation (6.1) and boundary conditions (6.4), (6.5), (6.6) at \(t = 0\). The annealed sharp interface of (6.8) is now an equilibrated and smoothed out interface, serving as the initial condition for our calculations. The upper boundary is now displaced by an amount \(u_0 = \frac{\tilde{k}}{k} L/2 + (\tilde{k} - \frac{\tilde{k}}{k})s\). The saw-tooth load is now applied starting from this reference state.

We will carry out various such programs of loading and/or unloading at various loading rates \(\dot{a}\).

We will calculate and plot graphs of the applied displacement \(\delta(t) = u(x_1, L/2, t)\) versus the corresponding average shear stress
\[
    \tau(t) =< T_{32} > = \frac{1}{L} \int_{-L/2}^{L/2} T_{32}(x_1, L/2, t) \, dx_1.
\] (6.9)

In order to determine the effective kinetic relation (in the present problem and in all subsequent problems) we proceed as follows: let \(P_D\) denote the overall rate of energy dissipation (per unit thickness) in the entire specimen. For all of the problems that we will consider, the couple stress boundary conditions are such that at each point on \(\partial \Pi\), either the prescribed couple \(\dot{n} = 0\) or the rate of change of \(\frac{\partial u}{\partial n}\) is zero. Thus, the rate of dissipation \(P_D\) may be defined by
\[
    P_D = \int_{\partial \Pi} t \dot{u} \, ds - \frac{d}{dt} \int_{\Pi} \phi \, dA,
\] (6.10)
where $t = T_\alpha n_\alpha$ with $T_\alpha$ given by (3.102); $\phi = W(k) + 2\lambda \kappa_\alpha \kappa_\beta$; $k = |\nabla u|$; and $\kappa_\alpha = -\frac{1}{2} \varepsilon_{\gamma\beta} u_{\gamma\alpha}$. One can readily show by using the field equations that $P_D$ can equivalently be written as

$$P_D = \int_{\Pi} \nu |\nabla \dot{u}|^2 \, dA. \tag{6.11}$$

In the present problem, the interface is straight and propagates entirely in the $x_2$ direction. The effective driving traction may thus be defined by

$$f = \frac{P_D}{V_n w}, \tag{6.12}$$

where $V_n$ is the propagation speed. When we compute $f$ and $V_n$ the interface will be propagating at a constant speed and $f$ will also be constant.

### 6.1.2 Propagation across an inhomogeneity

This next investigation will examine the role of inhomogeneities as obstacles to phase boundary propagation. In particular it will examine the effective kinetic relation when the body contains obstacles in the path of the propagating phase boundary. Figure 6.1 shows a schematic description of the problem.

Suppose that the cross-section $\Pi$ is a rectangle of dimensions $L \times 2L$; the longer length $2L$ here allows us to examine the propagation of the phase boundary over a greater length.
The body contains a concentric circular inclusion of radius $R$ which may either be a rigid particle or a cavity.

In order to motivate the boundary conditions which we will apply it is helpful to first consider the case where the body does not contain an inclusion and the material does not have couple-stress effects. A piecewise homogeneous displacement field which describes the steady downward motion of a planar phase boundary (location $x_2 = s(t)$, velocity $V_n > 0$) is described by equation (6.8), where

$$s = s(t) = \frac{L}{2} - V_nt.$$  

(6.13)

and the propagation velocity $V_n$ must be related to the stress $\tau$ through the kinetic relation.

This suggests that in the inclusion problem we prescribe the following boundary conditions on the outer boundary:

$$u = \begin{cases} 
\bar{k} x_2, & x_1 = \pm \frac{L}{2}, \ -L < x_2 < s(t), \\
\frac{\bar{k}}{k} x_2 + (\bar{k} - \frac{\bar{k}}{k}) s(t), & x_1 = \pm \frac{L}{2}, \ s(t) < x_2 < L, \\
\frac{\bar{k}}{k} \frac{L}{2} + (\bar{k} - \frac{\bar{k}}{k}) s(t), & x_2 = L, \ -\frac{L}{2} < x_1 < \frac{L}{2}, \\
-\frac{\bar{k}}{k} \frac{L}{2}, & x_2 = -L, \ -\frac{L}{2} < x_1 < \frac{L}{2},
\end{cases}$$

(6.14)

with $\tau$ prescribed, $V_n$ chosen consistently from the kinetic relation, and with $s(t), \frac{\bar{k}}{k}, \bar{k}$ given as discussed in the previous section. In this case the phase boundary will not be planar because of the inclusion. If the inclusion size is small compared to $L$ then near the right and left edges of the domain the phase boundary will be straight and horizontal and will deviate from this only in the central region. (The additional boundary conditions which must be prescribed because of couple stress effects depend on whether the inclusion is a particle or a cavity and will be described below.)

Once the initial-boundary-value problem has been solved, we then calculate the effective kinetic relation in the following manner: we first calculate the total energy dissipated during the process of propagating the phase boundary all the way across the entire cell. From this
we determine an averaged rate of dissipation, and hence an averaged value for the effective driving traction. By repeating the calculation for different values of the prescribed propagation speed \( V_n \) and/or stress \( \tau \), we are able to determine pairs of values for the propagation speed and the driving traction. This leads to the desired effective kinetic relation.

More specifically, for each given \( \tau \) and \( V_n \), we solve the initial-boundary-value problems numerically, and calculate the total rate of dissipation (per unit thickness) \( P_D \). The average driving traction \( \langle f \rangle \) is then given by

\[
\langle f \rangle = \frac{1}{V_n L} \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} P_D \, dt,
\]

where \( P_D \) is given by (6.11), the time \( t_0 \) corresponds to the instant when the interface enters the cell, and \( t_1 \) when it leaves the cell.

The specific problems of this type that we will solve are as follows:

**Propagation across a cavity**

When the body contains a circular cavity, we impose

\[
\hat{t} = 0, \quad \hat{m} = 0 \quad \text{on} \quad x_1^2 + x_2^2 = R^2.
\]

The additional boundary-conditions associated with couple-stress effects are

\[
\frac{\partial u}{\partial n} = \begin{cases} 
0, & x_1 = \pm \frac{L}{2}, \quad -L < x_2 < L, \ x_2 \neq s(t), \\
\frac{+}{k}, & x_2 = L, \quad -\frac{L}{2} < x_1 < \frac{L}{2}, \\
\frac{-}{k}, & x_2 = -L, \quad -\frac{L}{2} < x_1 < \frac{L}{2},
\end{cases}
\]

**Propagation across a rigid particle**

When the body contains a rigid particle, we must impose

\[
u = \text{constant}, \quad \hat{m} = 0 \quad \text{on} \quad x_1^2 + x_2^2 = R^2
\]

with global force balance of the particle (in the \( x_3 \)-direction) used to determine the value of this constant rigid translation. We also consider the case of a “fixed” rigid particle with
\( u = 0 \). The supplementary couple-stress boundary-conditions are

\[
\frac{\partial u}{\partial n} = \begin{cases} 
0, & x_1 = \pm \frac{L}{2}, \quad -L < x_2 < L, x_2 \neq s(t), \\
\dfrac{\kappa}{k}, & x_2 = L, \quad -\frac{L}{2} < x_1 < \frac{L}{2}, \\
-\dfrac{\kappa}{k}, & x_2 = -L, \quad -\frac{L}{2} < x_1 < \frac{L}{2}.
\end{cases}
\tag{6.19}
\]

This problem has some similarity with an analogous problem encountered in plasticity. There, particles trap a moving dislocation line and an extra amount of external work is required to free the dislocation and further plastically deform the body.

### 6.2 Nucleation

#### 6.2.1 Rigid particle in an infinite domain

In order to study nucleation at a rigid particle, the following problem was considered: suppose that the cross-section \( \Pi \) is a square, \( L \times L \), and that it contains a concentric rigid circular particle of radius \( R (<< L) \). The outer boundary of the body is subjected to a time dependent simple shear displacement and the inner boundary is held fixed. If the body had not contained the particle, the displacement field everywhere would have been \( u(x_1, x_2) = k_\infty(t)x_2 \) where \( k_\infty(t) \) is the prescribed amount of shear which we take to be a monotonically increasing function of time. By symmetry,

\[
u(x_1, x_2) = u(-x_1, x_2), \quad u(x_1, x_2) = -u(x_1, -x_2) \quad \text{for} \quad (x_1, x_2) \in \Pi.\tag{6.20}
\]

The displacement boundary conditions, as described above, require that on the outer boundary

\[
u = \begin{cases} 
k_\infty(t)x_2, & x_1 = \pm \frac{L}{2}, \\
k_\infty(t)\frac{L}{2}, & x_2 = \frac{L}{2}, \\
-k_\infty(t)\frac{L}{2}, & x_2 = -\frac{L}{2},
\end{cases}
\tag{6.21}
\]

and on the inner boundary

\[
u = 0 \quad \text{on} \quad x_1^2 + x_2^2 = R^2.\tag{6.22}
\]
Additional boundary conditions must be taken in the present couple-stress theory and for these we take

$$\frac{\partial u}{\partial n} = \begin{cases} 
0, & x_1 = \pm \frac{L}{2}, \\
k_{\infty}(t), & x_2 = \frac{L}{2}, \\
-k_{\infty}(t), & x_2 = -\frac{L}{2},
\end{cases} \quad (6.23)$$

on the outer boundary, and along the wall of the particle we take (the natural) boundary condition

$$\hat{m} = 0 \text{ on } x_1^2 + x_2^2 = R^2. \quad (6.24)$$

From the symmetry condition (6.20) one deduces that it is sufficient to perform the calculation on a quarter domain. A simple convergence analysis of the maximum value of strain versus the size of the computational domain $\Pi$ indicated that for domain sizes with $\frac{L}{R} \geq 40$ the finiteness of the body is unimportant and it behaves like an infinite medium. The problem formulated above concerns an infinitely long rigid fiber with circular cross-section loaded in anti-plane shear parallel to its longitudinal axis. It is a commonly studied first approximation for studying a dilute suspension of such inclusions. Additionally, the model serves to qualitatively characterize the effect of an elongated hard inclusion oriented in the $x_3$-axis.

### 6.2.2 Cavity in an infinite domain

This problem is complementary to the previous one, with the rigid cylindrical inclusion replaced by a cavity. The applied simple shear on the outer boundary again requires that

$$u = \begin{cases} 
  k_{\infty}(t)x_2, & x_1 = \pm \frac{L}{2}, \\
k_{\infty}(t)\frac{L}{2}, & x_2 = \frac{L}{2}, \\
-k_{\infty}(t)\frac{L}{2}, & x_2 = -\frac{L}{2},
\end{cases} \quad (6.25)$$

$$\frac{\partial u}{\partial n} = \begin{cases} 
0, & x_1 = \pm \frac{L}{2}, \\
k_{\infty}(t), & x_2 = \frac{L}{2}, \\
-k_{\infty}(t), & x_2 = -\frac{L}{2},
\end{cases} \quad (6.26)$$
whereas the cavity surface is now taken to be traction-free:

\[ \dot{t} = 0, \quad \dot{m} = 0 \quad \text{on} \quad x_1^2 + x_2^2 = R^2. \quad (6.27) \]

Again, the displacement field \( u \) satisfies the symmetry condition (6.20) throughout the whole domain \( \Pi \), allowing the analysis to be carried out on one quarter of the domain. A convergence analysis of the maximum strain versus the size of the computational domain again yields a ratio of \( \frac{L}{R} \geq 40 \) as being sufficiently large to successfully isolate the effects of the cavity.

If the cavity was replaced by an elastic inclusion, we expect that the response would be bounded by the preceding two problems pertaining to the rigid particle and the cavity.

### 6.2.3 Crack in an infinite medium

On the face of it, the problem to be considered here is merely a generalization of the preceding one, with the circular cavity replaced by a slender slot. Indeed, some of our results will take this point of view and address questions of nucleation and growth just as in the previous example. However, the principal purpose of the present problem is to address certain fundamental questions in the couple-stress regularization. Since we have the numerical solution of the sharp interface version of this problem from SILLING [74] and the analytical solution of ABEYARATNE [1] this is a particularly useful setting in which to address these questions.

In particular, as the material length scale \( l_m \) approaches zero, narrow transition layers usually become sharp interfaces. Is this always true? Is it true even when the microstructure is a fine laminate (SILLING) so that the sharp interface is one which goes back and forth a number of times. Or, does the couple-stress theory tend to some averaged solution like that of ABEYARATNE?

The body is again taken to have a square cross-section, \( L \times L \), and it now contains a slender slot (the crack) with its long axis aligned with the \( x_1 \)-axis. The prescribed simple
shear loading again requires on the outer boundary that

\[
\begin{align*}
  u &= \begin{cases} 
    k_\infty(t)x_2, & x_1 = \pm \frac{L}{2}, \\
    k_\infty(t)\frac{L}{2}, & x_2 = \frac{L}{2}, \\
    -k_\infty(t)\frac{L}{2}, & x_2 = -\frac{L}{2}, 
  \end{cases} \\
  \frac{\partial u}{\partial n} &= \begin{cases} 
    0, & x_1 = \pm \frac{L}{2}, \\
    k_\infty(t), & x_2 = \frac{L}{2}, \\
    -k_\infty(t), & x_2 = -\frac{L}{2}, 
  \end{cases}
\end{align*}
\]  

and the load-free condition on the crack surface requires that

\[
\hat{t} = 0, \quad \hat{m} = 0 \quad \text{on} \quad \partial \Pi_c. 
\]  

Here \( \partial \Pi_c \) is the curve which describes the boundary of the slot which is composed of two long straight segments which are parallel to each other and are joined together by two semicircular arcs:

\[
\partial \Pi_c = \{ (x_1, x_2) \mid x_2 = \pm c, \quad -(b - c) < x_1 < (b - c) \} \cup \{ (x_1, x_2) \mid (x_1 - (b - c)) = c \cos \theta, \quad x_2 = c \sin \theta, \quad -\pi/2 < \theta < \pi/2 \} \cup \{ (x_1, x_2) \mid (x_1 + (b - c)) = c \cos \theta, \quad x_2 = c \sin \theta, \quad \pi/2 < \theta < 3\pi/2 \}.
\]  

Thus the slot as shown in Figure 6.2 has an end-to-end length \( 2b \) and a width \( 2c \), \((c << b)\).

Numerical experimentation indicates that an aspect ratio of \( \frac{b}{c} = 50 \) was large enough for our purposes to model a sharp crack by a slender slot. A similar value was found by Silling in his study. Again, symmetry allows us to analyze just one quarter of the domain. In this
case we found that the region II essentially becomes an infinite domain if the ratio $\frac{L}{\delta}$ exceeds about 40.

### 6.2.4 Periodic array of particles

Suppose that one wishes to design a composite, in which the matrix is made of a SMA with a family of aligned stiff fibers which are relatively closely packed, so that the assumption of no mutual interaction does not hold anymore. It is then easy to extend the previous analyses to a periodic arrangement as shown in Figure 6.3. Such a configuration might also describe a periodic arrangement of defects.

