Modeling of Shape Memory Alloys: Phase Transformation/Plasticity Interaction at the Nano Scale and the Statistics of Variation in Pseudoelastic Performance

Dissertation

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By

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Abstract

Shape memory alloys (SMA) show two remarkable properties—pseudoelasticity and shape memory effect. These properties make them an attractive material for a variety of commercial applications. However, the mechanism of austenite to martensite phase transformation, responsible for these properties also induces plastic deformation leading to structural and functional fatigue. Micron scale experiments suggest that the plastic deformation is induced in part due to the local stress field of the fine martensite microstructure. However, the results are qualitative and the nature of transformation-plasticity interaction is dependent on factors like the width of the interfaces.

This thesis presents a new modeling approach to study the interaction between martensite correspondence variant scale microstructure and plastic deformation in austenite. A phase field method based evolution law is developed for phase transformation and reorientation of martensite CVs. This is coupled with a crystal plasticity law for austenite plastic deformation. The model is formulated with finite deformation and rotations. The effect of local crystal orientation is incorporated. An explicit time integration scheme is developed and implemented in a finite element method (FEM) based framework, allowing the modeling of complex boundary conditions and arbitrary loading conditions.
Two systematic studies are carried out with the model. First, the interaction between plasticity and phase transformation is studied for load-free and load-biased thermal cycling of single crystals. Key outcomes of this study are that, the residual martensite formed during thermal cycling provides nucleation sites for the phase transformation in the subsequent cycles. Further, the distribution of slip on different slip systems is determined by the martensite texture. This is a strong evidence for transformation induced plasticity. In the second study, experimentally informed simulations of NiTi micropillar compression are performed. The results reveal that the slip system activated, depends on the nature of the local deformation created by martensite CVs at the austenite-martensite interface. This is in qualitative agreement with the past analytical and experimental work. There are other factors like the width of the A-M interface, that influence the interaction between slip and phase transformation.

At the granular length scale, a systematic study of the factors influencing statistics of the pseudoelastic performance of the grains in a polycrystal SMA is performed. An existing grain scale microstructural FEM model calibrated to Ti-50.9at.%Ni is used to achieve this. Local crystal orientation of the grain, crystal orientation of the neighboring grains and the nature of the interfaces between the parent and the neighbors are the factors responsible for introducing a variation in the grain performance. A predictive function for the performance of a grain, as a function of the Schmid factors for transformation for the parent and neighbors is proposed. Two strategies are proposed to improve grain performance. The first is to reduce the number of interfaces, e.g. by constructing a bamboo or isostrain arrangement of grains. The second is to employ high-symmetry interfaces between grains, so that multiple
equivalent martensite plates can be activated at the interfaces, without compromising performance.
This dissertation is dedicated to my parents Smita and Madhukar Paranjape
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Chapter 1: Introduction

Recovery of the original shape of a sample on heating, irrespective of the deformation imposed at a lower temperature is known as shape memory effect. Alloys exhibiting this property are collectively known as shape memory alloys (SMAs). Au-47.5at%Cd was the first alloy found to exhibit the shape memory effect. Subsequently this phenomenon was observed in Cu-Al-Ni, Cu-Zn, In-Tl, Ni-Ti and other alloys. Today, Ni-Ti alloys remain the most popular class of SMAs [4]. Apart from metals, ceramics and polymers are known to exhibit shape memory effect [5, 6, 7].

The property of generation of large recoverable strain on loading and unloading is known as superelasticity (alternately referred to as pseudoelasticity). Many SMAs exhibit this superelastic behavior above a certain temperature characteristic of each alloy. The recoverable strain due to superelasticity varies from a few percent to 18% [4].

A solid to solid, displacive, reversible phase transformation, known as martensitic transformation, is responsible for the shape memory and superelasticity phenomena [8, 2]. The phase that is stable at higher temperature is generally referred to as austenite. The phase stable at lower temperature is referred to as martensite. Martensite phase possesses lower crystallographic symmetry compared to austenite. This leads to formation of multiple martensite variants (correspondence variants or CV), equivalent
in terms of energy. When no external stress is applied during cooling, the martensite variants tend to form a twinned microstructure such that the phase transformation does not produce any net shape change in the sample. A pair of martensite variants forming a twin is referred to as martensite plate or habit plane variant (hpv). When an SMA is stressed in the martensitic state, different martensite plates reorient into a single plate, resulting in macroscopic deformation. Such deformed sample, on heating, transforms back to the austenite phase, while completely recovering the deformation that occurred in the martensitic state. This roughly explains the mechanism of shape memory effect. When a SMA sample is stressed in the austenitic state, stress-induced martensite is formed. Such martensite is oriented in the sense that, certain plates are preferably formed based on the crystallographic orientation of the sample and the applied stress state. Formation of such oriented martensite results in a large strain, whose value is dependent on the SMA alloy system and the applied stress. This strain is recovered on removing the applied stress, owing to a reverse transformation from martensite to austenite. This roughly explains the phenomenon of superelasticity [2, 8]. The general terminology related to SMA is summarized in Figure 1.1.

The focus of this dissertation is to understand the performance of SMAs under various constraints. At the grain level this constraint can be due to the neighboring grains. At an even finer level, plastic deformation can constrain phase transformation and subsequently affect performance. In the spirit of understanding these effects, mechanical response exhibited by SMAs under various thermo-mechanical histories is summarized in the next Section. This is followed by a brief review of literature pertaining to the modeling of the mechanical behavior of SMAs. This review of modeling is focused on modeling the interaction between phase transformation and plastic
1.1 Response of SMA to Thermo-Mechanical Loading

Thermal cycling with or without external load, isothermal stressing and cyclic stressing (fatigue testing) are the three conventional modes of testing SMA for mechanical response. Each of these tests can provide information about the performance of SMA and the interaction between phase transformation and plasticity in the SMA.
Thermal cycling provides information about the evolution of microstructure. This type of measurement is important because actuators, the most popular application of SMA are subjected to such cyclic thermo-mechanical loading conditions. Isothermal stressing is the principal experimental technique of investigating superelastic behavior of SMA. Experimental response of SMA under these testing conditions is briefly discussed.

1.1.1 Thermal Cycling Without Biasing Load

Austenite to martensite transformation in a SMA initiates when the sample is cooled below a critical temperature. The undercooling provides necessary driving force to initiate the phase transformation. Figure 1.2 (a) shows a differential scanning calorimetry trace for a Ni-Ti SMA sample. The austenite to martensite transformation is marked by release of heat. The start and finish of the austenite to martensite transformation is usually marked on the temperature scale as $\theta_{MS}$ and $\theta_{MF}$ respectively. The transformation from martensite to austenite occurs during heating. The start and finish of this transformation is usually marked as $\theta_{AS}$ and $\theta_{MF}$ respectively. Alternatively, the forward and reverse transformation can be detected by measuring a physical property of the sample like electrical resistivity. Figure 1.2 (b) shows the variation of resistivity with temperature for a typical Ni-Ti SMA. Phase transformation can be identified by departure from linear trend in resistivity. The fact that $\theta_{MS}$ and $\theta_{AS}$ are not the same, can be explained by considering the necessity of undercooling required to initiate nucleation of each phase. Similarly, the range of temperatures necessary to complete each of the transformations can be explained by considering that, a continuous undercooling or superheating is needed to overcome the frictional
forces on the moving interfaces and the resistance of the local elastic fields to the growing phase [4].

![DSC traces](image1.png)

Figure 1.2: (a) Differential scanning calorimetry (DSC) traces used to determine the transformation temperatures for an SMA. (b) Electrical resistivity traces can provide similar information about the transformation temperatures. [2]

Martensite forms a twinned self-accommodating microstructure with triangular morphology [9, 10, 11]. Miyazaki et al [12] and Pelton et al [13] found that $\theta_{MS}$ decreases with cycling in solutionized polycrystalline NiTi SMA. They attributed this result to dislocations being generated at the austenite-martensite interface which resist the growth of martensite. In aged NiTi, $\theta_{MS}$ was found to be more stable, possibly because precipitates inhibit dislocation motion. Miller and Lagoudas [14] showed that plastic pre-deformation done in austenitic state ($T \gg \theta_{AF}$) generates an inhomogeneous stress state, which stabilizes martensite during bias-free thermal cycling, leading to some residual strain generation.
1.1.2 Thermal Cycling With a Biasing Load

In the presence of a biasing load, the hysteretic nature of SMA response is maintained, but the martensite microstructure is no longer self-accommodating. Preferred martensite plates are formed after cooling Ni-Ti SMA in the presence of a biasing load [15]. As the bias is increased, the transformation strain increases due to an increase in the formation of the preferred martensite plates [16, 17]. Apart from the transformation strain, there is some residual strain present which increases with cycling. In the absence of precipitates, the hysteresis is widened due to introduction of the dislocations at the austenite-martensite interface [15, 18]. Generation of dislocations suggests the possibility that some martensite is stabilized after each cycle which contributes to the residual strain [14]. These effects are observed in single crystals of Ni-Ti as well as polycrystals [15, 16]. Jones and Dye [17] report that the texture of martensite continuously changes with thermal cycling. This suggests that the martensite plate preference changes over thermal cycles due to the dislocations and stabilized martensite. Additionally, $\theta_{\text{MS}}$ decreases with cycling [17].

1.1.3 Isothermal Stressing at a Temperature Below $\theta_{\text{MF}}$

Martensite is the dominant phase in the SMA at $T < \theta_{\text{MF}}$. The deformation behavior of martensite has been extensively studied [10, 11, 14, 19, 20, 21, 22]. The observations in the literature indicate that the thermally produced martensite is self-accommodating. It exists in groups of twinned variants. At lower external stresses, some martensite plates grow into those plates which are more favorably oriented to the external stress. This process is referred to as martensite reorientation. Since the martensite plates are equivalent in terms of energy, this stage is not accompanied
by significant hardening. If the sample is unloaded at this stage, the deformation does not vanish. Further stressing results in the detwinning of martensite plates into individual variants. Since twinning is the source of shear accommodation in the martensite plates, once the detwinning has occurred, the shear is accommodated by introduction of dislocations. These dislocations stabilize the detwinned martensite, resulting in an elevation of $\theta_{AF}$ temperature. If the martensite is further loaded, it deforms by plastic slip.

Whether reorientation or detwinning occurs first seems to be not unambiguously verified in Ni-Ti SMA. However diffraction studies are capable of estimating contributions to the total strain from elastic, twinning and plastic deformation components [23].

1.1.4 Isothermal Stressing at a Temperature Between $\theta_{MF}$ and $\theta_{AF}$

Austenite and martensite phases coexist in the temperature range defined by $\theta_{MF} < T < \theta_{AF}$, in the stress free Ni-Ti SMA. The mechanical response is determined by reorientation and detwinning of martensite, and stress induced transformation of austenite into martensite. The former mechanism results in non-recoverable deformation. The latter mechanism may be able to recover some strain. [20, 24]. Nanoindentation based studies in this regime have shown that dislocation based plasticity is far smaller compared to phase transformation in Ti-50.7at.%Ni aged for 24 h at 1223K [25, 26]. This can be expected because mobility of dislocations is lower at lower temperatures and martensite is energetically favored compared to austenite.
1.1.5 Isothermal Stressing at a Temperature Greater than $\theta_{AF}$

Austenite is the stable phase at temperatures greater than $\theta_{AF}$ in the absence of external stress. Externally applied stress is capable of initiating a reversible austenite to martensite transformation. This reversible transformation gives rise to the phenomenon of superelasticity, which is previously discussed.

Stress-strain response of Ni-Ti SMA stressed to failure can be split into three distinct stages characterized by stress induced martensite (SIM) formation, SIM formation coupled with austenitic plasticity and martensitic plasticity respectively [20]. Figure 1.3 (a) shows such response of a Ti-50.6at.%Ni SMA. In stage I, since all the strain is generated by SIM, it is completely recovered on unloading. In stage II, some SIM is stabilized by the dislocations in austenite. This results in incomplete recovery of strain on unloading and even on heating to 373K. Though the authors of [20] claim the (dislocation based) plasticity to be the sole mechanism of martensite deformation in stage III, it is possible that martensite reorientation and detwinning are contributing. Heating to 373K might be insufficient to recover the strain imparted by stabilized martensite.

Critical stress for stress induced martensite transformation increases with temperature (in single crystals [27] and polycrystals [20, 28]). This is a manifestation of Clausius-Clapeyron relation. This can be seen in the stress-strain curves for polycrystalline Ni-Ti sample shown in Figure 1.3 (b). Residual strain on unload increases with temperature. This could be because of easier generation of dislocations at elevated temperature.
Figure 1.3: (a) Pseudoelastic response of Ti-50.6at.%Ni SMA. As the material is progressively subjected to higher strains, it goes to elastic, transformation and plastic deformation stages. (b) Pseudoelastic response of SMA at various temperatures. As the temperature increases, martensite becomes less and less energetically favored compared to austenite. This leads to rising critical stress (plateau stress) for transformation. [3]

The response of single crystals is strongly dependent on crystallographic orientation [29, 30, 31]. The dependence of superelastic response on crystal orientation suggests that the response of polycrystals would depend on the crystallographic texture [32]. Depending on orientation, some single crystals are very prone to austenitic slip and it is difficult to observe superelasticity unless care is taken to prohibit slip [27]. The residual strain on unloading is dependent on crystallographic orientation. This is due to the dependence of plastic slip on crystal orientation.