We characterize the unit cell II as being a square, $L \times L$ with a concentric particle of cross-sectional radius $R \ (< \frac{L}{2})$. Consider global coordinates $(X_1, X_2)$ for the body and local coordinates $(x_1, x_2)$ for a generic cell. The displacement $u$ obeys the earlier symmetry condition (6.20) within each cell, and globally it obeys the periodicity condition

$$u(X_1, X_2) = u(X_1 + mL, X_2), \quad u(X_1, X_2) = \left\{ \begin{array}{ll}
u(X_1, X_2 + nL) + nC, & X_2 = nL + X_2, \\
u(X_1, X_2 - nL) - nC, & X_2 = -(nL + X_2). \end{array} \right.$$  \hspace{1cm} (6.31)

where $m$ is an integer, $n$ is a non-negative integer and $C$ is a constant; $C$ denotes the difference in displacement between the rigid particle in one cell and the particle of the cell immediately above it.

The global loading is taken to be a simple shear $u = k_\infty(t)X_2$. Periodicity allows one to reduce the problem to a single cell, which we might as well take to be the one centered at the global origin so that $x_\alpha = X_\alpha \forall \ x_\alpha \in (-\frac{L}{2}, \frac{L}{2})$. Thus, the boundary conditions for the unit cell are, that on the outer boundary,

$$u = \left\{ \begin{array}{ll} k_\infty(t)x_2, & x_1 = \pm\frac{L}{2}, \\
k_\infty(t)\frac{L}{2}, & x_2 = \frac{L}{2}, \\
-k_\infty(t)\frac{L}{2}, & x_2 = -\frac{L}{2}. \end{array} \right.$$  \hspace{1cm} (6.32)

and

$$\frac{\partial u}{\partial n} = 0 \text{ on } x_1 = \pm\frac{L}{2}; \quad \hat{m} = 0 \text{ on } x_2 = \pm\frac{L}{2};$$  \hspace{1cm} (6.33)
on the particle wall we have

\[
\begin{align*}
  u & = 0 \text{ on } x_1^2 + x_2^2 = R^2 \\
  \hat{m} & = 0 \text{ on } x_1^2 + x_2^2 = R^2.
\end{align*}
\] (6.34)

Observe that the natural boundary conditions and the supplementary couple-stress bound-

![Diagram of periodic cells and symmetry](image)

Figure 6.3: Schematic of an ideal arrangement of periodic cells and the simplifications attained from periodicity and symmetry arguments.

ary conditions above are consistent with the periodicity assumption (6.31). On taking the symmetry condition (6.20) into account one can further reduce the computational effort to just one quarter of a unit cell. This problem differentiates itself from the preceding problems by having an additional length scale of significance (and this can be explored by examining the dependence of the results on the volume fraction).
In addition, we are able to study the interaction between particles, and therefore the interaction between two regions of nucleation. In presenting the results it is convenient to consider the average applied stress on the boundary of each cell as given by equation (6.9). We will not describe here the corresponding problem associated with a periodic arrangement of cavities since the physical interaction between cells is less intriguing.

### 6.3 Nucleation and growth

In this section we present a problem which incorporates both nucleation and subsequent propagation of interfaces. We consider, as in the preceding set of problems, a body with an inclusion. When the body is loaded the new phase nucleates near the inclusion and then develops, eventually into a band. Continued loading now leads to a propagation of the fronts of the band.

Consider a domain whose cross-section $\Pi$ is a square, $L \times L$, which contains at its center a concentric circular particle or hole of radius $R (<< L)$. The upper and lower sides $x_2 = \pm L/2$ are subjected to a time varying uniform displacement:

$$u = \pm \dot{a} \frac{L}{2} \quad \text{on} \quad x_2 = \pm \frac{L}{2},$$

(6.35)

The rate of shearing $\dot{a}$ is constant. When we wish to consider loading followed by unloading we simply change the sign of $\dot{a}$ at some instant $t^*$. The associated couple-stress boundary condition is taken to be

$$\dot{m} = 0 \quad \text{on} \quad x_2 = \pm \frac{L}{2}.$$  

(6.36)

The two vertical sides of the block are taken to be traction-free:

$$\dot{i} = 0, \quad \dot{m} = 0 \quad \text{on} \quad x_1 = \pm \frac{L}{2}.$$  

(6.37)

The symmetry of the loading and the geometry is expressed by (6.20).
6.3.1 Rigid particle

When the body contains a rigid particle we impose

\[ u = 0, \quad \dot{m} = 0 \quad \text{on} \quad x_1^2 + x_2^2 = R^2. \quad (6.38) \]

6.3.2 Cavity

When the body contains a hole we impose

\[ \dot{i} = 0, \quad \dot{m} = 0 \quad \text{on} \quad x_1^2 + x_2^2 = R^2. \quad (6.39) \]
Chapter 7

Results

Introduction

The solutions of the initial-boundary-value problems described in Chapter 6, obtained using the finite element method as described in Chapter 5, are presented here. As mentioned previously, these problems investigate a number of issues pertaining to nucleation and growth of a new phase.

In order to understand the physical significance of our results, it will be helpful to keep the various material, geometric and loading parameters in mind. Note first that the couple-stress theory that we use has a material-dependent length scale $l_m$ and a material-dependent time scale $t_m$ as follows:

$$ l_m = \sqrt{\frac{\lambda}{\mu}}, \quad t_m = \frac{\nu}{\mu}, $$

where $\mu$ is the infinitesimal shear modulus of the material, $\lambda$ is the strain-gradient parameter, and $\nu$ is the viscosity parameter. The length scale $l_m$ is a measure of the influence of couple stresses and has a small value when elastic effects are dominant. The time scale $t_m$ characterizes the relaxation time of the viscous contribution and is small when the elastic response dominates. A material-dependent velocity $v_m$ can be defined by

$$ v_m = \frac{l_m}{t_m} = \frac{\sqrt{\lambda \mu}}{\nu}. $$

For each problem the geometry of the domain and the rate at which the prescribed loading is applied introduces a geometric length scale $l_g$ and a loading-dependent time scale $t_l$. Thus
it is natural to define the *loading-dependent velocity* \( v_l \) by

\[
v_l = \frac{l_g}{l_t}, \tag{7.3}
\]

Since our interest is to examine certain questions pertaining to quasi-static phase transformations within the sharp interface theory, the time scales must be chosen so as to remain in the quasi-static regime, and the length scales must generally be chosen so as to contain couple-stress effects to phase boundaries. Thus let the non-dimensional parameters be defined as

\[
R_l = \frac{l_m}{l_g}, \quad R_v = \frac{v_l}{v_m}, \tag{7.4}
\]

where \( R_l \) characterizes the ratio of the material length scale to the geometric length scale, and \( R_v \) the ratio of the velocity of loading to the material velocity. In certain problems it is more convenient to replace the loading introduced velocity \( v_l \) with the propagation speed of the interface \( V_n \). For such problems we shall take

\[
R_t = \frac{l_m}{l_g}, \quad R_v = \frac{V_n}{v_m}, \tag{7.5}
\]

The organization of the present chapter parallels that of Chapter 6 where the various problems were formulated.

### 7.1 Kinetics of interfaces

In this section we will examine a propagating interface with a straight austenite/martensite interface and the effect of an inclusion which stands in the path of a propagating interface (see problems formulated in Section 6.1). For purposes of benchmarking, we will first consider a medium without an inclusion (Problem 6.1.1). We then consider the cases where the inclusion is a cavity, a rigid fixed inclusion and a rigid inclusion that is free to move (Problems 6.1.2).

Our main interest here concerns the *effective kinetic relation* of the propagating interface as it moves across the inclusion. As mentioned previously, the rate of dissipation (per unit
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thickness), \( P_D \), can be expressed as

\[ P_D = \int_{\Pi} \nu |\nabla \dot{u}|^2 \, dA, \quad (7.6) \]

and the effective driving traction \(< f >\) is then defined by equation (6.12) or (6.15), depending on whether the domain is homogeneous or not. In carrying out the calculations to determine the effective kinetic relation \(< f >\) to relate it to \( V_n \), we evaluate the total energy dissipated in moving the interface by using (7.6), and then use (6.12) or (6.15) to calculate the effective driving traction (corresponding to the known value of \( V_n \)).

Some insight into the structure of this kinetic relation can be obtained by dimensional analysis. The relationship involves the following list of parameters:

\[ < f > = f_0(V_n; \mu, \lambda, \nu, L, R), \quad (7.7) \]

which we can more conveniently write in the form

\[ < f > = f_1(V_n; \mu, l_m, v_m, L, V_f), \quad (7.8) \]

where \( \mu \) is the infinitesimal shear modulus and \( V_f = \pi R^2/2L^2 \) is the volume-fraction for a rectangular domain \( L \times 2L \) with a circular inclusion of radius \( R \). (Observe that the applied stress has not been included here explicitly because there is a one-to-one connection between it and \( V_n \) through the kinetic relation. Parameters other than \( \mu \) that are involved in the stress response function \( \tilde{\tau}(k) \) are all nondimensional, and are not important for our present purposes.) By invoking the Buckingham Pi Theorem of dimensional homogeneity, the form (7.8) can be reduced to

\[ \frac{< f >}{\mu} = f_2 \left( \frac{V_n}{v_m}; \frac{l_m}{L}, V_f \right). \quad (7.9) \]

When the system is not far from thermodynamic equilibrium, phase boundaries propagate relatively slowly and (7.9) can be linearized with respect to \( V_n/v_m \) to get

\[ \frac{< f >}{\mu} = \frac{V_n}{v_m} f_3 \left( \frac{l_m}{L}, V_f \right) \quad (7.10) \]
provided \( f_2(0; l_m/L, V_f) = 0 \). Finally, for relatively small values of the volume-fraction, we can expand \( f \) in a Taylor series with respect to \( V_f \) to obtain

\[
< f > \mu = \frac{l_m}{L} V_n \frac{V_m}{v_m} \left[ G_1 \left( \frac{l_m}{L} \right) + F_1 \left( \frac{l_m}{L} \right) V_f \right].
\] (7.11)

When it comes to plotting the results, (and also in order to have (7.11) in a form that is similar to equation (4.62)), it is convenient to divide both sides of equation (7.11) by the square of the transformation strain \( \gamma_f^2 \). We also note that the argument of the functions \( G_1 \) and \( F_1 \) can be replaced by \( R_t = l_m/l_g \), because a nondimensional parameter characterizing the shape of the cell, through a relation between \( L \) and \( l_g \), has not been included in (7.7). The linearized nondimensional kinetic relation then has the form:

\[
\bar{f} = \frac{< f >}{\mu \gamma_f^2} = \frac{V_n}{v_m} \left[ G (R_t) + F (R_t) V_f \right].
\] (7.12)

The function \( G \) can be found by considering the medium without any inclusion \((V_f = 0)\) and this is done in Section 7.1.2. The problems considered in Sections 7.1.6 provide information on the complete functional form.

### 7.1.1 Propagating interfaces

In the following sections we study the problem of a single propagating phase boundary as described in Section 6.1.1. We recall that in Chapter 4 a version of this problem was analyzed for a trilinear material. Here the trilinear material is replaced by the power-law material (5.46). In the numerical simulation a rectangular domain \( \Pi \) of width \( w (= l_g) \), and length \( L (= 10l_g) \) is considered. In the following we will characterize several geometric, mechanical, and thermodynamical properties of the regularized interface connecting austenite and martensite by means of a transition layer of thickness \( b \).

The numerical experiment was carried out with the body initially containing a stationary interface at the Maxwell stress \( \tau_0 \). The interface begins to propagate when the prescribed displacement

\[
\delta(t) = \frac{aL}{2} t + u_0,
\] (7.13)
is applied at \( x_2 = L/2 \). The opposite boundary at \( x_2 = -L/2 \) is fixed at all times \( t \). In order to describe loading followed by unloading (perhaps repeatedly) the “constant” shearing-rate \( \dot{\alpha} \) changes sign at periodic times \( t = nt^* \), \( n = 1, 2, \ldots \). The loading-dependent time scale \( t_l \) is taken to be

\[
    t_l = \frac{1}{\dot{\alpha}}. 
\]

Thus the non-dimensional parameters of (7.4) become

\[
    R_l = \frac{l_m}{l_g}, \quad R_t = \frac{\dot{\alpha} l_g}{v_m}. \tag{7.15}
\]

Since the original problem states that the domain is infinite the following conditions have to be enforced:

(i) The length \( L \) is much larger than the thickness \( b \), implying that

\[
    L \gg l_m. 
\]

(ii) The interface does not reach the boundaries at \( x_2 = \pm L/2 \).

(iii) The length scale introduced by the size of the element has to be at least of the order of \( b \). (The specific criteria constituting a sufficiently fine mesh will be discussed in Section 7.1.6 in a numerical convergence analysis.)

Under these conditions the ratio \( R_l = l_g/l_m \) no longer governs the problem, and solutions are solely characterized by the ratio \( R_t \). The linearized kinetic relation (7.12) reduces, for the case \( V_f = 0 \), to a linear function of constant slope with \( G(R_t) \) being that constant. The other results can be interpreted as calculations at a specified rate of loading \( \dot{\alpha} \), given shear modulus \( \mu \), and augmentation \( \lambda, \nu \) for each given nondimensional rate of loading \( R_t \).

### 7.1.2 Stress and kinetic relation

Figure 7.1(a) shows a typical force-deformation curve where the average elastic stress has been plotted versus the average strain increment \( (\delta(t) - \delta(0))/L \). The abscissa thus denotes
the change in boundary displacement per unit length measured from the initial position of the interface. In Figure 7.1(b) the nondimensional velocity $V_n/v_m$ and the position $s(t)$ of the interface are plotted versus the nondimensional time $t$. The markers $(b)$ to $(d)$ characterize the critical points at which the load is reversed, and correspond to the sequence shown in Figure 7.1(a).

![Graph A](image1.png)

![Graph B](image2.png)

Figure 7.1: (a) Average elastic stress versus the average strain. (b) Position and velocity of the interface during a cycle which includes two loading and one unloading sequence.

The cycle of loading begins at the state characterized by the Maxwell stress $\tau_0$, and as time increases ($t > 0$) the interface moves and attains a constant velocity of propagation $V_n/v_m$ (see Figure 7.1(b)). Austenite is transformed to martensite at a constant rate and the now constant stress level is greater than the Maxwell stress $\tau_0$. These corresponds in Figure 7.1(a) and 7.1(b) to segments $(a \rightarrow b)$. At point $(b)$ the loading is reversed and the strained phases respond elastically until the applied stress falls below the Maxwell stress $\tau_0$; the interface will start to propagate into the opposite direction, and the reversed transformation of martensite to austenite occurs. At point $(c)$ with $\delta(t_c) = \delta(t_a)$ the loading is once again reversed and after an initial elastic respond austenite is transformed to martensite. We note
that all cusps \((a), (c)\) and \((b), (d)\) are aligned along the vertical, so that the given loading varies between two fixed values \(\delta(t_a) = \delta(t_c)\) and \(\delta(t_b) = \delta(t_d)\). We will give later on a more accurate account on the kinematics of the interface and its dependency on \(R_t\).

\[\text{Figure 7.2: (a) Average elastic stress versus the average strain for several rates of loading } R_t. \text{ (b) The stress level associated with the steady transformation of austenite to martensite } (\tau_{AM}) \text{ and martensite to austenite } (\tau_{MA}) \text{ versus the rate of loading } R_t.\]

In Figure 7.2(a) we plot the average elastic stress that is necessary to sustain one complete cycle of loading \(\delta(t)\). The loops represent the first complete loading and unloading cycle, and show the increase of the size of the hysteresis loop with respect to a wide range of values \(R_t\). One observes that at the slower rates a steady state stress is approached at which the material transforms at a constant rate. Loading rates \(R_t > 0.006\) are too high (for the value of \(t^*\) chosen) for the specimen to reach a steady state transformation.

We also carried out calculations in which we cycled the specimen a large number of times. For the parameters chosen there was negligible difference between one loop and the next indicating that the specimen achieves a steady state loop very quickly. A typical value for the decrease in the average stress per cycle was, for the first hundred cycles, approximately \(10^{-7}\). For obvious reasons we have not plotted this data.
For the slower loading rates, the hysteresis loop possess two plateaus of constant stress: a stress $\tau_{AM}$ for austenite to martensite, and a stress $\tau_{MA}$ for martensite to austenite. The values of these two stress-levels for different loading rates were determined from the loops in Figure 7.2(a) and then plotted in 7.2(b). It is seen that these two stresses vary linearly with the loading rate. An interpolation yields

$$\begin{align*}
\tau_{AM} &= +7.492R_t + 0.2708, \\
\tau_{MA} &= -7.368R_t + 0.2685.
\end{align*}$$ (7.16)

This is what one would expect from the linear viscosity term $\nu \dot{u}_\alpha$ of (3.102). The viscous contribution governs the dissipative properties of the interface and thus (7.16). Nonlinear relations could be attained with a power law dependency on the strain rate $\dot{u}_\alpha$. This would better approximate the experimental results at faster rates, like those of Shaw & Kyriakides [76] for a thin wire of NiTi in uniaxial tension. This would not however be the real physical mechanism which gives rise to the nonlinearity in the dependency of $\tau_{AM}$ on the rate of loading which cannot be captured by a purely mechanical model. The real cause is the coupling between the exothermic (forward transformation at $\tau_{AM}$) and endothermic (reverse transformation at $\tau_{AM}$) transformation, at faster rates, between mechanical and thermal effects. The local heating alters the strength of the specimen (since the enthalpy of the interface varies with the velocity of propagation) and therefore the steady state stress necessary to propagate the interface changes.

An issue of importance in this study is the effective kinetic relation associated with the couple-stress theory. In the sharp interface theory one can specify this as part of the constitutive description, but in the couple-stress theory, as shown in Chapter 4, this is part of the constitutive statement relation stress to strain, strain-gradient and strain-rate. In the sharp interface theory the kinetic relation is, roughly, a propagation law relating the stress differential between the applied stress and the Maxwell stress to the propagation speed of the interface. The solid curve in Figure 7.3(a) shows a plot of the effective kinetic relation as determined from our calculations pertaining to the present problem. For small propagation
speeds this can be described by

\[ f = 0.147 \frac{V_n}{v_m}. \]  

(7.17)

\( (a) \) Effective kinetic relation. A graph of the driving traction \( f \) versus the propagation speed \( V_n/v_m \). \( (b) \) Three stress-strain relations, where the two trilinear materials provide bounds on the polynomial stress-strain curve. The kinetic relation for each model is shown in \((a)\).

In order to compare this result with the analytically determined kinetic relation in Chapter 4, we approximated the polynomial material model by two trilinear models as shown in Figure 7.3\((b)\). The associated kinetic relations as calculated from (4.62) in Chapter 4 are shown by the dashed curves in Figure 7.3\((a)\). The particular trilinear approximations of the polynomial stress-strain curve were obtained on the basis of the following criteria:

**Trilinear material 1**

a. The trilinear model has the same values of the strain-levels \( k_M \) and \( k_m \) as the power-law material (5.46).

b. The trilinear model has the same value of Maxwell stress \( \tau_0 \) as the power-law material (5.46).
c. The area of the loops above and below the Maxwell stress of the power-law material and the trilinear material are the same.

**Trilinear material 2**

a. The trilinear model has the same strain-levels $k_M$ and $k_m$ as the power-law material (5.46),

b. The trilinear model has the same Maxwell stress $\tau_0$ as the power-law material (5.46),

c. The trilinear stress-strain curve passes through the point $(k_0, \tau_0)$ which is the point at which the Maxwell line $\tau = \tau_0$ intersects the power-law stress-strain curve.

Thus material 1 attempts to mimic the dissipative nature of the power-law stress-strain relation, while material 2 approximates the shear modulus and the transformation strain $k_T$. All three stress-strain relations are shown in Figure 7.3(b). The kinetic relation for the power-law material is bounded by the kinetic relations of the two trilinear materials, with material 1 providing a somewhat closer approximation of the kinetic relation (presumably due to the similar dissipative properties build into the material).

### 7.1.3 Interface motion

During both loading and unloading, the propagation speed of the interface reaches a constant value as the interface reaches steady state propagation. Figure 7.4 shows how this steady speed varies with the loading rate $R_t$. It is seen that there is a linear relation between these quantities

$$\frac{V_n}{v_m} = S_{AM}R_t, \quad \text{Austenite \rightarrow Martensite}$$

$$\frac{V_n}{v_m} = S_{MA}R_t, \quad \text{Martensite \rightarrow Austenite}$$

(7.18)

From the figure, $S_{AM} = 56.55$ and $S_{MA} = 54.78$. Clearly, this discussion is only valid for steady state conditions. The fact that $S_{AM}$ differs from $S_{MA}$ can be explained as follows. Let us approximate the narrow transition zone by a sharp interface for purposes of this discussion.
Figure 7.4: Propagation speed $V_n$ as a function of the loading $R_t$ for the forward and reverse transformations.

As previously, let $\tau_{AM}$ and $\tau_{MA}$ denote the stress levels at steady state transformation (see Figure 7.2). Let $k_{AM}^A$ and $k_{AM}^M$ denote the strains on the austenitic and martensitic sides during the forward transformation, $\tau_{AM} = \hat{\tau}(k_{AM}^A) = \hat{\tau}(k_{AM}^M)$, and similarly let $k_{MA}^A$ and $k_{MA}^M$ denote the strains on the austenitic and martensitic sides during the reverse transformation, $\tau_{MA} = \hat{\tau}(k_{MA}^A) = \hat{\tau}(k_{MA}^M)$. Then the average strain is given by

\[
\frac{\delta}{L} = k_{AM}^M \xi_{AM} + k_{AM}^A (1 - \xi_{AM}), \quad \text{Austenite \rightarrow Martensite} \\
\frac{\delta}{L} = k_{MA}^M \xi_{MA} + k_{MA}^A (1 - \xi_{MA}), \quad \text{Martensite \rightarrow Austenite} \tag{7.19}
\]

where $\xi_{AM}(t)$ and $\xi_{MA}(t)$ are the volume fractions of martensite during the forward and reverse transformations. Differentiating these gives

\[
\frac{\dot{\delta}}{L} = (k_{AM}^M - k_{AM}^A) \dot{\xi}_{AM} = (k_{MA}^M - k_{MA}^A) \dot{V}_n w \quad \text{Austenite \rightarrow Martensite} \tag{7.20} \\
\frac{\dot{\delta}}{L} = (k_{MA}^M - k_{MA}^A) \dot{\xi}_{MA} = (k_{MA}^M - k_{MA}^A) \dot{V}_n w \quad \text{Martensite \rightarrow Austenite}
\]

Thus by combining (7.18) and (7.20) we get

\[
\frac{S_{AM}}{S_{MA}} = \frac{k_{MA}^M - k_{MA}^A}{k_{AM}^M - k_{AM}^A}. \tag{7.21}
\]

Consequently the slopes $S_{AM}$ and $S_{MA}$ are not expected to be identical though according to (7.21) they will be identical for a trilinear material. On the other hand if the strain
differential satisfies the inequality
\[
k_M^A - k_M^A > k_M^A - k_M^A,
\] (7.22)
then the rate at which the backward transformation occurs is smaller, and one concludes that \( S_{AM} > S_{MA} \). If one calculates the numerical values of \( k_A^A, k_M^A, k_A^M, k_M^M \) by using Figure 7.1 and (5.46) one finds that (7.21) holds with the values of \( S_{AM} \) and \( S_{MA} \) noted previously. The success of this argument reinforces the connection between the sharp interface theory and the couple-stress theory.

Figure 7.5: (a) Position of the interface versus time during cyclic loading for different loading rates \( R_t \). (b) The propagation speed \( V_n \) versus time during cyclic loading for different loading rates \( R_t \).

Next we consider the position (7.5(a)) and velocity (7.5(b)) of the interface as a function of time. As the rate of loading is increased, the motion of the interface is not synchronized with the prescribed motion of the boundary: when the prescribed loading reverses, the interface motion does not immediately turn around. This effect becomes more dominant at higher rates of loading \( R_t \); it is governed by the viscous contribution of the constitutive model and only vanishes if the rate of loading is precisely zero. After each load reversal the velocity
of the interface eventually approaches the steady state velocity asymptotically (see Figure 7.5(b)).

Finally, we examine the structure of the transition layer. Figure 7.6(a) shows a plot of the total strain $k = |\nabla u|$ along a line $x_1 = \text{constant}$. The profile shown indicates the smooth nature of the transition layer. The figure is drawn for an interface which has reached

![Graphs](image)

Figure 7.6: (a) A typical smooth transition zone in steady state which is a graph of $|\nabla u(x_1, \xi)|$ versus $\xi$ where $\xi = x_2 - V_n t$. (b) The thickness of the transition zone $b$ as a function of the rate of loading $R_t$.

a steady state. (During the course of a loading cycle the profile varies somewhat from this when the system is not yet in steady state). The thickness $b$ of the interface is defined as follows: recall the strain levels $k_m$ and $k_M$ associated with the stress-strain relation (see Figure 7.3(b)). Let $x_m$ and $x_M$ be the values of $x_2$ at which the strain $k$ takes on these two values: $|\nabla u(x_1, x_m)| = k_m$, $|\nabla u(x_1, x_M)| = k_M$. Then we define the thickness $b$ by

$$b = |x_M - x_m|;$$

see Figure 7.6(a). For various loading rates $R_t$ we calculated the thickness $b$ in the preceding manner. The result is shown in Figure 7.6(b). Observe that the interface thickness is
independent of the loading rate for \( R_t \leq 10^{-3} \). We will use this feature extensively in what follows.

### 7.1.4 Discussion

We will now attempt to relate some of the preceding results, and in particular to develop an understanding how the kinetic relation depends on the thickness of the transition zone wherein the dissipative processes occur. Suppose that the interface is perfectly straight and propagates in the negative \( x_2 \)-direction. The strain rate vector \( \dot{u}_\alpha \) of (7.6) has only one component \( \dot{\gamma}(x_2, t) \). If one introduces a coordinate system which moves with the interface, \( \zeta = x_2 + V_n t \), and the strain field is steady with respect to this frame, then

\[
\gamma = \gamma(\zeta) \tag{7.23}
\]

and the strain rate \( \dot{\gamma} \) becomes

\[
\dot{\gamma} = \gamma' V_n. \tag{7.24}
\]

The propagation speed here, \( V_n \), is constant and our previous results are applicable. Substituting equation (7.24) into (7.6) yields the rate of dissipation \( P_D \) as

\[
P_D = V_n^2 \int_{-b/2}^{b/2} \nu (\gamma')^2 w d\zeta, \tag{7.25}
\]

where \( w \) is the width of the specimen (i.e. the length of the interface). In choosing the limits of the integral we have assumed that most of the dissipation occurs in the band \(-b/2 < \zeta < b/2\); this will be re-visited shortly. The product of the driving traction \( f \), the velocity of propagation \( V_n \) and the width \( w \) equals the rate of dissipation \( P_D \). Hence, the kinetic relation \( f = \dot{f}(V_n) \) becomes

\[
f = \dot{f}(V_n) = V_n \int_{-b/2}^{b/2} \nu (\gamma')^2 d\zeta. \tag{7.26}
\]

Note that this expression is linear in \( V_n \) only if the integral is independent of \( V_n \). Next we estimate the integral by replacing the derivative \( \gamma' \) with the first order approximation

\[
\gamma' \approx \frac{k_m - k_M}{b}. \tag{7.27}
\]
Then the kinetic relation (7.26) reduces to

\[ f \approx \nu \left( \frac{k_m - k_M}{b} \right)^2 V_n. \]  

(7.28)

This expression can be brought in a nondimensional form by the usual substitutions:

\[ \bar{b} = \frac{b}{l_m}, \quad \bar{f} = \frac{f}{\mu \gamma^2}. \]

By dropping the overbars, the nondimensional driving traction \( f \) is given by the kinetic relation

\[ f \approx \frac{1}{\gamma^2} \left( \frac{k_m - k_M}{b} \right)^2 \frac{V_n}{v_m}. \]  

(7.29)

First, suppose that the transition zone thickness \( b \) is constant. According to our earlier numerical results \( b \approx 2.91 \) for \( R_t < 0.001 \). Then the estimate (7.29) yields

\[ f = 0.105 \frac{V_n}{v_m}. \]

The value of the driving traction given by this kinetic relation for some propagation velocity is significantly smaller than the true value given by (7.17) which is roughly \( f = 0.147 V_n/v_m \). This should be of no surprise, since the estimate (7.29) does not include the change in curvature associated with the transition layer smoothly connecting to the homogeneous states of deformation of the austenite and the martensite, i.e. with calculating the dissipation only in the band \(-b/2 < \zeta < b/2\). If we increase the range of integration to be over \(-C b/2 < \zeta < C b/2, \ C > 1\), the approximation (7.29) becomes

\[ f \approx C \frac{1}{\gamma^2} \left( \frac{k_m - k_M}{b} \right)^2 \frac{V_n}{v_m}, \quad C > 1. \]  

(7.30)

In the range \( R_t < 0.001 \) when \( b \approx 2.91 \) this now gives \( f = 0.105 C V_n/v_m \) so that we can match the numerical results by taking

\[ C = 1.41. \]  

(7.31)

Having fitted the above kinetic relation to the data in the range of small \( R_t(< 0.001) \), we now evaluate its validity beyond this range. The width \( b \) is now not constant and so we
write (7.30) as

\[ f \approx 1.41 \frac{1}{\gamma^2} \left( \frac{(k_m - k_M)^2}{b(V_n)} \right) \frac{V_n}{v_m}. \]  

(7.32)

We now compare this analytical kinetic relation with \( b = \hat{b}(R_t) \) taken from Figure 7.6 with the numerically calculated kinetic relation depicted in Figure 7.3. Both kinetic relations are linearly related to the nondimensional velocity \( V_n/v_m \) if \( R_t < 0.001 \) because in this case the transition layer has a constant thickness \( b \). At higher rates of loading, the interface becomes thicker (\( b \) increases with \( R_t \) and hence with \( V_n/v_m \) as shown in Figure 7.6) and the kinetic relation is no longer linear. Table 7.1 compares the analytical and numerical kinetic relations.