Tension-compression asymmetry is observed in the response of single crystals and polycrystals of Ni-Ti SMA [32, 33, 34, 35, 36, 37]. The critical stress for forward transformation is lesser and total superelastic strain is larger during tension. In single crystals, this asymmetry can be explained noting that different martensite plates are activated during tension and compression. This will become apparent when analytical models of superelasticity are explored. An interesting observation is that, in
the presence of fine precipitate particles, the tension-compression asymmetry is less apparent in single crystals [36, 37]. In polycrystals, depending on their crystallographic texture, this asymmetry is carried over [38].

Plasticity and martensitic phase transformation interact at macroscopic as well as microscopic scale. At the macro scale, there is strong evidence for stabilization of martensite due to plasticity [15, 20, 24]. This is demonstrated in the increasing residual strain with each cycle in Figure 1.3(a) and larger residual strain at elevated temperature in Figure 1.3(b). Stabilization of martensite by plastic pre-deformation in austenite state affects macroscopic response during subsequent loading [14, 39]. On a smaller length scale, plasticity and transformation are coupled at the grain level. This is manifested by an abnormal orientation dependence of the micro-hardness in the presence of a stress induced martensite \( T > \theta_{AF} \) [37] and a dependence of the degradation of the cyclic performance of single crystals on the crystallographic orientation [29]. At even smaller length scale, dislocations have been observed in the austenitic phase [13, 15, 31, 40, 41, 42, 43, 44]. These small length scale experimental studies of the interaction between phase transformation and plastic deformation are discussed below in further detail as they provide motivation for the work presented in this dissertation.

Hurley et al [44] performed cyclic pseudoelastic loading on Ti-50.5at.%Ni mm sized single crystal and later analyzed the microstructure of the specimen using TEM. They observed that the periodicity of the dislocations in austenite is similar to the internal twin width of the martensite plate. Based on this they concluded that the local stress field of the twinned martensite variants is responsible for the defect generation in austenite. A similar qualitative connection between the martensite twins and
austenite plasticity was made by Simon et al [41] using thermal cycling experiments of Ti-50.4at.%Ni microcrystals and in-situ TEM observations and by Pelton et al [13] using thermal cycling tests on Ti-50.5at.%Ni millimeter sized single crystals and ex-situ TEM analysis. Norfleet et al and Bowers et al performed compression tests on single crystal Ti-50.7at.%Ni micron sized pillars and analyzed the pillars ex-situ using STEM. Consistent with Hurley et al, they observed dislocation structure in austenite with periodicity matching that of the martensite twins. Using micromechanical modeling of the local stress state of the martensite, they were able to quantitatively predict the activated austenite slip systems. Additionally, they observed a sharp transition from elasticity to transformation during loading, concluding that there is little plastic deformation prior to transformation [40, 43]. Other proposed mechanism for defect generation in austenite is deformation twinning [42]. However, none of the experimental works discussed above have reported that deformation twinning. These experiments provide evidence for close connection between martensite fine microstructure and defect generation and accumulation in austenite. However, these are not predictive approaches and the characterization becomes challenging if multiple slip and transformation systems are active. Microstructural modeling provides a valuable tool for complementing the experiments.

1.2 Analytical Modeling of the Thermo-Mechanical Behavior of Shape Memory Alloys

At the continuum level, thermo-mechanical response of SMAs has been modeled at multiple length scales and with incorporation of varying level of details of the microstructure and constitutive laws. At the macro scale, phenomenological models simulate the response of SMA without incorporating details of the microstructure (For
example [45, 46]). Although these models have benefits in terms of relatively simple constitutive laws and computationally efficient implementation, they are not suitable for studying the physics behind microstructure-scale phenomena in SMA. At the nano and micro scale, microstructural models incorporate details of microstructure and crystallography to various degrees. This overview is focused on the microstructural modeling of SMAs.

Microstructural models generally develop a constitutive law for various mechanisms involved in the deformation of a single crystal. Response of a polycrystal is obtained from that of a single crystal, either through development of a homogenization approach or a finite element scheme. In the homogenization approach, the compatibility across the grains is not rigorously enforced. While in the finite element schemes, the effect of grain to grain compatibility is completely captured.

Early developments by Thamburaja and Anand [38] and Anand and Gurtin [47] incorporated crystallographic descriptions of the phase transformation. These were informed by empirical descriptions of nm-scale martensite plate interaction, based on Eshelby-type calculations [48]. This type of formalism was extended by Wang et al [49] to include crystallographic descriptions of plasticity in martensite, and by Manchiraju and Anderson [1] to include plasticity in austenite. The latter rather than former type of plasticity has been extensively documented in Ni-Ti [15, 40]. A conclusion by Manchiraju et al [16] is that such models can capture the effects of prior plastic deformation on polycrystalline shape memory response, but in plastically soft (solutionized) Ni-Ti alloys, they underestimate experimental values of plastic ratcheting during thermal cycling under load. To address this, Yu et al. [50] have recently
proposed a constitutive relation that can be fitted to empirically capture plastic ratcheting. These models, though excellent in predicting polycrystalline response, are not suitable for studying basic mechanism of plasticity-phase transformation interaction at the nano (martensite CV) scale.

Work of Thamburaja [51] and Pan et al [52] refined these models to a finer length scale by incorporating constitutive laws for martensite reorientation and detwinning. However, in these models, the starting microstructure was taken to be fully martensitic.

Phase field method is another approach used to study nano-scale microstructure development in the materials undergoing phase transformation (e.g. SMAs and steels). The assumption of diffuse phase interfaces is the key attribute that differentiates the phase field method from the microstructural methods described above. In this method, the microstructure is represented in terms of an array of order parameters. The rate of evolution of the order parameters is obtained in terms of a kinetic relation. This kinetic relation typically involves a driving force for phase transformation. The driving force is the work conjugate of the order parameter. Once the value of order parameter and stresses are obtained at a material point, various methods are used to obtain the response of the aggregate. Most popular schemes for this include fast Fourier transform based techniques, finite differences and finite element method.

Early work by Khachaturyan, Artemev, Wang and others consisted of development of 3D phase field models for the martensitic transformation in SMAs [53, 54, 55]. Levitas et al progressively worked on developing a similar model, implementing a finite element scheme, incorporating finite strains and rotations and incorporating coupled plastic deformation [56, 57, 58, 59, 60, 61]. However, the focus of their
work remained on developing sophisticated free energy functionals to capture physics of phase transformation. Additionally, continuum-scale plastic deformation is introduced through the incorporation of additional phase field order parameters. Other phase field efforts specific to SMAs included prediction of martensite microstructure on cooling ([62, 63, 64]) and the model of Richards et al [65] that generically studies phase transformation-slip interaction in a simpler setting of anti-plane shear and constant temperature.

Phase field based models have been developed to study interaction between phase transformation and plasticity in steels and Ni-based superalloys. Cottura et al developed a model incorporating strain gradient viscoplasticity to predict microstructure in Ni-based superalloys during creep [66]. Kundin et al developed a similar model for steels [67]. Yamanaka et al have developed a phase field based model for coupled plasticity and phase transformation in single and polycrystals [68, 69]. However they limit their studies to two dimensions and a finite difference based solver.

In summary, very few microstructural models exist that couple phase transformation with plasticity, incorporate finite strains and offer robust finite element implementation. And there is no existing work that explores interaction between phase transformation and plasticity at fine length scale in SMA using these analytical models.

1.3 Statistics of the Pseudoelastic Performance of Polycrystalline SMAs

The discussion in the preceding Sections has focused on the macroscale behavior of SMAs and fine-scale interaction between different deformation mechanisms. However at the intermediate length scale the grain scale response of SMA shows a complex
behavior as well. This Section reviews the literature related to quantifying factors influencing grain-scale performance in SMAs.

Experimental investigations show that the response of polycrystalline SMAs is highly dependent on alloy composition, heat treatment, mechanical work, and texture. However, response of an individual grain is influenced by its neighbors. The effect of texture on grain performance is highlighted by Yuan and Yi [70], who measured the pseudoelastic strain in Ti-50.4at.%Ni polycrystalline tensile test specimens cut at different angles to the rolling direction. The predicted values based on grain orientation deviated from measured values by 6.4%. The discrepancy was attributed to complex stress and strain states induced by the local grain neighborhood. Daly et al studied the local strain evolution in Ti-52wt.%Ni thin sheets using in-situ digital image correlation (DIC) [71]. They observed that transformation bands initiate in favorably oriented grains, but the subsequent growth of bands is constrained by poorly oriented grains. This underscores the potent effect of neighboring grains. Mao et al also observed the effects of neighboring grain constraint during isothermal deformation in Ti-50.8at.%Ni strips, using in situ electron back scattered diffraction (EBSD) [72]. Although the observed transformation system could be predicted well by the Schmid factor for transformation, the martensite volume fraction could not. A striking example is that grains with similar Schmid factors of 0.473 and 0.478 had a 5:2 relative ratio of martensite volume fraction under load. Merzouki et al studied a Cu-11.5wt%Al-0.5wt%Be SMA using DIC under pseudoelastic straining up to 0.8% [73]. They observed that within grains, the martensite plates with the largest Schmid factor did not always form first. The work underscores the local constraints imposed by neighboring grains and the need for simulations to account for local grain texture.
These constraints were reduced by Ueland and Schuh, by using oligocrystalline SMA wires [74, 75]. A clear benefit was the suppression of fatigue failure in their system.

Despite these various studies, the results are limited to observation of small numbers of grains, so that statistical information is lacking. At present, novel experimental techniques are in development to address this. In particular, neutron diffraction techniques are able to partition strain in polycrystalline SMA into elastic, transformation, and plastic components [23]. Likewise, X-ray based tomography techniques have advanced recently to spatially resolve strain at the grain scale [76]. Application of this technique to SMAs is particularly challenging, however, since the phase transformation introduces complexities in the interpretation of diffraction spectra.

In conclusion, at present, microstructural simulations can offer an advantage over experiments for studying grain performance statistics, because they can furnish detailed grain-level statistics for SMA performance.

1.4 Objectives and Scope

This dissertation has a twofold objective- to study the interaction between phase transformation and plasticity at the nano-scale and to study grain level statistics of phase transformation in polycrystalline SMAs using an existing meso-scale model.

Phase transformation-plasticity interaction at the martensite CV scale is studied by developing a microstructural model. This model combines a phase field based phase transformation law with the crystal based plasticity in austenite. The two deformation mechanisms interact with each other through the local stresses. The constitutive law incorporates finite deformations. It is implemented in a finite element method (FEM) framework. This allows modeling of complex boundary conditions.
Simulations incorporating cubic austenite to tetragonal martensite and a subset of the FCC slip systems in austenite are performed. Even though the simulations are carried out with a model tetragonal transformation system, the results are expected to be applicable to a wide range of SMAs.

Two hypotheses are tested with these simulations—

1. Plasticity affects martensite microstructure and transformation temperatures during load-free and load-biased thermal cycling.

2. Nature of the plastic deformation on various slip systems is determined by the martensite microstructure.

A systematic study of the transformation induced plasticity in NiTi SMAs is performed using the phase field approach. A subset of the cubic to monoclinic transformation system is modeled along with the slip in austenite. The aim of this study is to predict the austenite slip system activated and determine the mechanism for the transformation induced slip. This study is inspired by a recent experimental work investigating the transformation induced plasticity in micron-scale NiTi SMA specimen [40, 43].

A potential drawback of using the phase field approach to model phase transformation is that the diffuse interfaces modeled in this work may lead to unphysical results. For example, the stresses at a diffuse interface may be less concentrated compared to a sharper interface. Since an explicit time integration scheme is used to solve the field equations, small element size and time step is required. This makes this model computationally intensive and limits the spatial and temporal dimensions
of the phenomena that can be modeled. Based on the recent experimental evidence, plastic deformation is assumed to be limited to the austenite phase [40, 43].

The second part of this dissertation demonstrates how the statistics of pseudoelastic grain performance is affected by the local grain neighborhood in polycrystalline SMA. This is achieved using an existing microstructural FEM model calibrated to homogenized Ti-50.9 at%Ni SMA [46]. The results show a three-fold variation in the grain level axial transformation strain $p_T$ in randomly textured polycrystals, and a $\sim 20$ to $30\%$ reduction in average $p_T$ if plastically predeformed. A key outcome is a performance function to predict $p_T$ of a grain, based on the orientations of the grain and its neighbors. Two key strategies to improve polycrystalline SMA performance are identified. The first is to minimize the number of grain boundaries between high and low performing grains: plate and bamboo geometries achieve this. The second is to employ high symmetry orientation relationships between these grains. The results draw on recent experimental studies of grain level performance and provide a theoretical framework to interpret future diffraction tomography studies.

1.5 Dissertation Outline

This dissertation analyzes the performance of SMA across multiple length scale. First part of this dissertation explores interaction between phase transformation and plasticity in SMAs at the martensite CV scale. This study is performed using a new microstructural model that couples phase transformation and plasticity deformation mechanisms. The second part of this dissertation explores the effect of neighborhood on grain level performance in polycrystalline SMAs. This study is performed using an existing microstructural model for SMAs.
In Chapter 2 details of the microstructural phase field/finite element (PF/FE) model are given. The model combines a phase field based phase transformation law with the continuum crystal plasticity in austenite. The details of the explicit time integration scheme and implementation of the constitutive law in a user material subroutine in ABAQUS/Explicit finite element software [77] are provided.

A qualitative assessment of the model and a study of the interaction between phase transformation and plastic deformation is provided in Chapter 3. Martensite microstructure and the resultant plastic deformation are studied by employing a set of simulations with cubic austenite to tetragonal martensite transformation system.

In Chapter 4, the model described in Chapter 2 is utilized to model compression of NiTi micropillars. Model parameters informed by experiments are used. However, the model is not explicitly calibrated to a specific NiTi alloy. The dominant slip system induced by the phase transformation is identified.

In Chapter 5, a detailed study of the statistics of grain performance in a polycrystalline SMA is presented. This is achieved using a microstructural FEM model calibrated to homogenized Ti-50.9 at%Ni SMA. The grain pseudoelastic performance is quantitatively defined as the axial transformation strain in a grain at the maximum macro stress. The results show a three-fold variation in the grain performance. A key outcome of this study is a predictive performance function for the grain. Two key strategies to improve polycrystalline SMA performance are identified. The first is to minimize the number of grain boundaries between high and low performing grains: plate and bamboo geometries achieve this. The second is to employ high symmetry
orientation relationships between these grains. The results draw on recent experimental studies of grain level performance and provide a theoretical framework to interpret future diffraction tomography studies.

In Chapter 6 the contribution of this work to the SMA community is assessed. Possible extensions of this work are discussed.

The algorithm for the material constitutive law implementation is described in Appendix A.
Chapter 2: Constitutive Relations for the Coupled Phase Transformation/Plasticity Model

The constitutive relation or the material model relates the stress at a material point to the deformation gradient, temperature and other field parameters. In this Chapter a constitutive relation for SMAs is derived. Contributions to the deformation from elasticity, thermal expansion, phase transformation and plasticity are described. Since the focus of this work is to study plasticity induced by the local stress field of twinned martensite in SMAs, a phase transformation rule at the length scale of martensite CVs is derived. This is coupled with the continuum scale crystal plasticity in austenite. The choice of implementing plasticity in austenite is motivated by micron scale experimental studies that have shown evidence for dislocations on austenite slip systems in the vicinity of martensite [40, 43]. Anisotropic elasticity in austenite and martensite is considered. Thermal expansion coefficients are considered to be isotropic. This reduces the thermal expansion coefficient matrices to scalar values.

The deformation due to various mechanisms is represented in terms of the total deformation gradient at a material point. Let \( F \) be the deformation gradient that deforms a reference vector \( X \) into a distorted vector \( x \).

\[
dx = F \! dX
\]  

(2.1)
Following Lee [78] we multiplicatively decompose the deformation gradient into an elastic and an inelastic part. The multiplicative decomposition allows the deformation to be finite, as against an additive decomposition which is appropriate for infinitesimal deformations only.

$$F = F^e F^{\text{inel}}$$

(2.2)

Further, we can write evolution of inelastic deformation gradient in terms of inelastic velocity gradient as follows

$$\dot{F}^{\text{inel}} = L^{\text{inel}} F^{\text{inel}}$$

(2.3)

The inelastic velocity gradient $L^{\text{inel}}$ is approximated from the martensite evolution rate and slip rate weighted by austenite volume fraction $\nu_A$

$$L^{\text{inel}} = \sum_{t} \dot{\nu}_t S_t^{\text{trans}} + \nu_A \sum_{t} \dot{\gamma}_t S_t^{\text{slip}}$$

(2.4)

Here $\dot{\nu}_t$ refers to the rate of volume increase for the $t^{th}$ martensite CV and $S_t^{\text{trans}}$ is the Bain transformation strain for that CV. $\dot{\gamma}_t$ is the slip rate for the $t^{th}$ slip system and $S_t^{\text{slip}}$ is the Schmid tensor for that slip system. $N_T$ and $N_P$ are the number of transformation and slip systems respectively. Austenite volume fraction $\nu_A$ is calculated from the sum of volume fractions of all the CVs $\nu_A = 1 - \sum_{t=1}^{N_t} \nu_t$

So the task is to determine the martensite evolution and the slip rate. A rate-dependent phase field method based evolution law for austenite ↔ martensite transformation and reorientation of martensite CVs is describe in Section 2.1. Later in Section 2.2, a crystal plasticity based law for rate-dependent plasticity in austenite is described. Details of the implementation of this law in an FEM framework are described in Section 2.3. One of the key parameters used in the phase field method is the choice of the Landau polynomial. The Landau polynomial describes the energetic
landscape between austenite and martensite. The choice of the Landau polynomial in this model is described in Section 2.4.

2.1 Phase Field Method Based Martensite Evolution Law

We use the phase field method to model the growth of martensite. We take volume fraction of martensite CV as the order parameter ($\nu_t$). Following Artemev et al [55], we assume that the evolution of the order parameter follows the Ginzberg-Landau kinetic law

$$\dot{\nu}_t = M_{tu}f_{trans}^t$$  \hspace{1cm} (2.5)

Here $M_{tu}$ is the mobility matrix and $f_{trans}^t$ is the driving force for martensite transformation. We develop an expression for the driving force from the 1st and the 2nd law of thermodynamics.

Following Gurtin [79], we define following local quantities: microstress ($c_t$), internal microforce ($\Pi_t$) and external microforce ($\mu_t$). Each is doing work through the kinematical mechanism of phase transformation. We assume local microstres balance,

$$\text{div} c_t - \Pi_t + \mu_t = 0$$ \hspace{1cm} (2.6)

The work rate of microforce ($W_{\text{mic}}$) over a reference domain $P$ is given by

$$W_{\text{mic}} = \sum_{t=1}^{N_T} \left[ \int_{\delta P} (c_t \cdot n)\dot{\nu}_t da + \int_P \mu_t \dot{\nu}_t dV \right]$$ \hspace{1cm} (2.7)

Applying divergence theorem and using equation 2.6, we obtain

$$W_{\text{mic}} = \sum_{t=1}^{N_T} \int_P (c_t \nabla \nu_t \dot{\nu}_t + \mu_t \dot{\nu}_t) dV$$ \hspace{1cm} (2.8)
Now we write the expression for the 1\textsuperscript{st} law of thermodynamics
\[
\frac{d}{dt}\int_P \left( \frac{1}{2} \rho_R \dot{\mathbf{x}} : \dot{\mathbf{x}} + \rho_R \epsilon_R \right) dV = \int_P (\rho_R b \dot{\mathbf{x}} + \rho_R r_R) dV + \int_{\delta P} P N v da + \sum_{t=1}^{N_T} \int_P (c_t \nabla \dot{v}_t + \mu_t \dot{v}_t) dV
\]
(2.9)

Here the first term on the left hand side is the kinetic energy and the second term is the internal energy. \(\rho_R\) is the material density in the domain \(P\). On the right hand side, \(r_R\) is the internal heat generation rate and \(P\) is the 1\textsuperscript{st} Piola-Kirchhoff stress. Last term on the right hand side represents the work done by the microforces. Here we are assuming spatial uniformity of temperature. Hence in this energy balance expression, there is no term from the heat transfer.

Applying mechanical equilibrium, transport theorem, localization and mass conservation to equation 2.9, we get
\[
P \dot{F} + \sum_{t=1}^{N_T} \Pi_t \dot{u}_t + \sum_{t=1}^{N_T} c_t \nabla \dot{v}_t + r_R = \epsilon_R
\]
(2.10)

We can write an expression for the 2\textsuperscript{nd} law of thermodynamics as follows
\[
\dot{\eta}_R \geq \frac{r_R}{\theta}
\]
(2.11)

Here, \(\dot{\eta}_R\) is the entropy rate and \(\theta\) is the temperature. From equations 2.10 and 2.11,
\[
\dot{\eta}_R \theta \geq \dot{\varepsilon}_R - P \dot{F} - \sum_{t=1}^{N_T} \Pi_t \dot{v}_t - \sum_{t=1}^{N_T} c_t \nabla \dot{v}_t
\]
(2.12)

Applying Legendre transformation (\(\Psi_R = \epsilon_R - \theta \eta_R\) with \(\Psi_R =\) Helmholtz free energy) to equation 2.12,
\[
P \dot{F} + \sum_{t=1}^{N_T} \Pi_t \dot{v}_t + \sum_{t=1}^{N_T} c_t \nabla \dot{v}_t - \eta_R \dot{\theta} - \dot{\Psi}_R \geq 0
\]
(2.13)

We can relate the 1\textsuperscript{st} Piola-Kirchhoff stress \((P)\) and the 2\textsuperscript{nd} Piola-Kirchhoff stress \((T^*)\) using the following kinematic relations
\[
P = \det(F)TF^{-T}
\]
(2.14a)
\[ T = \left[ \det(F^e) \right]^{-1} F^e T^* F^{eT} \]  
(2.14b)

\[ D = \{F^e\}^{-T} \dot{E} \{F^e\}^{-1} \]  
(2.14c)

\[ \dot{F} = [\dot{\varepsilon} \{F^e\}^{-1} + \varepsilon^\text{inel} \{F^\text{inel}\}^{-1} \{F^e\}^{-1}] F \]  
(2.14d)

Hence, the first term in equation 2.13 can be re-written as

\[ P \dot{F} = T^* E^e + F^e T^* L^\text{inel} = T^* E^e + \sum_{t=1}^{N_T} F^e T^* S_t^\text{trans} \nu_t + \sum_{t=1}^{N_P} F^e T^* S_t^\text{slip} \gamma_t \]  
(2.15)

Let \( \Psi_R = \Psi_R(E^e, \theta, \nu_t, \nabla \nu_t) \). Using the chain rule, we can write

\[ \dot{\Psi}_R = \frac{\partial \Psi_R}{\partial E^e} \dot{E}^e + \frac{\partial \Psi_R}{\partial \theta} \dot{\theta} + \frac{\partial \Psi_R}{\partial \nu_t} \dot{\nu}_t + \frac{\partial \Psi_R}{\partial \nabla \nu_t} \nabla \dot{\nu}_t \]  
(2.16)

Using equations 2.13, 2.15 and 2.16 we have

\[ \left( T^* - \frac{\partial \Psi}{\partial E^e} \right) \dot{E}^e - \left( \eta + \frac{\partial \Psi}{\partial \theta} \right) \dot{\theta} - \sum_{t=1}^{N_T} \left( c_t - \frac{\partial \Psi}{\partial \nu_t} \right) \nabla \dot{\nu}_t + \sum_{t=1}^{N_T} \left( \Pi_t + F^e T^* S_t^\text{trans} - \frac{\partial \Psi}{\partial \nu_t} \right) \dot{\nu}_t + \nu \sum_{t=1}^{N_P} (F^e T^* S_t^\text{slip}) \dot{\gamma}_t \geq 0 \]  
(2.17)

The fields \( \dot{E}^e, \dot{\theta}, \dot{\nu}_t \) and \( \dot{\gamma}_t \) are independent and can be varied arbitrarily. This gives us the 2nd Piola-Kirchhoff stress, entropy and the internal stress.

2nd Piola – Kirchhoff stress :  \( T^* = \frac{\partial \Psi_R}{\partial E^e} \)  
(2.18a)

Entropy :  \( \eta = -\frac{\partial \Psi_R}{\partial \theta} \)  
(2.18b)

Internal stress :  \( c_t = \frac{\partial \Psi_R}{\partial \nu_t} \)  
(2.18c)

Finally, we also obtain the driving force for phase transformation

\[ f_t^\text{trans} = \Pi_t + F^e T^* S_t^\text{trans} - \frac{\partial \Psi_R}{\partial \nu_t} \]  
(2.19)
Assuming the external microstress equals zero, we obtain an expression for the internal microforce in terms of the microstress.

\[ \Pi_t = \text{div} c_t = \text{div} \left( \frac{\partial \Psi_R}{\partial \nabla \nu_t} \right) \quad (2.20) \]

So, the expression for the driving force for phase transformation becomes

\[ f_t^{\text{trans}} = \text{div} \left( \frac{\partial \Psi_R}{\partial \nabla \nu_t} \right) + F^{eT} F^{eT} S_t^{\text{trans}} - \frac{\partial \Psi_R}{\partial \nu_t} \quad (2.21) \]

Contributions from three terms are assumed to define the Helmholtz free energy. The first contribution is from the elastic strain energy. Second contribution comes from the chemical free energy difference between the constituent phases. The last contribution is from the energy of the phase interfaces in the system. We assume the following form for the Helmholtz free energy.

\[ \Psi_R = \frac{1}{2} E^{e} C E^{e} + f_{LP}(\nu_t, \theta) + \frac{1}{2} \sum_{t=1}^{N_T} \nabla \nu_t \sum_{u=1}^{N_T} K_{tu} \nabla \nu_u \quad (2.22) \]

In this expression \( C \) is the elastic stiffness tensor (units of Pa) and \( f_{LP}(\nu_t, \theta) \) is a Landau polynomial describing the chemical free energy landscape between stress-free austenite and martensite (units of energy/volume, or Pa). The choice of Landau polynomial is described in Section 2.4. \( K_{tu} \) is the coefficient for austenite-martensite and martensite-martensite interface energy (units of energy/length or N).