<table>
<thead>
<tr>
<th>Propagation Speed ( V_n/v_m )</th>
<th>Analytical Estimate of Driving Traction ( f )</th>
<th>Numerically Calculated of Driving Traction ( f )</th>
<th>% Deviation in values of ( f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.055063</td>
<td>-0.008086</td>
<td>-0.008050</td>
<td>0.453</td>
</tr>
<tr>
<td>-0.110068</td>
<td>-0.016005</td>
<td>-0.016080</td>
<td>-0.467</td>
</tr>
<tr>
<td>-0.165161</td>
<td>-0.023619</td>
<td>-0.023932</td>
<td>-1.306</td>
</tr>
<tr>
<td>-0.220273</td>
<td>-0.030787</td>
<td>-0.031492</td>
<td>-2.238</td>
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<td>-0.037399</td>
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</tr>
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</tr>
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<td>0.225238</td>
<td>0.031481</td>
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<tr>
<td>0.283253</td>
<td>0.038481</td>
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<tr>
<td>0.340995</td>
<td>0.044771</td>
<td>0.044812</td>
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</tr>
<tr>
<td>0.454238</td>
<td>0.054820</td>
<td>0.055810</td>
<td>-1.773</td>
</tr>
</tbody>
</table>

Table 7.1: Comparison of kinetic relations as determined numerically and analytically. The first column gives the propagation speed of the interface, the second column gives the corresponding value of the driving force \( f \) as calculated by the analytical kinetic relation (7.32) (with \( b = \hat{b}(R_t) \) taken from Figure 7.6), the third column gives the values of \( f \) as determined directly from the numerics (as in Figure 7.3), and the last column gives the relative deviation in these two values of \( f \).

in this case. The first column gives the propagation speed of the interface, the second column gives the corresponding value of the driving force \( f \) as calculated by the analytical kinetic relation (7.32) (with \( b = \hat{b}(R_t) \) taken from Figure 7.6), the third column gives the values of \( f \) as determined directly from the numerics (as in Figure 7.3), and the last column gives the
relative deviation in these two values of $f$. The agreement is seen to be remarkably good. (We have excluded the values for very small velocities since the analytical approximation was calibrated in this range and so the agreement is “perfect”. The data corresponding to $V_n/v_m < 0$ and $V_n/v_m > 0$ characterizes the reversed transformation (MA) and the forward transformation (MA), respectively.)

Since the width of the transition layer is different for the forward and the reverse transformations, we note that the ratio of the driving traction for the forward transformation $f_{AM}$ and the reverse transformation $f_{MA}$ (at the same propagation speed $V_n$) satisfies the relation

$$\left| \frac{f_{AM}}{f_{MA}} \right| = \frac{b_{MA}(V_n)}{b_{AM}(V_n)}. \quad (7.33)$$

This relates the geometric quantity $b$ to the thermodynamic quantity $f$. From Figure (7.6)(b) one deduces for the power-law material (5.46), that the thickness of the transition layer satisfies the inequality

$$b_{AM} > b_{MA}, \quad (7.34)$$

where $b_{AM}$ and $b_{MA}$ are the steady state thickness of the forward and reverse transformation, respectively. Consequently, equation (7.33) implies that

$$|f_{MA}| > |f_{AM}|. \quad (7.35)$$

This inequality (7.35) can be verified by forming the ratio of the numerical values of $f_{AM}$ and $f_{MA}$ given in Table 7.1

We also note that the results could be developed further by introducing the relation between the applied stress and the driving traction:

$$\left| \frac{f_{AM}}{f_{MA}} \right| \approx \left| \frac{\tau_{AM} - \tau_0}{\tau_{MA} - \tau_0} \right| \quad (7.36)$$

where $\tau_0$ is the Maxwell stress and $\tau_{AM}$ and $\tau_{MA}$ are the shear stresses during the two transformations. Now recalling that the augmentation also implies that the dimensional
steady state stress is linearly related to the imposed average strain rate as
\[ \tau_{AM} - \tau_0 \approx \text{Constant} \times \frac{\dot{\delta}}{L}, \quad \tau_{MA} - \tau_0 \approx -\text{Constant} \times \frac{\dot{\delta}}{L}, \]
then with the aid of equation (7.20) the following is true
\[ \left| \frac{f_{AM}}{f_{MA}} \right| \approx \frac{k_{AM}^M - k_{AM}^A}{k_{MA}^M - k_{MA}^A}. \]
Recalling that for the power-law material the denominator is for all rates of loading larger than the numerator, we once again attain the consistent result that \( f_{MA} > f_{AM} \). This little calculation can also be viewed as another check on the accuracy and consistency of our results.

### 7.1.5 Numerical convergence analysis

In Chapter 5 we verified our code by comparing the computed results to analytical solutions. The discretization of the domain with finite elements introduces an additional length scale, namely the characteristic size of an element. In order to gauge the importance of the element size and the necessary mesh refinement, several numerical experiments were carried out. The numerical experiments revealed, that quantities like the average stress, and the displacement field are sufficiently well approximated if the element size is of the order of the interface thickness \( b \). On the other hand the kinetic relation is strongly dependent on the size of the element, since it depends on the square of the strain rate and errors in the strain field are amplified. As a rule of thumb, a reasonably coarse mesh (size of element \( \approx b \) ) generally underestimates the average stress by a few percentage points and to a greater extent the value of the kinetic relation. In the remainder of this section we examine this more closely.

The computations involved in the problem at hand are relatively inexpensive, and therefore it is a particularly efficient problem in which to understand how the driving traction depends on the mesh. The conclusions drawn here will guide us in our mesh selection in the more complicated problems to be considered later.
The convergence analysis can be carried out in two ways. The most natural way is to progressively refine the mesh, solve the problem for each mesh and compare the results. An alternative indirect method is as follows: let $w$ be the width of the strip and let $L$ be its length. Since the problem is one dimensional, $w$ plays no role. Moreover if $b/L << 1$ the strip can be considered to be essentially infinite. Finally, as the material length scale $l_m$ increases so does the transition zone thickness $b$. We carried out a series of calculations for different values of $l_m/l_g$ were $l_g = L$ and the results are shown in Figure 7.7. Since the strip has essentially infinite length and since $b$ increases with $l_m/l_g$, it follows that effectively the number of finite elements contained within the transition zone increases with $l_m/l_g$. Thus the curves in Figure 7.7 can be interpreted as curves corresponding to increasingly finer meshes (as $l_m/l_g$ increases). The results show that as the mesh is refined the computed kinetic relation converges; in particular the driving traction $f$ converges to a unique value for each value of the interface speed $V_n/v_m$.

![Figure 7.7: The driving traction versus the propagatio speed (the kinetic relation) for several values of the length scales $R_t = l_m/l_g$.](image)

It should be noted that it is only in this problem where no true geometric length scale exists that this indirect procedure is meaningful. In the problems to be considered later, the
ratio \( l_m/l_g \) is an important parameter to quantify the thickness of the interface with respect to the size of particles and voids. In order to verify our procedure, we also carried out a few calculations following the first method where we actually considered a series of progressively more refined meshes. The results from both approaches agreed.

### 7.1.6 Propagation across inclusions of different type

The problems being solved in this section attempt to model an austenitic specimen which is subjected to a uniform constant stress \( \tau_3 = \tau \) with a straight austenite/martensite interface entering the specimen from its top boundary. If the applied stress is less than the Maxwell stress this phase boundary will retreat and the specimen will remain austenitic. However, if the stress exceeds the Maxwell stress this interface would like to propagate downwards through the specimen and transform it entirely into martensite. The inclusion has some retarding effect on this interface and this is what we are most interested in studying here. If the domain is sufficiently wide in comparison with the inclusion, then in two vertical strips near the sides of the specimen, the state of deformation will be approximately piecewise homogeneous with a straight horizontal interface that is propagating at a constant speed \( V_n \); the value of \( V_n \) is given by the kinetic relation. In the vicinity of the inclusion the interface will deviate from this shape.

The inclusion is circular (radius \( R \)) and is located concentrically in the rectangular domain \( L \times 2L \). For the geometric length scale \( l_g \), we will take

\[
l_g = R. \tag{7.37}
\]

The "applied loading" manifests itself through the stress \( \tau \) and the corresponding propagation velocity \( V_n \) which arises from the kinetic relation. The time scale associated with loading is therefore taken to be

\[
t_l = \frac{l_g}{V_n}. \tag{7.38}
\]
The nondimensionalized propagation velocity is taken to be

\[ \bar{v} = \frac{V_n}{v_m} \]  

(7.39)

where the material-dependent velocity \( v_m \) was defined earlier by equation (7.2). Finally, the temporal and spatial coordinates will be nondimensionalized as follows:

\[ \bar{t} = \frac{t}{t_l} = \frac{tV_a}{l_g}, \quad \bar{x}_a = \frac{x_a}{l_g}, \]  

(7.40)

and, as before, we will drop the overbar from here on, and if necessary distinguish between dimensional and nondimensional variables explicitly.

The two nondimensional parameters which control the details of this problem are the ratio of velocities \( R_v \) and the ratio of length scales \( R_l \):

\[ R_v = v = \frac{V_a}{v_m}, \quad R_l = \frac{l_m}{l_g}. \]  

(7.41)

The ratio \( R_l \) controls the thickness of the transition layer with respect to the size of the inclusion, and \( R_v \) determines the ratio between the interface’s velocity of propagation and the velocity inherent to the augmented material. In case the slowly propagating interface is sufficiently far removed from the inclusion the linearized kinetic relation (7.17) applies. This requires the ratio \( R_v \) to be much smaller than one \( (R_v << 1) \). The experiments were conducted for several values of \( R_l \) in the range \((0.025, 0.1)\).

Our main goal is to estimate the appropriate correction to the effective kinetic relation, in case particles and holes are encountered by the propagating interface. We also will explain the evolution of interfaces and correlate it to changes in the kinetic relation and rate of dissipation. In Figure 7.8(a) – (h) and Figure 7.9(a) – (g) the distribution of martensite and austenite is shown, when the propagating interface is influenced by an inclusion. In the contour plots of the total strain \( k \) shown, we characterize martensite \( (k > k_m) \) by the dark shaded region, austenite \( (k < k_M) \) by the light shaded region, and the transition layer \( (k_M < k < k_m) \) by the medium shaded region. Whenever we speak of an interface we mean the
location of the particular strain contour \( k = (k_M + k_m)/2 \). Before we elude to these contour plots it might be useful to recall the interrelation between the kinematical characteristics (velocity of propagation, length of an interface) and the mechanical and thermodynamic ones (kinetic relation, rate of dissipation).

Suppose that the interfacial motion can be modeled by a linear kinetic relation and that \( b = \bar{b}(R_t) \) is self similar and thus not a function of the rate of loading (see Figure 7.6(b) for \( R_t < 0.001 \)). Then the rate of dissipation depends quadratically on the velocity of propagation of the interface. If the process occurs sufficiently fast the linear range of the kinetic relation is not applicable. In case the interface undergoes a change in length the rate of dissipation and the kinetic relation change proportionately. Hence, two major effects can alter the rate of energy dissipation, and in our numerical experiments the following scenarios were encountered.

a. The rate of dissipation decreases:

i. The average velocity of the interface decreases, because the inclusion slows the interface down or even pins the interface.

ii. The effective length of an interface has shortened.

b. The rate of dissipation increases:

i. The average velocity of the interface increases, because the interface accelerates towards a region of highly strained martensite, or austenite.

ii. The propagating interface generates new interfaces of given mobility.

Typically, there will be multiple interfaces in the problems that we will discuss. The principal interface is the one that we drive through the specimen and we refer to it as the "forced interface". Other interfaces are nucleated near the cavity or particle and are of less interest in the present set of problems.
Propagation across a cavity

In Figure 7.8(a) a straight interface approaches the hole and austenite is transformed to martensite. The strain of the austenitic phase is amplified at the hole at \((x_1, x_2) = (\pm R, 0)\), and induces the formation of two small stationary regions of martensite (thus not contributing to the overall rate of dissipation). The kinetic relation for a straight interface is still valid. When the interface is sufficiently close to the hole the average speed of the forced interface decreases and the two small regions of martensite rotate towards the forced interface (see Figure 7.8(a) – (b)). The net effect is a small reduction in the rate of dissipation, since the drop in the average velocity of the forced interface outweighs the additional contributions of the two rotating interfaces in the vicinity of \((x_1, x_2) = (\pm R, 0)\).

Suddenly, the three regions of martensite coalesce and trap a triangular region of austenite near \((x_1, x_2) = (0, R)\). This fast process is shown in (c) and characterized by a significant spike in the rate of dissipation. Two mechanism are contributing to the brief but substantial increase in the rate of dissipation. First, the new configuration of phases increases the overall length of interfaces. Secondly, these interfaces propagate at velocities larger than \(V_n/v_m\).

During loading in the range (c) – (e) the forced interface is pinned at the perimeter of the hole. The average velocity of the two interfaces is about 50% smaller than \(V_n/v_m\), causing a significant drop in the rate of dissipation. In the range (c) – (f) this effect is counteracted by the shrinking of the triangular region of austenite. The overall rate of dissipation during (c) – (f) is smaller than the one of a straight interface propagating at a velocity \(V_n/v_m\). Hence, the additionally generated interface cannot compensate for the reduced rate of dissipation in the range (c) – (f).

In plot (f) the next fast process is developing. The pinned interfaces are breaking free at (g), and a new distribution of phases develops; a straight interface and two entrapped regions of austenite at \((x_1, x_2) = (0, \pm R)\) are formed. This process is at the instant of redistribution concomitant with a brief spike in the rate of dissipation. Later on, only the straight interface
Figure 7.8: Time evolution of martensite and austenite at different nondimensional positions $x_2 = s(t)$ of the forced interface at $x_1 = \pm L/2$ for the ratio $R_t = 0.05$, with (a) at $s(t) = 2.6$, (b) at $s(t) = 2.0$, (c) at $s(t) = 1.2$, (d) at $s(t) = 0.2$, (e) at $s(t) = -0.4$, (f) at $s(t) = -2.2$, (g) at $s(t) = -2.6$, and (h) at $s(t) = -3.2$. 
dissipates energy and the kinetic relation given by (7.17) is valid in the range beyond $h$.

The accumulative effect of this process can be expressed by (7.12). For the values of $R_l$ considered, the average dissipation is higher than the one associated with the motion of a straight interface propagating at a velocity $V_n/v_m$. The most significant contributions to the dissipation of energy occur during the two fast processes from $(b) - (c)$ and $(f) - (g)$. These increases were not compensated for by the drop of the rate of dissipation in the range $(c) - (f)$. The effective kinetic relation for a domain with a hole is estimated from these results to be

$$f = [0.147 + 5.1V_f] \frac{V_n}{v_m}. \quad (7.42)$$

**Propagation across a particle**

Next we replace the hole with a fixed rigid particle and carry out the same calculations as above. In Figure 7.9(a) – (g) a series of plots depicts the evolution of the phases. In Figure 7.9(a) a straight interface approaches the fixed particle. The strain field of the austenite phase is amplified near the particle, and this induces the formation of two symmetric regions of martensite near $(x_1, x_2) = (0, \pm R)$ as shown in (a).