From equations 2.21 and 2.22, the final expression for the driving force per unit volume for the martensitic phase transformation becomes

\[ f_t^{\text{trans}} = K_{tu} \nabla^2 \nu_u + F^{eT} F^{eT} S_t^{\text{trans}} - \frac{\partial f_{LP}(\nu_t, \theta)}{\partial \nu_t} \quad (2.23) \]

We can use this expression for the driving force in equation 2.5 to predict the evolution of martensite field variables.
2.2 Crystal Plasticity Law

Slip is modeled in terms of the crystal plasticity formulation of Peirce et al [80]. This formulation provides a rate dependent power-law type constitutive relation for plasticity, along with a phenomenological hardening rule in terms of a set of self and latent hardening parameters. The formulation, initially proposed by Peirce et al to study inhomogeneous deformation in metals has been widely used to model plastic deformation in metals and alloys. Some example applications include the prediction of texture evolution during processing of FCC metals [81] and the prediction of the pileup patterns during nano-indentation of Titanium [82]. Roters et al [83] provide a detailed overview of the applications of the crystal plasticity finite element models.

The slip rate $\dot{\gamma}_s$ is related to the resolved shear stress $\tau_s$ on the slip system $s$ and the slip hardness $g_s$.

\begin{equation}
\dot{\gamma}_s = \dot{\gamma}_0 \left(\frac{\tau_s}{g_s}\right)^{\frac{1}{m}} \text{sign}(\tau_s)
\end{equation}

\begin{equation}
\tau_s = F^e T^e T^* S^\text{slip}_t
\end{equation}

Here $\dot{\gamma}_0$ is the reference slip rate and $T^*$ is the 2nd Piola-Kirchhoff stress. The slip hardness $\tau_s$ evolves according to the following law

\begin{equation}
\dot{g}_s = \sum_{r=1}^{N_s} h_r (Q + (1 - Q)\delta_{sr}) |\dot{\gamma}_r| \quad (2.25a)
\end{equation}

\begin{equation}
h_r = h_0 \left(1 - \frac{g_r}{g_{sat}}\right)^a
\end{equation}

2.3 Numerical scheme and FEM implementation

The aim of the numerical procedure is to obtain the value of the Cauchy stress $(T(\tau))$, inelastic deformation gradient $(F_{inl}(\tau))$, martensite volume fraction $(\nu_t(\tau))$
for the transformation system $t$, slip $(\gamma_s(\tau))$ on the slip system $s$ and hardness $(g_s(\tau))$ of the slip system $s$ at the current time increment $\tau = t + \Delta t$, given the total imposed deformation gradient $F(\tau)$ and temperature $\theta$. This is achieved through a fully explicit numerical integration approach.

We start off by assuming a trial value of the inelastic deformation gradient ($F_{\text{inel}}(\tau)$) at $\tau$ equal to $F_{\text{inel}}(t)$; i.e. we assume the current deformation increment to be fully elastic. From this we obtain a trial value of the elastic deformation gradient through a multiplicative decomposition.

\[
F_{\text{trial}}^e = F F_{\text{trial}}^{-1}
\]  

(2.26)

With this trial value, the local elastic strain ($E^e$) and the stress ($T_{\text{trial}}^e$) are calculated.

\[
E_{\text{trial}}^e(\tau) = \frac{1}{2} (F_{\text{trial}}^e(\tau) F_{\text{trial}}^e(\tau) - I)
\]  

(2.27)

\[
T_{\text{trial}}^e(\tau) = C(E_{\text{trial}}^e(\tau) - A_{\text{therm}} \Delta \theta)
\]  

(2.28)

Here $C$ is the anisotropic elastic stiffness and $A_{\text{therm}}$ is the thermal expansion coefficient. An isotropic form is assumed for the thermal expansion coefficients $(A_{\text{therm}} = \alpha I)$ based on the experimental evidence which suggests the anisotropy in the stress-strain response is primarily introduced by elasticity [84]. For these parameters effective values are used, calculated using a rule-of-mixtures approach.

\[
C = \nu_A C_A + \nu_M C_M \quad \text{and} \quad A_{\text{therm}} = \nu_A A_A - \text{therm} + \nu_M A_M - \text{therm}
\]  

(2.29)

Here $\nu_A$ and $\nu_M$ are the austenite and martensite volume fractions respectively. Subscript A and M refer to the pure austenite and pure martensite material parameters respectively.
We calculate resolved stress on the candidate transformation systems ($\tau_{trans}^i$) and the slip systems ($\tau_{slip}^i$) from the local stress $T^*$.

$$\tau_{trans}^i(\tau) = F_{trial}^e(\tau) F_{trial}^e T^*(\tau) \cdot S_{trans}$$ (2.30)

$$\tau_{slip}^i(\tau) = F_{trial}^e(\tau) F_{trial}^e T^*(\tau) \cdot S_{slip}$$ (2.31)

Here $S_{trans}^i$ is the Schmid tensor for the $i^{th}$ transformation system and $S_{slip}^i$ is the Schmid tensor for the $i^{th}$ slip system. This stage represents the coupling between the mechanisms of phase transformation and plasticity through the local stress $T^*$.

With the resolved stresses known, the martensite volume fraction increment and the slip activity are calculated using the phase field evolution law (equation 2.5) and the crystal plasticity law (equation 2.24) respectively. Hardness of the slip systems is updated using equation 2.25.

Knowing the martensite volume increment and slip rate and using equations 2.3 and 2.4, we can calculate a new inelastic deformation gradient.

$$F_{inel}^e(\tau) = \left( 1 + \sum_{t=1}^{N_T} \dot{\nu}_t(\tau) S_{trans}^t + \nu_A \sum_{t=1}^{N_P} \dot{\gamma}_t(\tau) S_{slip}^t \right) F_{trial}^e(\tau)$$ (2.32)

With the new inelastic deformation gradient known, we can use equations 2.26, 2.27 and 2.28 to calculate an updated 2nd Piola-Kirchhoff stress and the Cauchy stress.

This numerical scheme is implemented as a user material subroutine (VUMAT) in ABAQUS FEM software [77]. At each time increment $t$, ABAQUS provides the field variables ($\nu_t$), inelastic deformation gradient $F_{inel}^e$, temperature $\theta$ and the imposed deformation gradient at $\tau = t + \Delta t$, $F(\tau)$. Using the constitutive laws and the numerical implementation described above, the updated stresses $T^*(\tau)$ and the inelastic deformation gradient $F_{inel}^e(\tau)$ are returned. The algorithm implemented in the VUMAT is listed in Appendix A.
An explicit time integration scheme is more computationally efficient than implicit
time integration. This is because, in the explicit time integration, there is no need for
construction of the global stiffness matrix and its inversion. The equations of motion
are solved as follows.

\[
\dot{u}^{(i+\frac{1}{2})} = \dot{u}^{(i-\frac{1}{2})} + \frac{\Delta t^{(i+1)} + \Delta t^{(i)}}{2} \ddot{u}^{(i)}
\]  

(2.33)

\[
u^{(i+1)} = u^{(i)} + \Delta t^{(i+1)} \dot{u}^{(i+\frac{1}{2})}
\]

(2.34)

\[
\ddot{u}^{(i)} = M^{-1} \cdot (F^{(i)} - I^{(i)})
\]

(2.35)

where \(M\) is the diagonal lumped mass matrix, \(F\) is the applied load vector, and \(I\) is
the internal force vector. The superscript \(i + 1\) refers to the current iteration; much
like the \(\tau\) time-instant in the notation used above. The superscript \(i\) refers to the
previous iteration, similar to the time-instant \(t\). Note that the displacement \(u\) at the
current iteration is completely defined in terms of various quantities at the previous
iteration.

The computational efficiency allows modeling with a fine mesh, which is essential
for capturing the spatial details of the fine martensite microstructure. Another ben-
efit of an explicit rather than an implicit scheme is that the calculation of material
Jacobian matrices (\(\partial F/\partial x\) and \(\partial F/\partial \theta\)) is not necessary. However, a drawback of an
explicit time integration scheme is that the solution is conditionally stable. In other
words, the time increment \(\Delta t\) used must be sufficiently small so that the solution is
stable. Another drawback of using the explicit time integration is that the resultant
simulation is solving a dynamic problem, rather than a static one. The information
about stresses in a dynamic explicit simulation propagates at the elastic wave speed in
the system. The elastic wave speed \(v^{\text{wave}}\) can be approximated in terms of isotropic
elastic modulus $E^\text{isotropic}$ and the density of the material ($\rho$), $v^\text{wave} = \sqrt{E^\text{isotropic}\rho}$.

However, the stable time increment $\Delta t^\text{stable}$ is given by, $\Delta t^\text{stable} = \Delta x/v^\text{wave}$, where $\Delta x$ is the size of the smallest element in the mesh. So in order to make the simulation computationally efficient, we want to use the largest possible density. But this adds kinetic energy to the system, potentially introducing inertial effects in the simulation. This is not desirable. This can be counteracted by adding a viscous drag to the model, which reduces rapid movement of material points.

A viscous drag is added to the simulations using the *viscous body force* option in ABAQUS/Explicit [77]. This applies a force ($f_v$) at each material point to oppose its motion. The magnitude of the force is proportional to the velocity of the material point.

$$f_v = -c_{vb}(v - v_{\text{ref}})V_e \quad (2.36)$$

Here $c_{vb}$ is the drag coefficient which determines the magnitude of the viscous force. $v$ is the velocity of a material point. $v_{\text{ref}}$ is a reference velocity, chosen to be zero in the simulations. $V_e$ is the volume of the element to which the material point belongs. The value of $c_{vb}$ is chosen such that the work done by the viscous forces, integrated over the whole model, is less than 10 per cent of the total energy of the model.

A computational challenge introduced by the incorporation of the gradient based interface energy term in Equation 2.22 and the large deformation approach is that the Laplacian ($\nabla^2 \nu_t$) of the order parameter $\nu_t$ must be calculated at each material point during each time increment. This is trivial if a uniform mesh is used like in the Fourier transform based approaches for solving field equations. However, due to the large deformation approach and large transformation strains involved, the location of each
material point is changing continuously. Due to this, the Laplacian is calculated by interpolating the field variable values. A modified Shephard’s interpolation algorithm (QSHEP3) by Renka is used for interpolation [85].

The discussion above involves a single crystal of austenite as the representative volume element. And the constitutive law so developed is for a single crystal. However, in the implementation, elastic stiffness \( C_A \) and \( C_M \) and Schmid tensors for transformation and plasticity \( S^{\text{trans}}_t \) and \( S^{\text{slip}}_t \) are rotated to the global coordinate system from the crystal coordinate system. For this the local crystal orientation is taken as input at each material point. Hence the implemented model can be applied to polycrystals as well as single crystals.

2.4 The Landau Polynomial

One of the parameters in formulating the Helmholtz free energy (Equation 2.22) of the austenite-martensite system is the chemical free energy of the aggregate. A Landau polynomial phenomenologically describes the chemical energy change as the austenite lattice is distorted to produce the martensite lattice. It is a function of the order parameter \( \nu_t \). The minima of the Landau polynomial describe the order parameter corresponding to stable or metastable phases. The form of the Landau polynomial can be informed by the density functional theory calculations [86], and it is typically taken to have minimum at pure austenite \( \nu_t = 0 \) and pure martensite \( \nu_t = 1 \). Additionally an activation barrier is included in between the stable phases [87, 58].

A temperature-dependent sixth order Landau polynomial is chosen as shown in Equation 2.37 and in Figure 2.1(a). At temperatures greater than the transformation
temperature \((\theta > \theta_T = 250K)\), austenite \((\nu_t = 0)\) is the stable phase and martensite \((\nu_t = 1)\) is the metastable phase. There is a small activation barrier between the two. As the temperature is lowered below \(\theta_T\), martensite becomes the stable phase.

\[
f_{LP}(\nu, \theta) = \lambda \left[ (\theta - \theta_{\text{trans}}) \left( p \sum_{i=1}^{N} \nu_i^2 + q \left( \sum_{i=1}^{N} \nu_i^2 \right)^2 \right) + \left( b \sum_{i=1}^{N} \nu_i^2 + d \sum_{i=1}^{N} \nu_i^4 + f \left( \sum_{i=1}^{N} \nu_i^2 \right)^3 \right) \right]
\]

(2.37)

With this form of the Landau polynomial and the driving force expression for phase transformation given in equation 2.23, we can expect the following behavior.

- During thermal cycling, as the temperature is lowered below the transformation temperature, all order parameters will start to gradually grow. A mixture of various martensite CVs will be obtained at a material point. The time scale over which the transformation takes place decreases as the mobility and driving force increase.

- During pseudoelastic loading \((\theta > \theta_{\text{trans}})\), the external stress will add a term proportional to \(\nu_t\) to \(\psi\). This will cause the order parameter to evolve by a small amount. When the external stress has completely overcome the activation barrier in the Landau potential, the order parameter will rapidly grow. This will lead to an instability in the stress-strain response of the model. The combined effect of external stress and chemical free energy (Landau term) during pseudoelastic loading is shown in Figure 2.1(b).
Figure 2.1: (a) Landau polynomial \( f_{LP}(\nu_t, \theta) \) plotted as a function of the order parameter \( \nu_t \) for various temperatures. Equilibrium transformation temperature is \( \theta_{\text{trans}} = 250K \). Note that \( \nu_t = 0 \) corresponds to pure austenite and \( \nu_t = 1 \) corresponds to pure martensite. (b) Effect of external stress on the total free energy of the system at \( \theta > \theta_T \).
Chapter 3: A systematic study of the interaction between phase transformation and plasticity

The phase field/finite element model described in the previous chapter is applied to load-free thermal cycling and load-biased thermal cycling. Evolution of martensite microstructure and interaction between phase transformation and plasticity is systematically studied. The aim of this chapter is to seek answers to three key questions.

1. Does the evolution of martensite microstructure result in generation of any slip activity in the austenite phase?

2. Does the slip activity in the material influence subsequent phase transformation at the microstructure level?

3. How does the interaction between phase transformation and plasticity result in any systematic changes to measurable quantities like the transformation temperatures, ratcheting response or the residual martensite?

To seek answers to these questions, a model transformation system involving cubic austenite to tetragonal martensite transformation is considered. The results for load-free thermal cycling and load-biased thermal cycling of single crystals are discussed
in Sections 3.3. The results and the model behavior are discussed in detail in Section 3.4. When a material model is developed, it is important to establish a length and time scale for the model. This is done in Section 3.5. Finally in Section 3.6, the strengths and weaknesses of the model are critically assessed.

3.1 Introduction: Transformation and Slip Systems

The aim of this chapter is to qualitatively study the transformation-plasticity interaction for various thermo-mechanical loading conditions. Hence the model is not calibrated for a particular SMA system. Rather, by simulating the formation of different martensite microstructures during load-free and load-biased thermal cycling, the resultant slip activity in austenite is studied. Even though a model transformation system is considered, a transformation strain magnitude of 6% is used. This is comparable to the magnitude of transformation strain in many typical SMAs including equi-atomic NiTi.

When a cubic austenite phase transforms to a tetragonal martensite, it forms three CVs that are energetically equivalent. The formation of three CVs makes the modeling of this system computationally more efficient than e.g. cubic to monoclinic, which involves twelve CVs. Cubic → tetragonal is the minimal full three-dimensional transformation system. This type of transformation is seen in In-23at.%Tl, Ni-36at.%Al, Fe-24at.%Pt and Fe-31at.%Ni-0.3at.%C [8].

The transformation strain matrices (in the cubic crystal coordinates) for the three CVs as used in the model are specified in Equation 3.1. The form of the transformation strain matrices is such that, there is no volume change involved when transforming from austenite to martensite. The transformation can be visualized to extend a
cube along either X, Y or Z crystal direction and bring a compression along the other two orthogonal directions.

\[
E_1 = \begin{pmatrix}
-0.03 & 0 & 0 \\
0 & -0.03 & 0 \\
0 & 0 & 0.06
\end{pmatrix}
\] (3.1a)

\[
E_2 = \begin{pmatrix}
-0.03 & 0 & 0 \\
0 & 0.06 & 0 \\
0 & 0 & -0.03
\end{pmatrix}
\] (3.1b)

\[
E_3 = \begin{pmatrix}
0.06 & 0 & 0 \\
0 & -0.03 & 0 \\
0 & 0 & -0.03
\end{pmatrix}
\] (3.1c)

### 3.1.1 Calculation of the M-M interface orientations

The resultant martensite-martensite (M-M) interface orientations in the cubic crystal coordinate system are calculated from the crystallographic theory of martensite. This procedure is formulated by Ball and James [88] and illustrated by Bhattacharya [8]. The strategy for finding a M-M interface is two-fold. The first step is to calculate the relative deformation of the second martensite CV with respect to the first. If the two CVs can form a coherent interface, then the second step is to find a plane that is relatively undistorted. The final result is a pair of vectors- \( a \) and \( n \) that determine a coherent interface between the two CVs. Steps of the procedure to determine \( a \) and \( n \) are presented below. For the details of this procedure, the reader is referred to Chapter 5 in Bhattacharya [8].

Given two CVs with the transformation strain matrices \( U_1 \) and \( U_2 \), we seek two vectors \( a \) and \( n \) and a matrix \( Q \) that satisfy the compatibility condition -

\[
QU_1 - U_2 = a \otimes n
\] (3.2)

The following procedure is followed to find such \( a \) and \( n \).
1. Calculate the matrix \( C = G^{-T}F^TFG^{-1} \).

2. If \( C = I \), then there is no solution to Equation 3.2.

3. If \( C \neq I \), calculate the eigenvalues \( \lambda_1, \lambda_2, \lambda_3 \) of the matrix \( C \). Automatically \( \lambda_i > 0 \). Number the eigenvalues so that \( \lambda_1 \leq \lambda_2 \leq \lambda_3 \).

4. Equation 3.2 has a solution if and only if the eigenvalues satisfy

\[
\lambda_1 \leq 1 \quad , \quad \lambda_2 = 1 \quad , \quad \lambda_3 \geq 1
\]  

(3.3)

5. If the condition in Equation 3.3 holds, then there are exactly two solutions given by

\[
\mathbf{a} = \rho \left( \sqrt{\frac{\lambda_3(1-\lambda_1)}{\lambda_3-\lambda_1}} \mathbf{e}_1 + k \sqrt{\frac{\lambda_1(1-\lambda)}{\lambda_3-\lambda_1}} \mathbf{e}_3 \right) \quad (3.4a)
\]

\[
\mathbf{n} = \frac{\sqrt{\lambda_3} - \sqrt{\lambda_1}}{\rho \sqrt{\lambda_3 - \lambda_1}} \left( -\sqrt{1-\lambda_1 U_2^T e_1} + k \sqrt{\lambda_3 - 1} U_2^T e_3 \right) \quad (3.4b)
\]

Here \( k = \pm 1 \), \( \rho \) is chosen to achieve \( |\mathbf{n}| = 1 \). \( \mathbf{e}_i \) are the eigenvectors corresponding to \( \lambda_i \).

The values for \( \mathbf{a} \) and \( \mathbf{n} \) calculated using Equation 3.4 are listed in Table 3.1.

### 3.1.2 Calculation of the A-M interface orientations

Similar to the M-M interfaces, the A-M interfaces can be analytically determined using the crystallographic theory of martensite. The crystallographic theory proposes that a mixture of two martensite CV in the proportion \( \lambda \) may form an interface with the austenite that is coherent in an average sense. In this case, the aim is to find a \( \lambda \) and two vectors \( \mathbf{b} \) and \( \mathbf{m} \) that determine a coherent interface. Once again, the final result from Bhattacharya [8] is summarized. For details, the reader is referred to the Chapter 7 of Bhattacharya [8] and the work of Ball and James [88].
Table 3.1: Martensite-martensite (M-M) interface orientations. The columns CV1 and CV2 refer to the pair of CVs forming the twin.

<table>
<thead>
<tr>
<th>CV 1</th>
<th>CV 2</th>
<th>Twin shear direction ((a))</th>
<th>Twin plane normal ((n))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>([0.00 \ 0.12 \ 0.13])</td>
<td>([0.00 \ 0.71 \ 0.71])</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>([0.00 \ 0.12 \ 0.13])</td>
<td>([0.00 \ 0.71 \ 0.71])</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>([0.12 \ 0.00 \ 0.13])</td>
<td>([0.71 \ 0.00 \ 0.71])</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>([0.12 \ 0.00 \ 0.13])</td>
<td>([0.71 \ 0.00 \ 0.71])</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>([0.12 \ 0.13 \ 0.00])</td>
<td>([0.71 \ 0.71 \ 0.00])</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>([0.12 \ 0.13 \ 0.00])</td>
<td>([0.71 \ 0.71 \ 0.00])</td>
</tr>
</tbody>
</table>

Given the transformation strain matrix \(U_1\) for a CV and the vectors \(a\) and \(n\) for a twin system, the task is to find two vectors \(b\) and \(m\) that satisfy the A-M interface compatibility equation -

\[
Q U_2 - U_1 = a \otimes n \tag{3.5a}
\]

\[
Q' (\lambda QU_2 + (1 - \lambda)U_1) = I + b \otimes m \tag{3.5b}
\]

A four stage procedure is proposed by Bhattacharya-

1. Calculate

\[
\delta = a \cdot U_1(U_1^2 - I)^{-1}n \quad \text{and} \quad \eta = \text{tr}(U_1^2) - \text{det}(U_1^2) - 2 + \frac{|a|^2}{2\delta} \tag{3.6}
\]

There exists an A-M interface only if

\[
\delta \leq -2 \quad \text{and} \quad \eta \geq 0 \tag{3.7}
\]

2. To find the solutions, calculate

\[
\lambda = \frac{1}{2} \left(1 - \sqrt{1 + \frac{2}{\delta}} \right) \tag{3.8}
\]
3. Calculate

\[ C = (U_1 + \lambda n \otimes a)(U_1 + \lambda a \otimes n) \]  

(3.9)

Find the eigenvalues \( \lambda_1 \leq \lambda_2 \leq \lambda_3 \) and the corresponding eigenvectors \( e_i \) of \( C \).

Automatically \( \lambda_2 = 1 \). Obtain \( b \) and \( m \) by solving

\[
\begin{align*}
\mathbf{b} &= \rho \left( \sqrt{\frac{\lambda_3(1 - \lambda_1)}{\lambda_3 - \lambda_1}} \mathbf{e}_1 + k \sqrt{\frac{\lambda_1(\lambda_3 - 1)}{\lambda_3 - \lambda_1}} \mathbf{e}_3 \right) \\
\mathbf{m} &= \frac{\sqrt{\lambda_3} - \sqrt{\lambda_1}}{\rho \sqrt{\lambda_3 - \lambda_1}} \left( -\sqrt{1 - \lambda_1} \mathbf{e}_1 + k \sqrt{\lambda_3 - 1} \mathbf{e}_3 \right)
\end{align*}
\] 

(3.10a)

(3.10b)

Just as in Equation 3.4, here \( \rho \) is chosen to make \( |m| = 1 \) and \( k = \pm 1 \).

4. If \( \delta < -2 \), repeat the above step by replacing \( \lambda \) with \( (1 - \lambda) \) to obtain two more solutions.

For the cubic to tetragonal system, equation 3.10 yields 24 A-M interfaces. The \( b, m \) values are reported in Table 3.2.

Six FCC slip systems with the slip plane belonging to the \{1 1 0\} family are considered in all the simulations in this chapter. The slip systems are listed in Table 3.5.
<table>
<thead>
<tr>
<th>CV1</th>
<th>CV2</th>
<th>Vector on invariant plane ((b))</th>
<th>Invariant plane normal ((m))</th>
<th>(\lambda)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>[0.04 0.00 0.04]</td>
<td>[0.78 0.02 0.68]</td>
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<tr>
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<td>2</td>
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</tr>
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<td>[0.04 0.04 0.00]</td>
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</tr>
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<td>0.35</td>
</tr>
<tr>
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<td>[0.78 0.02 0.68]</td>
<td>0.35</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
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<td>[0.78 0.68 0.08]</td>
<td>0.64</td>
</tr>
<tr>
<td>8</td>
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<td>[0.78 0.68 0.08]</td>
<td>0.64</td>
</tr>
<tr>
<td>9</td>
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<td>[0.02 0.73 0.68]</td>
<td>0.35</td>
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<tr>
<td>10</td>
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<td>[0.02 0.73 0.68]</td>
<td>0.35</td>
</tr>
<tr>
<td>11</td>
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<td>[0.68 0.73 0.08]</td>
<td>0.64</td>
</tr>
<tr>
<td>12</td>
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<td>[0.68 0.73 0.08]</td>
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</tr>
<tr>
<td>13</td>
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<td>[0.02 0.73 0.68]</td>
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<tr>
<td>14</td>
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<td>[0.02 0.68 0.73]</td>
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<tr>
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<td>[0.02 0.68 0.73]</td>
<td>0.35</td>
</tr>
<tr>
<td>22</td>
<td>3</td>
<td>[0.00 0.04 0.04]</td>
<td>[0.02 0.68 0.73]</td>
<td>0.35</td>
</tr>
<tr>
<td>23</td>
<td>3</td>
<td>[0.04 0.00 0.04]</td>
<td>[0.68 0.08 0.73]</td>
<td>0.64</td>
</tr>
<tr>
<td>24</td>
<td>3</td>
<td>[0.04 0.00 0.04]</td>
<td>[0.68 0.08 0.73]</td>
<td>0.64</td>
</tr>
</tbody>
</table>

Table 3.2: Austenite-martensite (A-M) interface orientations. The columns CV1 and CV2 refer to the pair of CVs forming the twinned microstructure in the martensite. The interface between twinned martensite and austenite is also known as the invariant plane because a line segment on the A-M interface does not deform, but it may rotate. \(\lambda\) is the ratio of the volume fractions of CV1 and CV2 forming the invariant plane.
3.2 Methods: Load-free Thermal Cycling and Load-biased Thermal Cycling Simulations

Two different modes of loading, load-free and load-biased thermal cycling are modeled in order to obtain different martensite microstructure and kinetic response. These simulations are described below.