Once the interface has propagated sufficiently close to the particle the martensite near $(x_1, x_2) = (0, R)$ starts to influence its evolution (see Figure 7.9(a) – (b)). First, the forced interface slows down, causing a minor drop in the rate of dissipation. Secondly, the martensite which is attached to the particle vanishes, and releases a small amount of energy. More importantly, the path to the particle has been cleared and the forced interface accelerates towards the particle and attaches itself to it. This process is characterized by a significant increase in the rate of dissipation. During further loading in the range $(c) - (e)$, the interface’s velocity along the perimeter of the particle decreases and the rate of dissipation is less than for a straight interface propagating at the velocity $V_n/v_m$. During this slow process the small region of martensite near $(x_1, x_2) = (0, -R)$ also vanishes at (e).

The next major change in the process occurs during $(f)$ and $(g)$, when the interface
Figure 7.9: Time evolution of martensite and austenite at different nondimensional positions $x_2 = s(t)$ of the forced interface at $x_1 = \pm L/2$ for the ratio $R_1 = 0.05$, with (a) at $s(t) = 2.2$, (b) at $s(t) = 1.8$, (c) at $s(t) = 1.4$, (d) at $s(t) = -1.8$, (e) at $s(t) = -3.8$, (f) at $s(t) = -5.0$, and (g) at $s(t) = -6.6$. 
detaches itself from the particle to form a nearly straight interface and generate an enclosed region of austenite. This region is relatively stationary and the additionally dissipated energy is rather insignificant. The straight interface can again be modeled by the kinetic relation (7.17).

The accumulative effect of a particle can be expressed by (7.12). For the range of values of \( R_t \) considered, the average dissipation is less than that associated with the motion of a straight interface propagating at a velocity \( V_n/v_m \). This is mostly due to the slowly evolving phases in the range \((d) - (f)\), where the average dissipation is significantly less than that for a straight interface. The two spikes in the rate of dissipation in the range \((b) - (c)\) and \((f) - (g)\) are not sufficient to compensate for the diminished dissipation. The effective kinetic relation in the presence of fixed rigid particles of a given volume fraction can be approximated, based on these calculations, as

\[
f = [0.147 - 5.6V_f] \frac{V_n}{v_m}. \tag{7.43}
\]

We repeated these calculations for the case of a rigid particle which is not held fixed (i.e. it is free to rigidly translate as might be needed). The differences at the beginning are rather minor. Only as the interface breaks free does the phases evolution change. This particle does not trap a region of austenite near \((x_1, x_2) = (0, -R)\) since the net force exerted by the particle on the surrounding material is zero. The effective kinetic relation in this case is approximately

\[
f = [0.147 - 5.8V_f] \frac{V_n}{v_m}. \tag{7.44}
\]
7.2 Nucleation

The first three problems pertain to an infinite medium containing a single inclusion, namely a rigid circular particle, a circular cavity and a crack. The geometric length scale \( l_g \) is taken to be the inclusion radius \( R \) in the first two problems and half the length \( b \) of the crack in the third problem. The fourth problem concerns an infinite medium containing a periodic array of rigid particles, and here we take \( l_g \) to be the particle radius and use the particle volume fraction per unit cell, \( V_f \), as an additional geometric parameter.

With regard to the loading, in each of these problems the body is subjected to a remotely applied simple shear displacement \( u(x_1, x_2) \sim k_\infty(t)x_2 \); the applied shear \( k_\infty(t) \) is taken to increase linearly with time,

\[
k_\infty(t) = \dot{\alpha} t,
\]

so that the shearing-rate \( \dot{\alpha} \) is constant. The loading-dependent time scale \( t_l \) is is thus taken to be

\[
t_l = \frac{1}{\dot{\alpha}}.
\]

The nondimensional parameters defined by (7.4) become

\[
R_t = \frac{l_m}{l_g}, \quad R_t = \frac{\dot{\alpha}l_g}{v_m},
\]

and characterize the ratio of the material length scale to geometric length scale, and material velocity to loading velocity respectively. In order to be in the regime of interest to us, we must take

\[
R_t \ll 1, \quad R_t \ll 1.
\]

In the results reported below we took \( R_t \sim 10^{-11} \), allowing us to analyze the effects of inclusions of very small dimensions at very slow loading rates \( \dot{\alpha} \). With respect to our previous results in Section 7.1.2 - Section 7.1.5 the linear kinetic relation is valid and the thickness of the transition layer between the austenite and martensite phase is independent of \( R_t \) for a straight interface. The results presented are found not to depend on the loading rate \( R_t \) for
the range of slow rates that we consider. Hence we only present results for the characteristic value \( R_t \sim 10^{-11} \). The ratio \( R_t \) was varied in the interval \([0.0125, 0.1]\), which is as small as our computational capabilities permitted.

With regard to the temporal and spatial variables of the problem, we nondimensionalize them using the geometric length \( l_g \) and the loading time \( t_l \):

\[
\bar{t} = \frac{t}{t_l} = t\dot{a}, \quad \bar{x}_\alpha = \frac{x_\alpha}{l_g}.
\]  

A typical velocity \( v \) in the problem will be no-dimensionalized as

\[
\bar{v} = \frac{v}{l_g\dot{a}}.
\]  

For simplicity of writing, from here on we shall drop the overbars, and if necessary, distinguish variables by using the explicit wording nondimensional.

Note that, by choosing the time scale \( t_l \) to form the nondimensional time \( t \) the strain \( k_\infty(t) \) is equal to the nondimensional time. Thus, for example, when the reader views in the following sections a graph of some quantity versus the nondimensional time, that graph could also be interpreted as portraying the variation of that quantity with the applied strain \( k_\infty \).

Finally a word about some terminology. In all our calculations we will be starting with a body which is entirely in the parent phase (austenite). As the body is loaded, we say that the product phase (martensite) is nucleated when some point in the body attains the strain-level \( k_m \). We will use the term nucleation strain to refer to as the value of the remotely applied strain \( k_\infty \) at which such nucleation occurs; it refers to the global strain, the local strain level at this instant always being \( k_m \). At some instant after nucleation, there will typically be some region of the body which continues to be untransformed \( (k < k_M) \), another region which has transformed \( (k > k_m) \) and these regions would be separated by a transition zone which is the region bounded by the strain contours \( k = k_M \) and \( k = k_m \). The thickness of the phase boundary or transition zone refers to some suitable measure of the thickness of this region.
Finally, when we wish to calculate the propagation speed of the phase boundary we will calculate the propagation speed (at a suitable location) of the strain contour \( k = (k_M + k_m)/2 \).

### 7.2.1 Rigid particle in an infinite domain

We now consider the problem formulated in Chapter 6.2.1 pertaining to an infinite medium containing a rigid circular particle; the medium is subjected to a remotely applied simple shear \( u(x_1, x_2) \sim k_\infty(t)x_2 = \dot{a}tx_2 \). Initially the body is composed of the parent phase austenite. As the applied shear \( k_\infty(t) \) increases, the body continues to be composed of austenite for some initial period of time. At a critical value of \( k_\infty \), martensite is nucleated at the points of stress concentration \((x_1, x_2) = (0, \pm R)\). This nucleation value of shear strain depends on the material length scale \( l_m \) in the manner shown in Figure 8.1. As \( k_\infty \) continues to increase, the phase boundary propagates into the austenitic region and the martensitic region grows.
Figure 7.10: Time evolution of martensite and austenite for $l_m/l_g = 0.05$, with (a) at $t = 0.026$, (b) at $t = 0.028$, (c) at $t = 0.036$, (d) at $t = 0.032$, and (e) at $t = 0.034$. 
The subsequent growth of the new phase is described in Figure 7.10, which shows a chronological sequence of contour plots of the total strain $k$, describing the time evolution of the two phases. The calculations are carried out for $l_m/l_g = 0.05$. The dark region represents the martensite phase $k \geq k_m$, and the light region the untransformed austenite phase $0 \leq k \leq k_M$; the phases are separated by a narrow, smooth, transition layer where $k_M < k < k_m$. At the instant of nucleation one observes that the interface emerges almost instantaneously in the form of an arch-like domain.

The value of the applied strain at nucleation depends on the material parameter $l_m$; this can be seen qualitatively by comparing Figure 7.10 with Figure 7.11, where in the latter figure we have decreased the ratio $l_m/l_g$ to 0.0125. This is shown quantitatively in Figure 8.1.

Once the new phase has established itself, its rate of growth is influenced by the steepness of the strain gradient in front of the interface. This is best depicted in Figure 7.12(a) and 7.12(b), in which we plot the position of the interface at different times $t$; as mentioned previously, in discussions such as this, “the interface” refers to the strain contour $k = \frac{k_M + k_m}{2}$. In this figure, the time increment between two adjacent positions is $\Delta t = 0.002$. The change in position between two consecutive contours is thus a measure of the current propagation velocity field of the interface. At the point where the phase boundary meets the particle it is normal to the particle surface. Moreover, one observes that the phase boundary propagation velocity at the rigid particle decreases rapidly with time and eventually the phase boundary gets pinned at a certain location on the surface of the particle. This pinning effect is caused by the adverse strain gradient along the perimeter of the particle which is inherent to the problem at hand. The strain $k$ vanishes at $\theta = 0$ and increases with $\theta$ along the particle surface until the phase boundary is reached. This makes it increasingly more difficult for the phase boundary to move further along the particle surface. As the loading continues to increase, the interface becomes almost immobile along the particle surface, and instead begins to extend itself by bulging horizontally above this point of attachment.
Figure 7.11: Time evolution of martensite and austenite for $l_m/l_g = 0.0125$, with (a) at $t = 0.022$, (b) at $t = 0.024$, (c) at $t = 0.026$, (d) at $t = 0.028$, (e) at $t = 0.030$, (f) at $t = 0.032$, and (g) at $t = 3.034$. 
Figure 7.12: Time evolution of a sharp interface: (a) from $t = 0.026$ to $t = 0.034$ for the material parameter $\frac{l_m}{l_g} = 0.05$, and for (b) from $t = 0.022$ to $t = 0.034$ for the material parameter $\frac{l_m}{l_g} = 0.0125$, where one chooses the strain $k = \frac{k_M + k_m}{2} = 0.075$ as the location of the sharp interface.

Figure 7.13(a) shows the propagation velocity of the phase boundary along the vertical line $x_1 = 0$. Observe that after some initial transient, it increases linearly with time (and therefore linearly with the applied strain $k_\infty$.) The different curves in Figure 7.13 correspond to several values of the ratio $R_t$. The initial transient, which corresponds to the initial nucleation process, depends strongly on the material parameter $l_m$. On the other hand the acceleration of the interface after the transients have decayed, for the range of loading considered, appears to be (roughly) independent of $l_m$.

In Figure 7.13(b) we plot the variation of the thickness $b$ of the transition layer; here, the thickness is defined as the distance along the $x_2$-axis between the strain contours $k = k_M$ and $k = k_m$. We conclude from this figure that the material length scale $l_m$ determines the thickness of the transition layer; this follows from the fact that the ratio $\frac{b}{l_m}$ changes only slightly over a wide range of values of the ratio $\frac{l_m}{l_g}$. This conclusion that the transition layer thickness scales with the material length scale $l_m$ supports our assumption that the
transition layer in couple stress theory replaces the sharp interface of the classical theory with a smooth transition layer.

Figure 7.13: (a) Normal velocity of the interface for a motion along the $x_2$-axis for different ratios of $l_m/l_g$, (b) nondimensional thickness $\frac{b}{l_m}$ of the interface's transition layer for different ratios $\frac{l_m}{l_g}$, in which measurements were taken at the intersection with the $x_2$-axis.

### 7.2.2 Cavity in an infinite domain

We now turn to the problem formulated in Chapter 6.2.2 concerning an infinite medium which contains a circular cavity; the medium is subjected to a remotely applied simple shear $u(x_1, x_2) \sim k_\infty(t)x_2 = atx_2$. As in the previous problem, initially, the body is composed of the parent phase austenite. As the applied shear $k_\infty(t)$ increases, the body continues to be composed of austenite for some initial period of time. At a critical value of $k_\infty$, martensite is nucleated at the point of stress concentration $(x_1, x_2) = (\pm R, 0)$. As $k_\infty$ continues to increase, the phase boundary propagates into the austenitic region and the martensitic region grows.
Figure 7.14: Time evolution of martensite and austenite for $l_m/l_g = 0.05$, with (a) at $t = 0.026$, (b) at $t = 0.028$, (c) at $t = 0.030$ and (d) at $t = 0.032$. 
In the present problem the nature of the loading causes the largest strain to be found at 
\((x_1, x_2) = (\pm R, 0)\), whereas the strain vanishes at \((x_1, x_2) = (0, \pm R)\). Nucleation occurs at 
\((x_1, x_2) = (\pm R, 0)\) when the local strain there reaches the value \(k_m\). The value of the applied 
strain \(k_\infty\) when this happens depends on the material length scale in the manner shown in 
Figure 8.1. After the new phase nucleates at the location of the strain concentration, it 
grows horizontally along the \(x_1\)-axis where the adverse strain gradient is smaller than along 
the free surface of the hole.

In Figure 7.14 we display the evolution of the phases as determined from our solution. The 
calculations pertain to \(l_m/l_g = 0.05\). The martensitic phase \((k \geq k_m)\) is represented by the 
dark region and the austenitic phase \((0 \leq k \leq k_M)\) by the light region. The transition layer 
depicted by the region of medium darkness separates these two phases. The time increment 
between the four Figures 7.14(a–d) is kept constant at \(\Delta t = 0.002\). Martensite nucleates at 
the free surface of the hole at \((x_1, x_2) = (\pm R, 0)\) and extends itself at a rapid rate along the 
\(x_1\)-axis. Observe that the transformed region has a needle like form. The initial transients 
associated with nucleation persist only for a very short time and the primary elongational 
motion of the martensitic needle along the \(x_1\)-axis begins very soon after nucleation. The 
growth of the martensitic region along the perimeter of the cavity is very small since a steep 
adverse strain gradient has to be overcome in this direction. Thus the needle grows with 
essentially no thickening.

The tip of the phase boundary \((x_2 = 0)\) propagates along the \(x_1\)-axis at a speed \(v\) as 
shown in Figure 7.15. Again, the phase boundary here refers to the strain contour 
k(x_1, x_2) = (k_M + k_m)/2. Due to high propagation speed, the tip of the phase boundary approaches the 
domain boundary rather quickly, and its motion is presumably affected by this. This is 
probably the reason why the tip acceleration is seen in Figure 7.15 to decrease after some 
time.

In order to accurately interpreted this data, one must take into account the fact that 
the position of the interface is highly sensitive to the (high) velocity of the tip, as well as
the fact that the nucleation strain depends noticeably on the ratio \( \frac{l_m}{l_g} \). For example, at time \( t = 0.03 \), the three simulations shown in Figure 7.15 have propagation velocities which have the same order of magnitude. However, the phases are at very different stages of their evolution: the interface associated with \( \frac{l_m}{l_g} = 0.1 \) has barely nucleated and has just propagated to \( x_1 = 1.96 \). On the other hand with \( \frac{l_m}{l_g} = 0.05 \) (see Figure 7.14) the new phase already displays a needle like structure which reaches \( x_1 \approx 4.37 \). In the third case \( \frac{l_m}{l_g} = 0.025 \) (which is the one with the least amount of regularization) the needle tip is found at \( x_1 = 5.56 \).

Because the phase boundary propagates rapidly, the solution shows an increased dependency on the material length scale \( l_m \). Since our interest here is in fact with the sharp interface theory, it is sufficiently small values of \( l_m \) that we are interested in, small enough that the couple stress theory is sufficiently close to the sharp interface theory. In terms of, say Figure 7.15, for each value of \( l_m \) there is a different curve, but as \( l_m \rightarrow 0 \) these curves converge to some limiting curve. The question of numerical importance is how small should we take \( l_m \) so that the curve obtained is sufficiently close to the limiting curve. The figure
suggests that this is true for $l_m/l_g \leq 0.05$.

We used the data to observe how the thickness $b$ of the fully developed transition zone varies with loading. When the thickness referred to is the thickness in the vicinity of the hole, it was found that $b$ scales as the material length scale $l_m$ thus indicating that the smooth transition layer of couple-stress theory corresponds to a sharp interface in the classical theory.

![Graph showing the nondimensional thickness of the interface's transition layer for different ratios $l_m/l_g$.](image)

Figure 7.16: Nondimensional thickness $\frac{b}{l_m}$ of the interface's transition layer for different ratios $l_m/l_g$. Measurements were taken at the intersection with the $x_1$-axis.

However, the thickness of the transition layer at the tip of the martensitic needle, is found not to be scaled by the material parameter $l_m$, as can be seen from Figure 7.16. One notes that the data in this figure does not scale with $l_m$. On the contrary, if the needle tip is sufficiently far removed from the nucleation site, the transition layer has a thickness at the tip which is largely independent of $l_m$. This leads us to conclude that the physics at the tip are independent of the amount of augmentation, and not simply the result of smoothing a sharp interface. Therefore, as the sharp interface theory limit of the present theory is taken, the transition layer near the martensitic needle tip does not converge to a simple sharp interface, but to some more complex microstructure. This issue will be expanded upon in the next problem.
7.2.3 Crack in an infinite domain

Next we consider the Mode-III crack-problem formulated in Chapter 6.2.3. We recall that the crack is modeled as a slot of length \(2b\) and thickness \(2c\) consisting of parallel faces joined by semi-circular arcs at the ends. We take \(\frac{b}{c} = 50\). The medium is subjected to a remotely applied simple shear \(u(x_1, x_2) \sim k_\infty(t)x_2 = \dot{\alpha}tx_2\). Initially the body is composed of the parent phase austenite. As the applied shear \(k_\infty(t)\) increases, the body continues to be composed of austenite for some initial period of time. At a critical value of \(k_\infty\), martensite is nucleated at the crack-tip point of stress concentration \(x_1 = \pm b, x_2 = 0\). As \(k_\infty\) continues to increase, the phase boundary propagates into the austenitic region and the martensitic region grows.

Nucleation occurs at \((x_1, x_2) = (\pm b, 0)\) when the local strain there reaches the value \(k_m\). The value of the applied strain when this happens depends on the material length scale in the manner shown in Figure 8.1.

Figure 7.17 document the subsequent time evolution of the martensite and austenitic phases, and the intermediate transition layer, in their respective shades of gray. The calculations were carried out for \(l_m/l_g = 0.05\). The time increment from one figure to the next is \(\Delta t = 0.001\).

On comparing the nucleation characteristics of the crack problem with the hole problem several interesting and sometimes nonintuitive observations can be deduced. First, as one would expect, the value of the applied strain needed to nucleate a phase transformation is lower for the crack problem because the higher local curvature at the crack tip amplifies the applied strain \(k_\infty\) more significantly. Second, by comparing the results of several such calculations for various values of \(l_m/l_g\) it is found that (the steepness of the strain field induces more significant higher order stresses at the crack tip and therefore) the nucleation value of applied strain depends more strongly on the material length scale \(l_m\) than in the equivalent problem of the cavity.

Consequently, in order to observe a self-similar behavior, we must use smaller values of
Figure 7.17: Time evolution of martensite and austenite for $l_m/l_g = 0.05$, with (a) at $t = 0.025$, (b) at $t = 0.026$, (c) at $t = 0.027$, (d) at $t = 0.028$, (e) at $t = 0.029$, (g) at $t = 0.030$, (g) at $t = 0.031$ and (h) at $t = 0.032$. 
$l_m/l_g$. This phenomenon is clearly depicted, for example, in Figure 8.1, which we will discuss in Chapter 8.

Thirdly, the initial growth of the martensitic phase immediately after nucleation differs from that observed at the circular cavity, since the strain field in front of the crack-tip decays rapidly and this adverse strain gradient inhibits the initial growth of the martensitic region.

![Graph](image)

Figure 7.18: Normal velocity of the interface for a motion along the $x_1$-axis for different ratios of $l_m/l_g$.

This can be seen from Figure 7.18 where we have plotted the velocity of propagation of the tip of the phase boundary along the $x_1$-axis. (As before, for the present purpose, we are identifying the phase boundary with the strain contour $k = (k_M + k_m)/2 = 0.075$.) Nucleation is observed at the time $t = 0.016$ for the case $l_m/l_g = 0.05$ that we consider. Observe from this figure that the initial growth is extremely slow (in comparison with the cavity problem), and it is only at times greater than $t = 0.025$ that this interface is able to detach itself from the crack-tip region and begin to accelerate continuously and penetrate the rest of the domain. After this, the features of such a well-established interface are very similar to those documented in Figure 7.15 for the cavity. The speed attained by the phase boundary tip is still considerable lower than that for a hole, but if the loading is increased
Figure 7.19: Nondimensional thickness $\frac{b}{l_m}$ of the interface's transition layer for different ratios $\frac{l_m}{l_p}$. Measurements were taken at the intersection with the $x_1$-axis.

Further, the progress of the interface becomes less dependent on its initiation details and similar speeds should be attained. The thickness of the transition layer behaves similarly to that in the cavity problem. In particular, its thickness measured in the $x_2$-direction at a point in the middle of the elongated martensitic needle (once it has formed) scales with the material length scale $l_m$. Therefore in the limit of the sharp interface theory this portion of the transition layer will collapse into a sharp interface. On the other hand, Figure 7.19 shows how the thickness of the transition zone at the phase boundary tip (in the $x_1$-direction) varies with time. In this tip region, transition zone thicknesses do not scale with $l_m$, but rather, are self similar for a range of $l_m$. Therefore in the transition zone tip region the transition layer thickness does not vanish in the sharp interface limit. It should therefore be interpreted as a region of microstructure and not as a smoothed sharp interface. This conclusion is in keeping with the numerical solution of SILLING [74] where he found a complicated microstructure in a region ahead of, and removed from, the crack-tip. One can not identify a well-defined phase boundary in the region and there is instead a fractal like mixture of phase. The limiting solution we find here is similar to that in ABNEYARATNE [1]'s analytical solution where he
found a region of transition material in a domain ahead of the crack-tip.

7.2.4 Periodic array of particles

Here we turn to the problem formulated in Chapter 6.1.4 concerning an infinite medium containing a periodic array of rigid circular particles. Each square unit cell contains a concentric rigid circular particle; the particle volume fraction is denoted by $V_f$. The medium is subjected to a remotely applied simple shear $u(x_1, x_2) \sim k_\infty(t)x_2 = \dot{a}tx_2$. Initially the body is composed of the parent phase austenite. As the applied shear $k_\infty(t)$ increases, the body continues to be composed of austenite for some initial period of time. At a critical value of $k_\infty$, martensite is nucleated at the points of stress concentration $(x_1, x_2) = (0, \pm R)$. As $k_\infty$ continues to increase, the phase boundaries in each cell propagate into the austenitic region and the martensitic region grows. Eventually the phase boundaries from different cell coalesce.

In addition to examining questions similar to those looked at for the previous three problems, we are also interested here in examining the “effective stress-strain response” of the composite body.

The calculations will explore, in addition, the influence of the two main parameters – the volume fraction $V_f$ and the ratio of length scales $l_m/l_g$. In particular take all combinations of $l_m/l_g = 0.025, 0.05, 0.1$ and $V_f = 0.20, 0.35$.

At a critical value of the applied shear strain $k_\infty$, martensite is nucleated at the points $(x_1, x_2) = (\pm R, 0)$. This value of shear strain at nucleation depends on the material length scale $l_m$ in the manner shown in Figure 8.1.

Figure 7.20 shows the subsequent growth of martensite by showing the position of the phase boundary at various instants of time. The figure pertains to the volume fraction $V_f = 0.20$. At this volume fraction, and for the load-levels shown, the evolution in the present periodic array is very similar to that in the infinite medium considered in Section 7.2.1. One observes from Figure 7.20 that here too the phase boundary tends to become
Figure 7.20: Time evolution of the sharp interface from $t = 0.022$ to $t = 0.034$ for the parameters $l_m/l_g = 0.05$, and $V_f = 0.20$, where one chooses the strain $k = \frac{k_M + k_m}{2} = 0.075$ as the location of the sharp interface.

pinned at a certain point along the surface of the particle.

The propagation velocity of the phase boundary along the vertical $x_2$-axis is plotted as a function of time in Figure 7.21. After an initial transient phase, the phase boundary velocity varies more or less linearly with the applied strain ($\sim$ time). The value of the propagation speed in this case is somewhat smaller than that in the infinite medium problem (Figure 7.21(a)) but the values are generally of the same order of magnitude. The difference between the propagation velocity in an infinite domain and in a periodic array of finite cells increases with the ratio $l_m/l_g$; this can be explained by the fact that the relative thick transition layer (which occurs for large values of $l_m/l_g$) is closer to the upper boundary of the cell than is a thin zone.

Figure 7.21(b) plots the variation of the transition layer thickness with time where the thickness has been measured along the vertical $x_2$-axis. The transition layer thickness is seen to scale with the material length scale $l_m$. Consequently, in this problem the transition layer converges to a sharp interface in the limit of the classical theory.

The interaction between neighboring cells becomes more pronounced at higher volume
Figure 7.21: (a) Normal velocity of the interface for a motion along the $x_1$-axis, (b) the nondimensional thickness $\frac{b}{l_m}$ of the interface’s transition layer, where measurements were taken at the intersection with the $x_2$-axis. Both figures give curves for ratios $\frac{l_m}{l_g}$ at $V_f = 0.20$.

fractions. Figure 7.22 shows the evolution of the phase transformation at the higher value of volume fraction $V_f = 0.35$. During the initial stages (as shown in Figure 7.22(a) – (d)) the response in one cell is not particularly affected by that in a neighboring cell. However, during the latter stages (as shown in Figure 7.22(e) – (h)) the martensitic regions in neighboring cells are seen to interact and eventually coalesce. Figure 7.23 shows the consecutive positions of the phase boundary at a sequence of times. Observe that once the interface sees its counterpart in the cell above it, it begins to accelerate and propagates faster than it had been up to that point. After coalescence the martensitic region begins to propagate by elongating more or less horizontally. (Along the particle surface the interface has been pinned by now and is at rest.)

A characteristic of the composite material here that is of particular interest is its “effective stress-strain response”. The shear strain $k_1$ along the top surface of the cell being analyzed is uniform. The shear stress $\tau_{32}$ however varies along this lines and its linear average gives the effective shear stress. Figure 7.24(a) shows a plot of this average shear stress versus
Figure 7.22: Time evolution of martensite and austenite for the ratio $l_m/l_g = 0.05$ at $V_f = 0.35$, with (a) at $t = 0.026$, (b) at $t = 0.028$, (c) at $t = 0.030$, (d) at $t = 0.032$, (e) at $t = 0.034$, (f) at $t = 0.036$, (g) at $t = 0.038$, and (h) at $t = 0.040$. 
Figure 7.23: Time evolution of the sharp interface from $t = 0.020$ to $t = 0.040$ for the parameters $\frac{l_m}{l_g} = 0.05$, and $V_f = 0.35$, where one chooses the strain $k = \frac{k_m + k_m}{2} = 0.075$ as the location of the sharp interface.

the applied shear strain (for the case when the volume fraction is $V_f = 0.35$). For purposes of reference the figure also shows the stress-strain relation for the matrix material. The symbols (a)-(h) on the effective stress-strain curve can be correlated with the corresponding plots (a)-(h) in Figure 7.22.

Initially, the elastic stress dominates the response and the couple stress effects are minimal. This is because in our theory, and for the small value of the material length scale $l_m$ chosen, couple stress effects only play a role in the vicinity of phase boundaries. The effective stress-strain curve in this range is stiffer than that for the matrix material purely because of the presence of the rigid particle. For all practical purposes, the effective elastic modulus in this range is solely dependent on the volume-fraction $V_f$ of the particle. The nucleation of martensite initiates at $k_\infty = 0.16$, close to where the slope of the stress-strain curve suddenly changes. The stress continues to increase as the new phase grows (see range $(a - e)$) until it reaches point $(e)$. Here the martensitic regions in adjacent cells coalesce (see Figure 7.22) and during this process the stress decreases. Once the coalescence of the martensitic regions has fully developed at $(g - h)$ the stress again begins to rise. Thus the "effective stress-strain
response" is the up-down-up curve shown in Figure 7.24(a). Figure 7.24(b) shows a series of effective stress-strain curves for different values of the material length scale (all at the same volume-fraction $V_f = 0.35$).

Figure 7.24: (a) Comparison between the stress-strain relation of the homogeneous matrix and the nondimensional elastic average stress required to propagate the interface at a constant rate of loading for $\frac{l_m}{l_g} = 0.05$ at $V_f = 0.35$, (b) dependency of the nondimensional elastic average stress on the ratio of $\frac{l_m}{l_g}$. 
7.3 Nucleation and propagation

In this section we examine a boundary-initial-value problem where the specimen has an inhomogeneity and it is loaded from a state of austenite to a state of martensite. The specimen is square and has a concentric circular inhomogeneity; it is subjected to a shear loading on two opposite faces, the remaining two faces being traction-free. We examine the macroscopic load-deformation response of the material as the specimen is loaded and then unloaded. During this process initially the austenite deforms elastically, martensite is then nucleated at the inhomogeneity and the martensitic region begins to develop. After some further loading, the martensitic region has developed into a band which runs across the specimen and contains the inhomogeneity; the martensitic band is parallel to the faces of the specimen that are sheared. On continued loading the leading edges of the band propagate normal to itself and eventually the entire specimen is composed of martensite. The specimen is then unloaded and roughly, though not in precise detail, it repeats this response in reverse.