To model thermal cycling, a cylindrical model is created with 114,000 hexahedral reduced integration elements (C3D8RT in ABAQUS FE suite). Figure 3.1 shows the cylinder geometry with the boundary conditions. The boundary conditions on the base of the cylinder are solely to avoid rigid body motion. All other surfaces are free. A fixed viscous body force is applied at all the material points to dampen the elastic waves generated due to the inertial effect. The form of the viscous body force is specified in Equation 2.36. A viscosity coefficient \( (c_{vb}) \) of 35 N·m/s is chosen so that the total viscous dissipation in the model is less than 10% of the total internal energy of the model.

Two load-free thermal cycle simulations are carried out. In the first simulation, plasticity is turned off by setting the yield stress to a very high value. This is referred to as the without-plasticity case. In the second simulation, the yield stress for plasticity is set to 160 MPa. This is referred to as the with-plasticity case.

Two load-biased thermal cycling simulations are carried out. In each case, a biasing stress of -60 MPa is applied along the Y global direction. These two simulations are identical to the with-plasticity and the without-plasticity cases described for the load-free thermal cycling simulations. The only exception in this case is that, there is a biasing stress applied.
In each case, the temperature is varied between 400 K and 150 K for two cycles. The rate of temperature variation is fixed and equals approximately 16.7 K/s. All material points in the model have the same temperature at a given time instant. This automatically satisfies the thermal equilibrium and hence the thermal diffusion equation is not solved. At the start of the first cycle, inhomogeneous nucleation is simulated by specifying non-zero order parameter value at two nucleation sites. A fixed crystallographic orientation is assigned to all the elements in the model. The local to global correspondence relation is: \([1 0 0] \parallel X, [0 1 0] \parallel Y\) and \([0 0 1] \parallel Z\). All other simulation parameters are listed in Table 3.3.

The rationale behind choosing to perform these four simulations is as follows. The load-free no-plasticity simulations provides a reference case. Here the martensite microstructure is random and it is not influenced by plasticity. In the load-free with-plasticity case, the martensite microstructure is still random, but there is slip activity possible, presumably due to the stress field of the A-M interfaces. The load-biased with-plasticity case has textured martensite, because the applied bias favors only certain CVs. Additionally, the crystal orientation of the sample is chosen such that the Schmid factor for plasticity along the loading direction is zero for all the slip systems modeled. This ensures that the slip activity is due to the textured martensite microstructure. The critical stress for slip for various orientations is shown in Figure 3.2.

For each of the simulations, following quantities are stored in the results at each material point- (1) The martensite volume fraction for the three CVs \((\nu_1, \nu_2, \nu_3)\). (2) The slip activity increment on each slip system \((\Delta\gamma_s)\), (3) The resolved shear stress
Figure 3.1: Geometry of the model used to simulate load-free and load-biased thermal cycling. The nodes on the base of the cylinder cannot displace in Y direction. The origin, located at the center of the base is fixed.

on each slip system ($\tau_{\text{slip}}$), (4) The temperature ($\theta$), (5) The stresses ($\sigma_{ij}$) and (6) the strains ($\epsilon_{ij}$).

To make the simulations computationally efficient, two strategies are employed. First the coarsest possible mesh is used. To determine this, a step-quench type of simulations are carried out with the mesh size varying from 50 000 to 2 000 000 tetrahedral elements. In a step-quench simulation, the sample is frozen at a fixed temperature below the transformation temperature and the evolution of the microstructure is observed. In these simulations, the samples are frozen at $\theta = \theta_T - 100K = 150K$. Figure 3.3 shows that the microstructure is qualitatively similar for mesh sizes varying between 500 000 and 2 000 000 elements. In the results discussed in the next Section, the choice is made to use octahedral elements. This is because about 100 000 octahedral elements give around the same mesh density as 500 000 tetrahedral elements. The second strategy employed to make the simulations efficient is to set the interface
Critical stress for plasticity ($\sigma_{\text{crit}(\text{pl})}$) along the loading direction in the load-biased thermal cycling simulations. $\sigma_{\text{crit}(\text{pl})}$ is calculated in terms of the initial flow shear strength for austenite ($g_0^s$) and the maximum Schmid factor for plasticity ($S_P$). $\sigma_{\text{crit}(\text{pl})} = g_0^s / S_P$. For the load-biased case modeled, the critical stress for slip is infinite in the loading direction [0 1 0]. The loading direction is shown by a solid circle.

Energy term to zero ($K_{tu} = 0$). This eliminates the need to calculate the gradient of the order parameter at each time increment. This reduces the simulation time by around 50%. Even though the interface energy term is set to zero, the interfaces still have a non-zero energy associated with them owing to the elastic strain energy in the elements at the interfaces. To study the effect of setting the interface term to zero, two simulations are carried out with an identical mesh. In the first simulation, the interface term is set to zero. In the second simulation, the interface energy term is set to $1 \times 10^{-3}$ J/m. In both cases, a step-quench type of temperature history is imposed. Figure 3.4 shows the microstructures for the two cases. The two microstructures are qualitatively similar. An analysis of the length scale of the microstructure, even when the interface term is zero, is presented later in Section 3.5.
<table>
<thead>
<tr>
<th>Elastic and thermal</th>
<th>Elastic constants (GPa): $C_{11(A)} = 130$; $C_{22(A)} = 98$; $C_{44(A)} = 21$; $C_M = C(A/2)$</th>
<th>Thermal expansion coefficients ($10^{-6}/K$): $\alpha_A = 11$; $\alpha_M = 6.6$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Equil. transf. temp. (K): $\theta_T = 250$</td>
<td>Latent heat of transf./unit vol. (MPa): $\lambda_T = 20$</td>
</tr>
<tr>
<td></td>
<td>Landau polynomial coefficients in Eqn. 2.37: $p = 1.0$, $q = -0.5$, $b = 1.0$, $d = -2.0$, $f = 1.0$</td>
<td></td>
</tr>
<tr>
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<td>Mobility in Eqn. 2.5 (/s): $M = 3.5 \times 10^{-2}$</td>
<td>Number of martensite CVs: $N_T = 3$</td>
</tr>
<tr>
<td></td>
<td>Transformation strains for CVs: Listed in Eqn. 3.1</td>
<td>Interface energy term in Eqn 2.23, $K_{tu} = 0.0$</td>
</tr>
<tr>
<td>Phase transformation</td>
<td>Reference shear strain rate (1/s): $\dot{\gamma}_0 = 0.02$</td>
<td>Strain rate exponent: $m = 0.5$</td>
</tr>
<tr>
<td></td>
<td>Initial slip system flow shear strength (MPa): $g^0_s = 160$ for the with-plasticity cases and $\infty$ for the without-plasticity cases.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Self-hardening coefficient (MPa): $h_0 = 1250$</td>
<td>Ratio of self to latent hardening: $Q = 1.4$</td>
</tr>
<tr>
<td></td>
<td>Hardening exponent: $a = 0.1$</td>
<td>Saturation shear strength (MPa): $g_{sat} = 1000$</td>
</tr>
<tr>
<td></td>
<td>Number of slip systems: $N_S = 6$</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.3: Material values for the simulations used to systematically study thermal cycling. A model set of parameters are chosen for the phase transformation. Elasticity and slip parameters are for solutionized Ti-50.9at.%Ni. Adapted from Manchiraju and Anderson [1].
Figure 3.3: Effect of mesh refinement on the martensite microstructure. The microstructure is shown for a step-quench type of simulations, where the sample is frozen at a $\theta = 150K$. (a) 500 000 elements, (b) 800 000 elements, (c) 2 000 000 elements. In each of the simulations tetrahedral elements are used.

Figure 3.4: Effect of the interface energy term ($K_{tu}$) on the martensite microstructure. (a) The interface energy term is set to zero. (b) Non zero interface energy term. The microstructure in this case is similar to the one shown in (a) in terms of the feature size.
3.3 Results: Martensite Microstructure and Plasticity Evolution During Thermal Cycling

3.3.1 Load-free Thermal Cycling

Plot of total martensite volume fraction ($\nu_{\text{tot}} = \nu_1 + \nu_2 + \nu_3$) against temperature ($\theta$) is shown in Figure 3.5(a) for the without-plasticity case, and in Figure 3.5(b) for the with-plasticity case. For both cases, the austenite does not completely transform to martensite at the end of cooling during the first cycle. These points are marked as $A$ and $A'$. The transformation completes soon into the heating part. Towards the end of the heating part, the martensite volume fraction shows fluctuations that diminish gradually. This is the part of the curve between points $P$ and $Q$ for the without-plasticity case; and points $P'$ and $Q'$ for the with-plasticity case. This effect is due to the inertial effects. During the end-stage of the cooling part, the kinetic energy of the model is large; almost comparable to the total energy. It is less than 10% of the total energy during other parts of the cycle, including the end-stage of the heating part. At the end of the first cycle, there is 3.8% residual martensite.

The residual martensite at the end of the first cycle grows during the cooling part of the second cycle. Due to this, the undercooling that otherwise would be required to nucleate martensite, is reduced. At the end of the cooling part of the second cycle, the austenite is completely transformed to martensite. During the heating part of the second cycle, for the without-plasticity case, the $\nu_{\text{tot}}$ vs. $\theta$ curve shows behavior that is identical to the first cycle. In the with-plasticity case, the response towards the end of heating is slightly different for the two cycles.

Figure 3.6 shows the volume fractions of individual martensite CVs against the temperature. The six representative points $A$ to $D$ and $P$, $Q$ from Figure 3.5
are shown again in this Figure. There are three key observations. First, the volume fractions of all CVs grow equally during cooling. Once the total martensite fraction has reached 1, CV 1 coarsens at the expense of CV 2 and CV 3. This is true for both cycles and for with-plasticity and without-plasticity cases. Second, the dominance of CV 1 is higher for the second cycle compared to the first. And third, the dominance of CV 1 is diminished in the with-plasticity case compared to its no-plasticity counterpart. Another observation is that, when the martensite volume fraction is fluctuating between points $P$ and $Q$, the oscillations in CV 1 fraction are complementary to those in CVs 2 and 3.

For the points marked $A$, $B$, $C$ and $D$ in Figure 3.5; the martensite microstructure is shown in Figure 3.7. At point $A$, bands of martensite have grown from the two nucleation sites $N_1$ and $N_2$. However, large parts of the model have a mixture of all three CVs. In those regions, the total martensite fraction is around
50%. All three martensite CVs grow to an equal sample-averaged volume fraction. After this point, reorientation of CVs starts to occur and volume fraction of one of the CVs grows at the expense of others. At point (B), austenite in the whole sample is transformed to martensite. CV 1 has coarsened to dominate. At the peak of the second cycle, at the point marked as (C), all the austenite is transformed to martensite. The martensite is present in narrow bands. At point (D), again first CV is dominant. However at (D), the volume fraction of CV 1 is larger than what it were at point (B). This is reflected in Figure 3.6 as well. Corresponding microstructure evolution for the with-plasticity case is shown in Figure 3.8. In this case the microstructure evolution is qualitatively similar to the without-plasticity case.

Evolution of the sample-averaged equivalent plastic strain ($e_{\text{plas}(eq)}$) vs. temperature for the with-plasticity case is shown in Figure 3.9(a). The equivalent plastic
strain is defined as,

\[ e_{\text{plas(eq)}} = \sqrt{\frac{1}{2}[(\epsilon_{11} - \epsilon_{22})^2 + (\epsilon_{22} - \epsilon_{33})^2 + (\epsilon_{33} - \epsilon_{11})^2] + 3(\epsilon_{12}^2 + \epsilon_{23}^2 + \epsilon_{31}^2)} \]  

(3.11)

e_{\text{plas(eq)}} produced over two cycles is small (\(\sim 2 \times 10^{-3}\)) compared to the strain produced by phase transformation (0.06). Smaller plastic strain (\(\sim 7 \times 10^{-4}\)) is produced during the first cycle than that during the second cycle (\(\sim 1.3 \times 10^{-3}\)). The rate of plastic strain generation is higher between 150-160 K and 250-280 K in the heating part of the first cycle; between 170-150 K of the cooling part of the second cycle and between 250-290 K of the heating part of the second cycle. These are the temperature ranges during which most of the phase transformation occurs.

Variation of the sample-averaged equivalent plastic strain as a function of the total martensite volume fraction is shown in Figure 3.9(b). In the first cycle, the rate of plasticity production is higher when the martensite volume fraction is greater than 0.6. The rate of plasticity generation is also higher in the region bounded by the points \(P'\) and \(Q'\). This perhaps suggests that there is some plasticity generation due to the inertial effects, which are dominant in that temperature range. During the cooling part of the second cycle, there is plastic strain generation at a fixed rate.