In our calculations, the cross-section $\Pi$ is a square $L \times L$ and contains either a rigid particle (Section 7.3.1) or a cavity (Section 7.3.2) of radius $R$ at the center of $\Pi$. For the geometric length scale we take $l_g = R$. We also choose $L >> R$, to reduce the dependency of the results on volume fraction; specifically we take $L = 10l_g$. On the upper and lower sides we prescribe a uniform time-dependent displacement

$$u(x_1, \pm L/2, t) = \pm \delta(t), \quad \delta(t) = \frac{\dot{a}L}{2}t, \quad \text{for } 0 < t < t^*. \quad (7.51)$$

The rate of shearing the two sides is measured by $\dot{a}$. When we wish to unload the specimen at time $t^*$ we simply change the sign of $\dot{a}$. The sides $x_1 = \pm L/2$ are traction-free. See Sections 6.3.1 and 6.3.2 for a more complete description of the problem. As in the previous problem in Section 7.2, we take for the loading-related time scale

$$t_l = \frac{1}{\dot{a}}.$$
and the nondimensional length and velocity ratios $R_l$ and $R_t$ are taken to be
\[ R_l = \frac{l_m}{l_g}, \quad R_t = \frac{\dot{d}l_g}{v_m}. \]

We use $R_l = 0.05$ and use $R_t$ as our measure of the loading rate.

The main objective here is to calculate the macroscopic force-deformation response associated with a complete cycle of loading and unloading and to correlate its features with the local features of the phase evolution. The quantities that we will use in these plots are the nondimensional average traction $\bar{\tau}$ as a force-like quantity and the nondimensional displacement $\bar{\delta}$ as the kinematic variable:
\[ \bar{\tau} = \frac{<\tau>}{\gamma_r \mu}, \quad \bar{\delta} = \frac{\delta}{l_g}, \]  

(7.52)

where the average traction $<\tau>$ was defined previously by (6.9). Note that the nondimensional displacement $\bar{\delta}$ here is related to the average strain used in Section 7.1.1 by the ratio $L/l_g$ and ten times larger than the average strain. The nondimensional coordinate $\bar{x}_\alpha$ is defined as
\[ \bar{x}_\alpha = \frac{x_\alpha}{l_g}. \]  

(7.53)

We will drop the overbar from hereon; if confusion may arise, we will refer to the nondimensionality of the variable explicitly.

### 7.3.1 Rigid particles

Consider first the case where the inclusion is a rigid particle. Figure 7.25 shows a plot of the macroscopic load-deformation response.

The three different loops in 7.25(a) correspond to three different values of the maximum displacement to which the loading is carried out before unloading commences; the loading rate for the three curves is $R_t = 0.005$. The three curves in Figure 7.25(b) show the dependence of the hysteresis loop on the loading rate ($R_t = 0.004, 0.005, 0.006$), all for the same loading amplitude $\delta_{max} = 0.35$. The general behavior is rather independent of the rate of loading and only minor changes are observed:
a. The critical value of the applied displacement $\delta$ at the instant of nucleation varies with $R_t$.

b. The ensuing drop in the load is indirect proportional to $R_t$, since the necessary applied average stress at point (c) seems to be independent of $R_t$, but the steady state force increases linearly with the rate of loading $R_t$.

c. The jump in force at the final stage of the backward transformation decays with the rate of loading $R_t$.

These overall changes are generally minor, except if the rate of loading $R_t$ exceeds approximately the value of 0.01.

Figure 7.25: (a) Average elastic stress versus the displacement $\delta$. The three curves correspond to different values of the maximum prescribed displacement with a loading rate $R_t = 0.005$.

(b) Average elastic stress versus the displacement $\delta$ for different rates of loading $R_t$. The maximum displacement amplitude is the same for all curves: $\delta_{\text{max}} = 0.35$.

Figures 7.26(a) – (h) show a series of contour plots which depict the corresponding evolution of the phases during loading and unloading. The points marked (a) – (h) on the hysteresis loop in 7.25 correspond to the contour plot with the same label. In the contour
plots, the dark region is occupied by martensite (i.e. points where \( k > k_m \)), the lightly shaded region is occupied by austenite (i.e. points where \( k < k_M \)) and the transition layer \((k_M < k < k_m)\) corresponds to the medium shaded region. When we speak of an interface, we refer to the particular strain contour \( k = (k_M + k_m)/2 \).

In Figure 7.26(a) the applied value of \( \delta \) has reached a value which is sufficient to nucleate martensite at \((x_1, x_2) = (0, \pm R)\). On continuing to increase \( \delta \), the martensitic region expands outwards at a fairly uniform rate. Since \( k = 0 \) at the points \((x_1, x_2) = (\pm R, 0)\) the front gets pinned at some point along the surface of the particle; (see Figure 7.26(b)). A further increase of \( \delta \), corresponding to the range \((b)-(c)\), causes the martensitic region to expand horizontally in an elongated shape, extending towards the free surfaces at \( x_1 = \pm L/2 \). This dramatic change in the manner in which the martensitic phase grows is concomitant with an additional softening of the material. During the interval \((c)-(d)\) an increase in \( \delta \) induces a fast horizontal expansion of martensite and is accompanied by a drop in the applied stress when the martensitic region reaches the free surfaces at \( x_1 = \pm L/2 \). At stage \((d)\), martensite has formed two stable bands that are attached to the particle near \((x_1, x_2) = (0, \pm R)\). The two outer surfaces of the two bands are “free” to continue moving, the two inner surfaces are more or less “fixed”.

As \( \delta \) continues to increase correspondingly to \((d) - (e)\) (and beyond) the average stress remains constant and the force-displacement curve has a plateau. The effect of the particle is now secondary to the macroscopic response of the material and a continued increasing of \( \delta \) results in the free interfaces propagating vertically in the \( \pm x_2 \) direction. The response can now be modeled by the results of Section 7.1 for a straight interface propagating in a homogeneous strip. The fixed interfaces are now almost stationary and they entrap a band of austenite between them; the motion of the free interfaces increases the volume fraction of martensite to accommodate the change due to the loading. By further inspecting the data at \((e)\) one notes that the free interfaces are still curved at \( x_1 = 0 \) and the average stress \( \tau = 0.298 \) is lower than the prediction \( \tau = 0.308 \) for the straight interface for the same
loading rate $R_t = 0.005$. The reason for this slight discrepancy in the value of the average stress could be twofolded. First, the velocity and shape of the interfaces are not in full correspondence with a straight interface. Second, the mesh used here is rougher than the previous one causing the average stress to be underestimated by a few percentage points.
Figure 7.26: Time evolution of the martensitic (dark) and austenitic (light) regions at different instants during loading and unloading: (a) $\delta = 0.14$, (b) $\delta = 0.2$, (c) $\delta = 0.22$, (d) $\delta = 0.26$, (e) $\delta = 0.34$, (f) $\delta = 0.26$, (g) $\delta = 0.18$, and (h) $\delta = 0.14$. The transition zone has the medium shading. The figures (a) – (h) correspond to the similarly labels in Figure 7.25(a).
Upon beginning to unload, the response of the material is initially elastic. Thereafter the free interfaces reverse direction and propagate inwards towards the particle (behave like straight interfaces in a homogeneous domain; see Figure 7.26(f) and 7.25(a)). The free interfaces are also straighter during the unloading than they were during loading, and do not exactly retrace the same path (see Figure 7.26(e), (f)). The stress level at which this motion occurs is nearly constant and is approximately 8% larger than the result given by equation (7.16) for a straight interface. The fixed interfaces in turn are now more mobile and begin to propagate along the particle and free surfaces towards the corresponding free interfaces. The trapped layer of austenite starts to grow at a higher rate than it shrunk during the forward transformation. Between (f) – (g) the fixed interfaces detach themselves from the particle and connect with their mirror images, leaving the particle in the austenitic phase. This process is accompanied by a shallow drop of the load as the fixed interfaces accelerate towards their images. Consequently, two narrow bands of martensite have been created, by the simultaneous motion of the fixed and free interfaces (see Figure 7.26(f)). This evolution of the interfaces is unique to the reversed transformation. In Figure 7.25(a) we show that to complete the martensite/austenite transformation an additional amount of work has to be invested before the parent phase of austenite is recovered and the material responds once again purely elastic.

### 7.3.2 Cavity

In this section we consider the same problem as the preceding one but now with the particle replaced by a cavity. In Figure 7.28(a) – (k) a series of contour plots are depicted, to illustrate several important events during the evolution of the phases. Each plot (a) – (k) can be associated with the points (a) – (k) of the force-displacement Figure 7.27(a).

In Figure 7.27(a) we show three loading-unloading cycles with different amplitudes $\delta_{max}$, all at the same rate of loading $R_t = 0.005$. The dependency on the loading rate $R_t$ is described in Figure 7.27(b) where the three loops shown correspond to four loading rates, all
Figure 7.27: (a) Average elastic stress versus the displacement $\delta$ for a rate of loading $R_t = 0.005$. The three curves correspond to different values of the maximum prescribed displacement. (b) Average elastic stress versus the displacement $\delta$ for a range of different rates of loading $R_t$.

at a displacement amplitude $\delta_{max} = 0.45$. As expected from our previous results in Section 7.1, the hysteresis loop expands more or less linearly with respect to the rate of loading. Nevertheless, the increase in the rate of loading causes several characteristic features of the force-deformation relation to wash out, for example:

a. The point (b) at which nucleation occurs undergoes a horizontal shift and a vertical reduction, and

b. as $R_t$ increases the drop in the average stress at point (e) gets smaller, and the jump in the force between (j) and (k) becomes smaller.

We now discuss the contour plots (7.28) keeping the associated features of the load-deformation plot (7.27) in mind. In Figure 7.28(a), the value of the prescribed displacement has been sufficiently high so as to nucleate martensite at $(x_1, x_2) = (\pm R, 0)$. As $\delta$ continues to increase, the martensite expands rapidly towards the free boundaries (see Figure 7.28(a) –
(c)). At (b), the martensitic region is in contact with the free boundaries \( x_1 = \pm L/2 \); the stress drops as the martensite accelerates towards the boundary and eventually the martensite establishes itself as a uniform band of nearly constant width. This relatively fast process comes to an end at point (c).

When \( \delta \) continues to increase ((c) – (e)) the interfaces struggle to overcome the adverse strain gradient along the boundary of the cavity. The ends of the interface at the free boundaries move about three times as fast as the end on the cavity wall. This exemplifies itself by a linear increase in the materials macroscopic resistance in the range (c) – (d). Point (e) marks the instant when the interfaces connect with each other leaving behind a small pocket of austenite. These pockets are enclosed by part of the cavity wall and by newly generated interfaces (see Figure 7.28(f)). For sufficiently slow rates of loading as shown in Figure 7.27(b) one observes that the joining of the two interfaces at (e) is accompanied by a small drop in the average elastic stress. The plateau of the applied stress between points (e) and (f) has a similar value to the one calculated in Section 7.1. The parallel interfaces are now sufficiently far removed from the cavity.

In order to simplify our writing, let us refer to a long interface parallel to the loading axis as a “free” interface and the smaller interface surrounding the pocket of austenite as the (relatively) “fixed” interface. After point (f), the loading is reversed and the free interfaces reverse their direction of propagation and straighten up further as shown in (g). The fixed interfaces mostly expand vertically but remain fixed at their point of pinning along the perimeter of the cavity. The associated stress reaches a steady state value of the order of magnitude predicted in Section 7.1.2 for a straight interface. At point (h) it becomes clear that the process is different from that during the forward transformation: observe that the fixed and free interfaces approach each other and continously reduce the size of the thin band of martensite at \( x_2 \approx \pm 2 \). The mobility of the fixed interfaces has increased considerably, but is still less than that of the free interfaces.
Figure 7.28: Time evolution of the martensitic (dark) and austenitic (light) regions during loading and unloading: (a) $\delta = 0.16$, (b) $\delta = 0.18$, (c) $\delta = 0.20$, (d) $\delta = 0.34$, (e) $\delta = 0.38$, (f) $\delta = 0.44$, (g) $\delta = 0.40$, (h) $\delta = 0.32$, (i) $\delta = 0.26$, (j) $\delta = 0.16$, and (k) $\delta = 0.10$. The loading rate is $R_t = 0.005$. The transition layer has the medium shading. The Figures (a) – (k) correspond to the similarly labeled point in Figure 7.27(a).
As the imposed displacement $\delta$ continues to decrease, at point $h$ another fast process occurs, when the fixed and free interfaces merge. Each single free interface has separated into two parts and attached itself to the cavity (see Figure 7.28(i)). This process is concomitant with a brief rise in the applied stress at point $h$. The distribution of phases is then rather similar to the one characterized by $(d)$. Thus the interfaces retrace in the range $(i) - (j)$ of unloading a path that is similar to that during the loading stage $(c) - (d)$. Of course the stress field in the specimen is different during these two processes which one can deduce from Figure 7.27(a) which shows that the stresses $\tau_{MA}$ for the forward transformation and $\tau_{MA}$ for the reverse transformation are different. As the evolution approaches point $(j)$ another fast process is starting to develop. The remaining band of martensite has to be squeezed out of the domain, requiring a certain amount of work as illustrated by the momentary rise in the applied stress in Figure 7.27(a) in the range $(j) - (k)$. Further unloading is then purely elastic and the material is in the austenitic phase.
8.1 Discussion of mathematical models

In Chapter 2 we reviewed the sharp interface theory for thermoelastic martensitic transformations. This theory requires, in addition to the elastic potential, the specification of a kinetic relation and a nucleation criterion. The former describes the dissipative properties of an existing interface, and the later is the condition which characterizes the initiation of the transformation. These additional assumptions are required in order to completely model dynamic processes involving phase transformation.

In Chapter 3 we developed a couple stress theory in order to consistently regularize sharp interfaces. The richer description of the kinematics allows one to generalize the concept of "forces", and introduce a stored energy function that depends on the lagrangian strain $E$ and the tensor $K$ ($K$ is a measure of the change in curvature). In order to model the dissipative nature of the process the constitutive relation for the stress tensor involves a dependency on the strain rate. Thus the smooth interface has been given structure and it dissipates energy.

Next we established the correspondence between the sharp interface theory and the couple stress theory, by considering the one dimensional problem of a traveling shear wave. The elastic part of the material model here involves a trilinear stress-strain curve in shear. The main results of this analyses can be summarized as follows:

- The couple stress theory can be used to describe a smooth interface which connects
martensite and austenite through a thin transition layer.

- The couple-stress theory has an effective kinetic relation.

- The sharp interface theory and the couple stress theory will yield equivalent results if the preceding effective kinetic relation is specified as the appropriate kinetic relation for the sharp interface theory.

## 8.2 Kinetics of interfaces propagating in a homogeneous medium

In Section 7.1 we numerically simulated this problem. Rather than the trilinear material, we used here a power-law relation (5.46) with similar characteristics. The domain was sufficiently long to be considered infinite and it contained a single smooth interface. The analytical results of Chapter 4, were verified and several additional points were illuminated:

- The straight interface smoothly connected austenite and martensite.

- The steady state stress of the sheared slab is linearly related to the steady state speed of the propagating interface as shown in Figure 7.2; e.g. the stress increases for the forward transformation (austenite $\rightarrow$ martensite) and decreases for the reverse transformation (martensite $\rightarrow$ austenite).

- The couple stress theory (with the power law stress-strain relation) implies the effective kinetic relation shown in Figure 7.3.

- The effective kinetic relation for the power-law material was well approximated by a trilinear material with equal dissipative properties. We hypothesize that an arbitrary stress-strain relationship can be well modeled by a piecewise linear model provided the following two criteria hold: (i) the equivalent trilinear material has the same Maxwell stress as the power law material, and (ii) the area enclosed by the loop of the stress-strain relation above (or below) the Maxwell line is the same for both stress-strain
relations. Clearly, better approximations can be obtained for each individual case, but we doubt that the method is as simple and consistently transferable.

- The steady state velocity of propagation is linearly related to the rate of loading, and indirectly proportional to the transformation strain at the corresponding steady stress level (see Figure 7.4 and Section 7.1.3 for more detail).

- The thickness \( b \) of the transition layer is inversely proportional to the driving force given by the kinetic relation of the material (see analytical approximation (7.29)).

- The smooth interface has a minimal constant thickness \( b \), which is approached asymptotically for decreasing velocities of propagation of the interface (see Figure 7.4 and 7.6).

- We also showed how the different data are related to each other and a good understanding of the interrelation of the unknown quantities was developed by dimensional analysis. We illustrated this in two separate discussions. We first related the transformation strain to the velocity of propagation for the forward and reverse transformations. Secondly, we developed the dependency between the driving traction \( f \) and the interface thickness \( b \) to attain a simple relation for the kinetic relation (7.32).

Based on this study several conclusions on the adequacy of the model can be reached. The couple-stress theory has proven to be able to capture under isothermal conditions the most characteristic effects of pseudoelasticity in Shape Memory Alloys. One of the shortcomings of the model is its linear dependency on the rate of the shear strain \( k_{\alpha} \). This gives rise to a monotonic kinetic relation with \( f = 0 \) when \( V_n = 0 \), as shown in Figure 7.3. This behavior appears not to be consistent with experimental results of uniaxial tension by Shaw & Kirakides [76], who have observed a finite driving traction for nonpropagating interfaces, so that \( f \neq 0 \) when \( V_n = 0 \). (Simple shear and uniaxial tension have the same governing equations, thus one should expect a qualitatively similar kinetic relation). This deficiency
is inherent to the model and could be eliminated by a nonlinear dependency on the strain rate, which "anticipates" the nucleation of interfaces. Workers like ROSAKIS [73] currently attempt to find a more appropriate augmentation for uniaxial tension.

The forte of both theories lies in the evaluation of micromechanical effects in the continuum framework. In this context the sharp interface theory has proven to be a useful tool. Its strength is its concise formulation, and independence it affords in specifying the phase's bulk behavior, and the interface's properties. The major reason to pursue a higher-order strain gradient approach is the simplifications one attains in multidimensional problems. In a purely mechanical setting a single governing equation now incorporates the nucleation and evolution of interfaces throughout the domain. The simplicity and richness of the approach has been illustrated in several numerical problems, to which we will refer next.

8.3 The role of inhomogeneities

A large part of this study has been focused on the effect of inclusions (of different types and shapes) on the response of a Shape Memory Alloy. We investigated four specific issues:

- First, we considered the effect of an inhomogeneity upon the initial nucleation of martensite.

- Second, we analyzed a periodic array of particles and examined the influence of the particle volume fraction $V_f$ on the macroscopic response of the material. Based on these problems we also established the influence of the material length scale $l_m$ with respect to the inherent geometric length scale $l_g$.

- Third, we examined how an inclusion which stands in the path of a propagating interface obstructs its motion.

- Lastly, we examined the complete problem of nucleation, development and propagation of a martensitic band beginning from an inclusion.
Each of these problems has been discussed in detail in Chapter 7. In the following sections we will summarize the most significant observations and results.

### 8.3.1 Nucleation of martensite

Particles, holes, and cracks play a very distinct role at the initial stage of nucleation. Let us first concentrate on the nucleation and subsequent development of martensite. Martensite nucleates at points with the highest strain concentration. For a particle we observe the following:

- Martensite nucleates at \((x_1, x_2) = (0, \pm R)\) and forms two small regions which are partly bounded by the particle and by an austenite/martensite interface (for a description of the geometry and loading see Section 7.2).

- When the load is increased, interfaces become pinned at some points along the perimeter of the particle, causing the interface thereafter to expand horizontally above the point of pinning (see Figure 7.12).

- The transition layer has a thickness that is similar to that of a straight interface (see Figure 7.13).

- The highest velocity of propagation of the arc like austenite/martensite interface is greater than that for a corresponding straight interface (see Figure 7.13 and 7.4).

For a hole and a crack, the results are quite distinct from that for a particle. The point with the highest strain is now rotated by 90°. For the hole the most obvious observations are briefly summarized as follows:

- The nucleated region of martensite is a needle like structure reaching into the austenitic domain as shown in Figure 7.14.

- The velocity of propagation of the tip of this structure is several orders of magnitude higher than the velocity of propagation of the straight interface or interface nucleated
at a particle (see Figure 7.15).

- Along the long sides of the needle-like martensitic region, the transition layer's thickness \( b \) is scaled by the material length scale \( l_m \).

- Around the tip of the martensitic region, the transition layer is not scaled by the material length scale \( l_m \), but is rather characteristic of a microstructure (see Figure 7.14 and 7.16).

The crack generates a similar distribution of phases to the hole. Nevertheless, several differences exist:

- The macroscopic strain of nucleation is lower, due to the larger curvature at the tip of the crack.

- The nucleated martensite is initially arrested by the crack, retarding its penetration into the austenitic domain (see Figure 7.17 and 7.18).

When the martensite has penetrated sufficiently deep into the austenitic domain the differences between a hole and crack as a nucleation site vanish. On the other hand the martensitic region nucleated by a particle is quite distinct, and is such that the amount of transformed martensite is less than that for the other two inclusions. Also, they are locally bounded if other effects do not perturb the current equilibrium configuration. The importance of some of those external influences have been studied and are summarized in the next section.

### 8.3.2 Periodic arrangement of particles

Now let us consider what occurs if a periodic array of circular particles of given size and volume fraction \( V_f \) are placed in a domain. We assume the volume fraction \( V_f \) to be relatively high and studied two cases with \( V_f = 0.20, 0.35 \). In Section 7.2.4 we described the results of a periodic arrangement of cells which was continuously sheared. Initially, the response was
similar to the one observed for the single particle in an infinite domain, but once the applied shearing was sufficiently large to cause the martensitic region in one cell to interact with the martensitic region in another cell we observed that:

- The regions of martensite connected with each other, forming an alternating pattern of martensite and particles in an austenitic matrix (see Figure 7.22).

- The process is characterized by a macroscopic response with several distinct features as shown in Figure 7.24.

- The contribution of the couple stress is negligible if the domain is composed of austenite.

- The nucleation of martensite is concomitant with a softening of the macroscopic response.

- As the regions of martensite coalesce the average stress necessary to expand the single region of martensite between the two particles drops (for more detail see Section 7.2.4).

### 8.3.3 Influence of the material length scale

As mentioned previously, the numerical values of the ratio \( l_m/l_g \) (where \( l_m \) is the material length scale and \( l_g \) is the geometric length scale) that were used in our calculations were smaller than those used by researches whose interest is in the couple stress theory per se (without phase transformation) and so they had significant couple stress effects in the bulk response of the material. In contrast, for the small values of \( l_m/l_g \) that we consider, bulk couple stress effects are only noticeable in the immediate vicinity of a phase boundary. The significance of this is further illustrated by the results in Figure 8.1. This figure shows the value of the remotely applied shear strain at the instant when nucleation occurs; it shows this for each of the four problems 6.2.1-6.2.4, and for a range of values of \( l_m/l_g \). For small values of \( l_m/l_g \), we observe for example that the remote strain level at nucleation is much
Figure 8.1: Nondimensional nucleation strain to observe the initial occurrence of martensite for the previously discussed problems at different ratios of $\frac{\ell_m}{\ell_g}$.

smaller for the crack in comparison with the cavity. This is not surprising of course since the crack has a much higher strain concentration effect. However observe that for larger values of $\ell_m/\ell_g$ this difference in strain-levels has more or less disappeared. Couple stress effects are now significant even prior to nucleation, and this cancels out the differences between the strain concentration effects of the different inclusions. It is this latter range of values of $\ell_m/\ell_g$ that those principally interested in couple stress effects have focused on; in contrast it is the former range that we have focused on here, because in our point of view couple stresses are simply a device for regularizing the sharp interface theory.

8.3.4 Propagating across an inclusion

In Section 7.1.6 we studied the effects of particles and holes that stand in the way of an approaching interface. The main question that we addressed pertained to the effective kinetic relation of the domain. We illustrated the evolution of the phases, examined when the
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effect of the inclusion becomes significant, and interpreted the contribution of these local occurrences to the effective kinetic relation. More specifically, it was shown how the hole induced the nucleation of several additional interfaces of sufficient mobility, so that the average effective kinetic relation is steeper with respect to the average velocity of propagation. On the other hand a particle reinforced domain yielded a flatter kinetic relation with respect to the average velocity of propagation. We concluded, that the additional interfaces do not compensate for the significant reduction in the velocity of the primary interface during the extended period of pinning.

8.3.5 Nucleation and growth

From the problems studied under this category (Section 7.3) we have gained some important insights into the process of nucleation and growth of martensite during a stress-induced transformation. In particular, we have been able to relate various characteristics of the macroscopic force-displacement curve to local events. We have also seen the difference between nucleation at a rigid particle versus at a cavity. In both cases, once a nearly straight interface has developed, the results pertaining to the propagation of a straight interface in a homogeneous body discussed in Section 7.1 are applicable. The principal macroscopic characteristics of the response in the two problems are depicted in Figure 7.27 and 7.25. The detailed process of nucleation, and the subsequent development of a martensitic band are rather different in the two cases.

For the rigid particle, the initial nucleation of martensite occurs at a displacement \( \delta \approx 0.14 \). This is followed by a continuous expansion of the martensitic region which is accompanied by a considerable softening of the response until the peak stress is attained at \( \delta \approx 0.22 \). At this point the interfaces suddenly break-free. Thereafter, the stress necessary to propagate the interfaces drops to the value associated with propagating a straight interface in a homogeneous body.

In the case of a cavity, the formation of the martensitic band is a longer lasting process.
Initial nucleation of martensite occurs at $\delta \approx 0.16$, with a brief period of transition to $\delta \approx 0.18$, at which point the interfaces connect to the free surfaces of the specimen. This is followed by a stage of linear hardening until the stress level has risen sufficiently to support a straight interface; this occurs at $\delta \approx 0.38$ (see Figure 7.27(a) point (e)). The stress level now is consistent with that necessary to propagate a straight interface in a homogeneous body.

Our calculations related to unloading showed that, while the main evolution of the phases is similar, several unique features are associated with the reverse transformation. In the presence of a rigid particle, the process is very much like that for a straight interface, except in the immediate vicinity of the particle (approximately as close as half the particle diameter away from the particle). An additional amount of work has to be done (see Figure 7.25(a) at (g) — (h)) to recover austenite.

In case of the cavity, a more complicated process occurs during unloading (Figure 7.27). First, the straight interface gives results of good agreement with results of Section 7.1, but later on, a small rise and linear softening of the specimen is encountered. The final transformation of martensite $\rightarrow$ austenite can now be accomplished by a stress increase of half that in the case of the particle, which occurs at a considerably smaller displacement $\delta \approx 0.1$ than for the particle (which occurs at $\delta \approx 0.14$).

We conclude that a one-dimensional model would be quite successful in predicting many aspects of the material response. This is seen from the agreement between the results in the presence of an inhomogeneity and that in its absence (Section 7.1). Once the martensitic band has developed, the stress plateau in the macroscopic response is the same as that corresponding to a straight interface in a homogeneous body. Nevertheless, the phenomena (such as the local stress maximum) associated with nucleation and the development of the band are intrinsically higher-dimensional phenomena.
8.4 Future work

In conclusion, we describe some projects that we are currently working on and some others that are awaiting future research.

A boundary-value problem that we are currently investigating is designed to illuminate the serrated stress-displacement graphs which are observed experimentally. The problem is a combination of the problems discussed previously in Chapter 6.1.2 and 6.3. Here, we prescribe a constant stress on two faces of the specimen and observe the evolution of a pre-existing straight interface as it encounters and crosses through an inclusion. For small values of the applied stress the interface gets stuck at the inclusion and does not proceed. If the applied stress is sufficiently large, the interface is able to pass through the inclusion and then transform the entire specimen. This calculation is being carried out for several different values of applied stress, and the results will allow us to find the effective kinetic relation of the medium. The phenomenon just described makes it clear that a finite value of driving force is required in order to make the transformation occur, and the kinetic law is therefore similar to a "frictional model" as calculated by Abeyaratne, Chu & James [8].

As emphasized previously, our use of the couple-stress model has been viewed solely as a technique for regularizing the problem to allow numerical solution of the "sharp interface theory". In this sense, our model included only the most necessary ingredients for this purpose. Several assumptions were made, such as the assumption that the energy potential depended on the kinematic quantity $\kappa$ (which led to a simple form for the stresses (3.102) and the governing equation (3.100)). A couple-stress model that is built on physical considerations should be addressed in future work.

Our analysis has been limited to quasi-static motions. The theory should be extended to account for inertia (in order to model, for example, the impact induced phase transformations studied by some researchers). Inclusion of the concept of inertia is not as straight forward as in the theory without couple stresses. One has to account for rotational and translational
kinetic energy of a particle as well as rotational and linear momentas. It would be of interest to see if the change of the rotational momenta and kinetic energy of a particle are ultimately negligible. Then a reduced theory with inertia solely implied in the usual way would be sufficient.

A number of effects in pseudoelasticity require that one account for the coupling between the mechanical and thermal responses of the material. One will first have to determine a regularized version of thermoelasticity with an explicit dependency on the temperature $\theta$. This model would capture the \textit{self heating} of specimens due to latent heat and non-equilibrium effects at propagating interfaces, and allows for thermal interactions with the environment. This varying temperature field induces anisotropic mechanical properties, which could be fundamental to the proper understanding of the relation between the applied force, loading rate, and nucleation of new interfaces.

Our study, while rather comprehensive, has been limited to anti-plane shear. Clearly, other modes of deformation should be investigated. One task of interest is to adapt the three-dimensional couple-stress theory to the cases of plane stress and plane strain. The numerical parts of this work should be facilitated by the recent development of higher order finite elements by \textsc{Xia \& Hutchinson} [89]. These elements have been developed for a strain-gradient plasticity theory with similar underlying kinematics.

The numerical simulations that we presented were obtained on non-adaptive meshes. Thus the largest possible size of an element was determined by the desired resolution of the smoothed interface with steep gradients. Since those interfaces propagate throughout the domain, the mesh has to be refined only in the areas that the interface is presently moving through. The number of necessary elements could be significantly reduced by including an adaptive mesh generation, which tracks the interface and refines the mesh in the vicinity of it.

\textsc{James} and his co-workers are currently developing two-dimensional experiments for Shape Memory Alloys. In their experiments a thin rectangular plate of SMA is biaxially
stretched in a soft device. Our work would benefit from some simple-shear or pure-shear experiments, that could be extended to include nucleation and propagation of phase boundaries as discussed in Chapter 7.3. Such experiments are also being carried out and should be used to validate our model.
Bibliography