### 3.3.2 Load-biased Thermal Cycling

The martensite volume fraction evolution for the load-biased thermal cycling is shown in Figure 3.10. At the start of the cooling part, there is already some martensite. This martensite is stabilized due to the biasing stress. The transformation completes at \(\sim 175\) K, compared to the incomplete transformation during the cooling part of the first cycle of the load-free thermal cycling. During the heating part, the reverse transformation is abrupt, compared to the smooth forward transformation.
The macro response in terms of the martensite fraction evolution is almost identical for the with-plasticity and the without-plasticity cases. The data for the second cycle is incomplete for the load-biased simulations. This is because, the simulations encountered a numerical instability in the second cycle. However, the available data for the second cycle of the with-plasticity case suggests that the transformation starts earlier in the second cycle.

Evolution of the volume fraction of individual CVs is shown in Figure 3.11. Only CV 1 and 3 appear during transformation. This is because, those CVs are favored by the biasing stress. During the early part of the cooling, both CVs grow equally. At the end of cooling, CV 1 is dominant. It continues to grow in the heating part, until the temperature reaches \( \sim 250 \) K. The evolution of the individual CVs is almost identical in the without-plasticity and the with-plasticity cases. During the second cycle, for the with-plasticity case, the path followed by the two CVs in terms of the volume fraction is essentially identical to the first cycle. The only difference being an earlier onset of transformation.

The martensite microstructure for the without-plasticity case at the end of cooling of the first cycle is shown in Figure 3.12. The orientation of the interface between CV 1 and CV 3 is of the type \([1\ 0\ 1]\). This is consistent with the results of the crystallography calculations listed in Table 3.1. The martensite microstructure at the end of cooling of the first and the second cycle for the with-plasticity case are shown in Figure 3.13. The microstructure in the second cycle is finer than that in the first cycle.

Figure 3.14(a) shows the equivalent plastic strain averaged over the model as a function of temperature. During the cooling part of the first cycle, there is a gradual
increase in the plastic strain. During the heating part, between 250 K and 300 K, there is a rapid rise in plastic strain. This corresponds to the temperature range when the reverse transformation is taking place. The plastic strain accumulation during the cooling part of the second cycle is similar to the first cycle. In Figure 3.14(b), the variation of plastic strain as a function of the martensite volume fraction is shown. The trend seen here is similar to that in the load-free thermal cycling case. There is a rapid accumulation of plastic strain when the martensite fraction is small (<0.2). This potentially corresponds to the slip activity induced by the inertial effects. The plastic strain generated in the first cycle ($1.1 \times 10^{-3}$) is larger than the plastic strain generated in the first cycle of load-free thermal cycling ($0.7 \times 10^{-3}$).
Figure 3.7: Martensite microstructure at the temperatures marked as A, B, C and D in Figure 3.5(a). Volume fractions of the three CVs are plotted on the model with a cut along the XY plane. Without-plasticity load-free thermal cycling case. The results for the corresponding with-plasticity case are shown in Figure 3.8 and they are qualitatively similar.
Figure 3.8: Martensite microstructure at the temperatures marked as A’, B’, C’ and D’ in Figure 3.5(b). Volume fractions of the three CVs are plotted on the model with a cut along the XY plane. *With-plasticity* load-free thermal cycling case.
Figure 3.9: Plot of equivalent plastic strain averaged over the model vs. (a) temperature and (b) martensite fraction, for the load-free thermal cycling simulations. (with-plasticity case).

Figure 3.10: Evolution of total martensite volume fraction during the load-biased thermal cycling simulations. The without-plasticity case is shown in (a) and the with-plasticity case is shown in (b). The two curves are almost identical.
Figure 3.11: Evolution of the martensite volume fraction of the three CVs during load-biased thermal cycling simulations. The without-plasticity case is shown in (a) and the with-plasticity case is shown in (b). The two set of curves are almost identical.

Figure 3.12: Martensite microstructure at 150K during the first cycle for load-biased thermal cycling (without-plasticity case). Only CV 1 and CV 3 are present, due to the external stress.
Figure 3.13: Martensite microstructure at 150K for the load-biased thermal cycling (\textit{with-plasticity} case). Only CV 1 and CV 3 are present, due to the external biasing stress.

Figure 3.14: (a) Macro equivalent plastic strain vs. temperature for the load-biased thermal cycling. (b) The equivalent plastic strain plotted against the martensite volume fraction.
3.4 Discussion: Analysis of the Thermal Cycling Simulations

3.4.1 Load-free Thermal Cycling

The martensite fraction vs. temperature curves in Figure 3.5 show a hysteretic response typical of SMAs. The incomplete transformation during cooling in the first cycle is due to insufficient time available for the phase transformation to complete. A larger mobility value or a slower cooling rate would have allowed the transformation to complete. During the first cycle, the phase transformation does complete shortly into the heating part. At the end of heating part of the first cycle, the driving force for reverse transformation is small. Small driving force coupled with fast heating rate does not allow reverse transformation to complete. This leads to a residual martensite fraction of about 2.4% in the case of with-plasticity case and 3.8% in the without-plasticity case. Holding at high temperature for longer time would allow the reverse transformation to complete. During the cooling part of the second cycle, these existing domains of the residual martensite essentially make a large number of nucleation sites available. This abundance of nuclei, compared to only two nuclei at the start of the first cycle, makes transformation complete to 100% during the second cycle. Further, these nuclei distributed across the sample, rapidly grow into bands of martensite. This causes the emergence of finely fragmented microstructure at the peak of the second cycle as shown in Figure 3.7 (C) as well as Figure 3.8 (C').

The fragmented microstructure formed during the first and the second cycle coarsens so that $\nu_1 > \nu_2, \nu_3$. The coarsening happens despite the interfacial energy term, $K_{tu}$ in Equation 2.23 being set to zero. This can be rationalized as follows. Even though the gradient-based interface energy term is set to zero, there is an energy associated with the interfaces at a finer length scale. The finite elements at the
interface are distorted elastically. This elastic energy can be reduced by a coalescence of the fragments of martensite into thicker bands. This happens for all the CVs, as seen in Figure 3.7 (C) and (D), and its with-plasticity counterpart. The dominance of CV 1 intern of the volume fraction is potentially statistical, in the sense that CV 2 or 3 had an equal chance of growing in volume.

The residual martensite at the end of the first cycle essentially causes the \( \theta_{MS} \) and \( \theta_{MF} \) temperatures to rise. To quantify this, \( \theta_{MS} \) is defined to be the temperature at which the martensite volume fraction reaches 0.2. \( \theta_{MF} \) is defined as the temperature at which the total martensite fraction reaches 0.8. The values of the transformation temperatures calculated from the macro data are listed in Table 3.4. \( \theta_{MF} \) values for the first cycle are unavailable for the load-free thermal cycling case, because the sample did not completely transform to martensite. From this data, we can also observe that for the with-plasticity case, the transformation temperatures in the second cycle are slightly higher vs. the without-plasticity case.

<table>
<thead>
<tr>
<th></th>
<th>Transformation temperatures (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \theta_{MS} ) 1\textsuperscript{st} cycle 2\textsuperscript{nd} cycle</td>
</tr>
<tr>
<td>Load-free without-plasticity</td>
<td>166.1 177.8 -</td>
</tr>
<tr>
<td>Load-free with-plasticity</td>
<td>166.2 180.6 -</td>
</tr>
<tr>
<td>Load-biased without-plasticity</td>
<td>222.2 - 180.9 -</td>
</tr>
<tr>
<td>Load-biased with-plasticity</td>
<td>222.5 227.2 181.2 189.1</td>
</tr>
</tbody>
</table>

Table 3.4: \( \theta_{MS} \) and \( \theta_{MF} \) temperatures for the thermal cycling simulations calculated from the macroscopic data.
Experimental data for load-free thermal cycling of Ni-Ti polycrystals suggests that these transformation temperatures are lowered and the difference between $\theta_{MS}$ and $\theta_{MF}$ increases [89]. This is possibly due to the stress field of the dislocations hindering growth of martensite. This is not observed in the with-plasticity case, possibly because of the small amount of plastic strain and because the simulations presented here involved single crystals. However, the same experimental work reports a rise in the $\theta_{MS}$ temperature on thermal cycling for samples that were plastically pre-strained.

If we repeat the exercise of determining the $\theta_{MS}$ and the $\theta_{MF}$ temperatures for all the individual material points in the model, we reach the same conclusion as above - that the transformation temperatures are elevated in the second cycle vs. the first and they are slightly higher for the with-plasticity case in the second cycle vs. the without-plasticity case. Figure 3.15 shows the distribution of $\theta_{MS}$ and $\theta_{MF}$ for all the material points in the samples. However, an interesting result is obtained if this analysis is repeated, but while considering only the 1000 material points in the with-plasticity case which have the highest local equivalent plastic strain. In this case, the with-plasticity case has the transformation temperatures shifted to lower values. Figure 3.16 shows the histograms of $\theta_{MS}$ and $\theta_{MF}$ for top 1000 plastically deformed material points. For the without-plasticity case, 1000 points are arbitrarily chosen. This trend suggests a deleterious effect of plastic strain on the local phase transformation, perhaps in principle similar to the experiments-based hypothesis of Miyazaki et al discussed above [89].

Based on the observation that, the plastic strain has a deleterious effect on transformation, we would expect that the transformation would be hindered more at the
material points with a large plastic strain. To test this hypothesis, the difference in the $\theta_{\text{MS}}$ and $\theta_{\text{MF}}$ temperatures is plotted against the plastic strain for the top 1000 plastically deformed points. However material points with a specific dominant slip system are chosen. The result is shown in Figure 3.17(a). There is a weak but interesting correlation between the magnitude of the equivalent plastic strain and the transformation temperature range. For small plastic strains, the difference $\theta_{\text{MS}} - \theta_{\text{MF}}$ decreases with an increasing plastic strain. After a cutoff value of strain, the difference becomes wider. So, there is a range of plastic strains, where the plasticity is helping transformation; but at larger plastic strain, it hinders transformation. There are factors other than the plastic strain that may affect the transformation temperature spread. These are the position of the material points in the interior vs. the...
Figure 3.16: A histogram of the (a, b) $\theta_{MS}$ and the (c, d) $\theta_{MF}$ temperatures for top 1000 plastically deformed material points in the load-free thermal cycling simulations. $\theta_{MS}$ and $\theta_{MF}$ shift higher for the second cycle vs. the first. With-plasticity case has lower $\theta_{MS}$ vs. without-plasticity case.

surface of the sample and the type of the residual martensite present at the start of the second cycle. The dominant slip system active at the material points did not show a correlation with the spread in the transformation temperatures.

There is a spatial correlation between the spread $\theta_{MS} - \theta_{MF}$, the regions of slip activity and the martensite microstructure. Figure 3.18 shows the martensite microstructure that formed in the first cycle, the difference $\theta_{MS} - \theta_{MF}$ in the second cycle and the spatial distribution of slip activity in the first cycle. The difference $\theta_{MS} - \theta_{MF}$ is higher ($\sim 30$ K) in the regions where M-M interfaces were present during the first cycle. The plastic strain is also localized in the regions of M-M interfaces.

Another effect of residual martensite and the resultant fragmented microstructure during the second cycle is that, additional plastic strain is produced during the cooling part of the second cycle vs. the first cycle (shown in Figure 3.9). Fragmented
Figure 3.17: The difference in the $\theta_{MS}$ and $\theta_{MF}$ temperatures against the equivalent plastic strain at the top 1000 plastically deformed points. Material points with a specific dominant slip system, (10\(\overline{1}\))[010] are chosen. (a) load-free and (b) load-biased thermal cycling. There is a weak correlation between the magnitude of the plastic strain and the transformation temperature range. For small plastic strains, the difference between the transformation strain reduces with plastic strain. However, after a cutoff value, the difference widens.

Martensite microstructure means that more A-M interfaces are present where the local stress field potentially causes plastic deformation to occur. Widespread plastic deformation accompanying the evolution of fragmented martensite is shown in the image sequence in Figure 3.19. During the first cycle, two nucleation sites lead to relatively coarse martensite microstructure and hence lower plastic strain during cooling. Since the martensite microstructure coarsens during the early part of heating (points \(\mathbb{B}\) and \(\mathbb{D}\) in Figure 3.7), there are approximately same number of interfaces during the reverse transformation in the first and the second cycle. Due to this, the plastic strain produced during heating stage is comparable across the two cycles.
Figure 3.18: There is a spatial correlation between the martensite microstructure formed in the first cycle, $\theta_{MS} - \theta_{MF}$ spread in the second cycle, and the regions of slip activity formed in the first cycle of load-free thermal cycling. (a) Martensite microstructure in the first cycle. This is at a temperature slightly higher than the point labeled as $B'$ in Figure 3.8. (b) The difference $\theta_{MS} - \theta_{MF}$ in the second cycle with the interfaces between the martensite CVs in (a) superimposed in solid black lines. (c) Contour plot of the equivalent plastic strain at the same temperature in the first cycle as (a). These bands match with the position of M-M interfaces in (a).

All slip systems make comparable contributions to the total slip activity observed. This is evident when the dominant slip system in terms of the slip produced is determined at various material points. Table 3.5 lists the number of material points where each of the six slip systems is dominant. For the load-free thermal cycling, the dominance is almost equally distributed among the six candidate slip systems. This can be rationalized based on the fact that all martensite CVs are activated leading to the formation of a large number of A-M and M-M interfaces. Based on the hypothesis that the local stress field of the martensite twins is responsible for transformation induced plasticity, a large number of interfaces would favor a wide variety of slip systems. Activation of a limited number of martensite variants may reduce the number of favored slip systems.
Figure 3.19: An image sequence showing the evolution of martensite and the plastic strain during the second cycle of load-free thermal cycling. As the fragments of martensite grow from $G'$ to $I'$, plastic strain increases in the same regions.

3.4.2 Load-biased Thermal Cycling

During the load-biased thermal cycling, the biasing compressive stress is applied along the Y direction. Since CV 1 and 3 produce compressive strain along Y direction they are favored; while CV 2 is not favored because it produces tensile strain along Y (see Equation 3.1). Additionally, as shown in Figure 3.2, external stress does not favor slip activity on any of the six modeled slip systems.
Table 3.5: Dominant slip systems in terms of slip activity at 1000 material points with the largest plastic strain in each of the load-free and load-biased simulations (with-plasticity case).

At the start of the first cycle, there is some martensite present (~15%) due to the biasing stress. This can be explained in terms of the reduction in the free energy of the martensite due to the bias stress. Figure 3.20 shows a schematic free energy curve for austenite-martensite system. Here we assume that the gradient based interface energy is zero. In the absence of a biasing stress, the free energy curve is solely described by the Landau polynomial. When an external stress of -60 MPa is present, it lowers down the free energy curve. Because of this, a new minimum occurs at an intermediate value of the order parameter. In the schematic this minimum is exaggerated. An exact value of this minimum can be numerically calculated by setting the driving force in Equation 2.23 to zero and solving for the order parameter.

The transformation temperature are elevated in the case of load-biased thermal cycling simulations vs. load-free simulations due to the bias stress. This is reflected in the $\theta_{\text{MS}}$ and $\theta_{\text{MF}}$ values in Table 3.4. $\theta_{\text{MS}}$ temperature is approximately 50 K higher compared to the load-free case, while the $\theta_{\text{MF}}$ is around 30 K higher.
Figure 3.20: A schematic of the stabilization of martensite facilitated by an external biasing stress.

Figure 3.21 shows the variation in $\theta_{MS}$ and $\theta_{MF}$ respectively for all the material points in the model. These plots reflect the trend seen in the macro data for the transformation temperature, in the sense that, the transformation starts earlier in the second cycle. The $\theta_{MS}$ temperature is spread over a wider range in the second cycle, compared to the first. Consideration of only top 1000 plastically deformed material points in this case leads to similar conclusions as the load-free case in part - the plastically deformed points tend to have a lower elevation in the $\theta_{MS}$ temperature. The data for the $\theta_{MF}$ temperature does not provide such results. Results for top 1000 plastically deformed material points are shown in Figure 3.22.

The correlation between the difference $\theta_{MS} - \theta_{MF}$ and the plastic strain at a material point is poorer compared to the load-free case. Figure 3.17(b) in general shows that, large plastic strain correlates with narrower difference in the transformation
temperatures. One reason for the weak influence of the plastic strain on the transformation temperatures could be the external bias stress. Perhaps the added driving force from the biasing stress makes the plasticity less relevant as far as progress of the transformation front is involved.

Figure 3.21: A histogram of the (a, b) $\theta_{MS}$ and (c, d) $\theta_{MF}$ temperature for all material points in the load-biased thermal cycling simulations. $\theta_{MS}$ and $\theta_{MF}$ shift higher for the second cycle vs. the first. Only the With-plasticity case is shown.

A comparison of Figures 3.14 and 3.9 suggests that the evolution of the plastic strain in the load-biased case has a similar trend as the load-free case. However the magnitude of the plastic strain at the end of the first cycle is higher for the load-biased case ($\epsilon_{pl(eq)} = 1.1 \times 10^{-3}$) than the load-free case ($\epsilon_{pl(eq)} = 0.7 \times 10^{-3}$). This could presumably be due to the longer time taken for completion of the transformation in the load-biased case. $\theta_{MS} - \theta_{MF}$ is $\sim 40$ K for the load-biased case vs. $\sim 20$ K for the load-free case. This is because the plasticity formulation implemented in this model is time-dependent.
Figure 3.22: A histogram of the (a, b) $\theta_{\text{MS}}$ and (c, d) $\theta_{\text{MF}}$ temperature for the top 1000 plastically deformed material points in the load-biased thermal cycling simulations. $\theta_{\text{MS}}$ and $\theta_{\text{MF}}$ shift higher for the second cycle vs. the first. Only the With-plasticity case is shown.

The nature of slip systems activated in this case is drastically different compared to the load-free case. Table 3.5 shows the dominant slip systems in 1000 most plastically strained material points. Slip systems with Burger’s vector along [0 1 0] are dominant in the load-biased case. This can be rationalized on the basis on activation of only two CVs - 1 and 3. This plastic deformation is not at a sharp interface between austenite and twinned martensite. Rather, during the reverse transformation of martensite during heating, there form bands of austenite which grow as the temperature increases. The plastic deformation is predominantly in these trapped bands of austenite. Figure 3.23 shows the location of plastic zone relative to the martensite microstructure.
Figure 3.23: An image sequence showing the evolution of the martensite microstructure and the plastic strain during the heating part of the load-biased thermal cycling. Traces of the M-M boundaries at \( J' \) are superimposed on the sample shape at \( L' \). The position of the slipped regions matches with the M-M interfaces that vanished from \( J' \) to \( L' \).
3.5 Establishing a Time and Length Scale for the Model

The parameters used in the constitutive relation lend a length and a time scale to
the model. However, the implementation itself essentially uses “effective” values for
time step and grid length. In this Section, a length scale for the model is established on
the basis of the interfacial and the bulk energy terms used in the phase transformation
law. Then a time scale is established in terms of the kinetic coefficient used in the
phase transformation law.

Figure 3.24: A schematic of the volume and interfacial energy terms associated with
a martensite plate. A cross-section of a plate that spans a cylindrical sample is
shown. $T$ is the plate thickness and $t$ is the twin thickness. $\lambda_t$ and $\lambda_i$ are the energies
for the twin (M-M) interface and the plate (A-M) interface respectively. $\lambda_{ev}$ is the
elastic strain energy stored in the austenite matrix due to the local stress field of the
martensite twins.

A length scale is established in the model due to the competing nature of the
chemical free energy of the phases, the interfacial energies and the elastic strain
energy. A plate forms when the martensite has a lower chemical free energy than
the austenite. Formation of a twinned plate leads to creation of interfaces between
the twinned variants and between the austenite and the martensite. It is desirable to reduce the area and hence the energy of the interfaces. The twins produce a stress field in the neighboring austenite due to the incompatibility between the austenite and a martensite variant. Based on the Saint-Venant’s principle, the stress field can be argued to extend into the austenite to a length comparable to the twin width \( t \). This implies that a coarse twin microstructure would lead to a larger volume of elastically deformed austenite and consequently generate larger stored elastic energy compared to a fine microstructure. The competition between the interfacial energies and the elastic strain energy in austenite leads to an equilibrium twin width \( t_{\text{equilib}} \).

Note that the interfacial energies need not be contributed by the gradient based term \( K_{tu} \) in the phase transformation law (Equation 2.23). They can be contributed by the local deformation of the FEM mesh at the interfaces.

The total energy of a representative volume consisting of the plate can be written as follows.

\[
E_{\text{ref}} = \Sigma \epsilon^T \pi r^2 T + \lambda_c \pi r^2 T + \lambda_i \frac{2r}{t} T + \lambda_{\text{ev}} \pi r^2 t \tag{3.12}
\]

Here \( \Sigma \) is the local stress, \( \epsilon^T \) is the transformation strain, \( \lambda_c \) is the chemical free energy change between austenite and martensite, \( \lambda_i \) is the A-M interface energy and \( \lambda_t \) is the M-M interface energy. The equilibrium twin thickness \( t_{eq} \) corresponds to a \( t \) that minimizes the energy \( E_{\text{ref}} \). We use the condition for minimization of E, \( \delta E/\delta t \big|_{t=t_{eq}} = 0 \) to find \( t_{eq} \).

\[
\frac{\delta E}{\delta t} \bigg|_{t=t_{eq}} = -\lambda_i \frac{2r}{t^2} T + \lambda_{\text{ev}} \pi r^2 = 0 \tag{3.13}
\]

This gives,

\[
t_{eq} = \sqrt{\frac{\lambda_i T}{\lambda_{\text{ev}} \pi r^2}} \tag{3.14}
\]
The form of $t_{eq}$ can be rationalized as follows: higher M-M interface energy would favor coarser twin structure, while higher elastic strain energy coefficient would favor finer twin structure. Further, $\lambda_{ev}$ can be written in terms of the elastic stiffness constants for the austenite matrix.

An effective time scale can be constructed for the model in terms of the mobility coefficient ($M$) in Equation 2.5 and the latent heat ($\lambda$).

$$\tilde{t} = \frac{1}{M\lambda} \tag{3.15}$$

With $M \sim 10^{-2} m^3/J \cdot s$ and $\lambda \sim 10^6 J/m^3$, the time scale for the model is of the order of $10^{-4} s$.

### 3.6 Conclusions

In this chapter, a systematic study of the martensite microstructure development and the interaction between phase transformation and slip activity in austenite is presented using the phase field/finite element model developed in Chapter 2. This is achieved by performing load-free and load-biased thermal cycling simulations with a model cubic ↔ tetragonal transformation system and six \{1\ 1\ 0\} type slip systems in austenite.

A mixture of all CVs is formed during load-free thermal cycling. Slip activity is observed at the sites of M-M interfaces. The slip activity is equally distributed on all the six slip systems due to the lack of martensite texture. During load-biased thermal cycling, textured martensite comprising of CVs 1 and 3 is formed. Slip activity in this case is predominantly on the slip systems with \[0\ 1\ 0\] type Burger’s vector.

A coarse martensite microstructure is formed in the first cycle and the microstructure is fragmented during the second cycle. This is due to the residual martensite at
the end of the first cycle that did not have opportunity to reverse transform due to fast thermal cycling rate. This is observed for both, load-free and load-biased thermal cycling.

The transformation temperatures, $\theta_{\text{MS}}$ and $\theta_{\text{MF}}$, shift to higher values in the second cycle compared to the first. This is due to the residual martensite that promotes phase transformation in the second cycle. At the macro scale, the elevation of transformation temperatures is slightly higher for the cases where slip activity was present.

However at the local scale, slipped regions tended to have lower transformation temperatures compared to their unclipped counterparts. Additionally, the difference between $\theta_{\text{MS}}$ and $\theta_{\text{MF}}$ is increased in the regions of the sample that were plastically deformed. Quantitatively, the material points with plastic strain above a threshold tended to have $\theta_{\text{MS}} - \theta_{\text{MF}}$ proportional to the plastic strain. This spatial and quantitative correlation between the $\theta_{\text{MS}} - \theta_{\text{MF}}$ spread and the plastic strain is observed in the load-free thermal cycling simulations.

Though the simulations capture the martensite microstructure and plasticity, there are two issues. First, the predicted A-M interfaces are diffuse, even though the M-M interfaces are sharper. Second, inertial effects are present in the simulations, which may be influencing the observed plastic response. However, the inertial effects are predominant primarily in the full transformed state at the peak cooling and additionally at the end of heating stage. In the prior situation, slip activity is impossible, because plasticity is only present in austenite.
Chapter 4: Modeling of NiTi Micropillar Compression

Ni-Ti SMAs have received substantial attention due to their suitability for various industrial applications. However, poor dimensional stability is in part restricting wider adaption of this material. Over the years, experimental evidence has grown to suggest that one of the factors responsible for generation of defects is the local stress field of the martensite microstructure (see Section 1.1.5 for an overview of the literature). In that sense, it is desirable to understand the mechanism by which these defects are generated. This knowledge can then be used to suppress the defect formation or accumulation (For example, by tailoring the alloy composition so that a wide variety of compatible A-M interfaces can be formed [90], or by mechanical treatment [91]).

In this study the PF/FE framework based modeling is combined with compression tests on Ni-Ti micropillars (described in [40, 43]). With this three key questions are answered.

1. What is the martensite microstructure on loading the pillar?
2. Which slip system is activated due to the stress field of martensite twins?
3. How does the slip system activated accommodate deformation at the interface?
4.1 Methods

4.1.1 PF/FE Modeling

The PF/FE approach described in Chapter 2 is used to model the compression of a Ni-Ti micropillar. Figure 4.1(a) shows the geometry of the pillar and platen modeled. The platen compresses the pillar at a constant strain rate of $\dot{\varepsilon}_y = 3.5 \times 10^{-3} / s$ for two loading-unloading cycles. The loading is done at a temperature that is 40 K above the transformation temperature. The platen is misaligned with the top of the pillar by $3^\circ$ and it is modeled as a rigid body. Contact between the platen and the pillar is frictionless. The pillar is meshed into 25 thousand hexahedral elements (C3D8RT in ABAQUS). The material properties assigned to the pillar are listed in Table 4.1. Nodes on the bottom surface of the pillar ($y = 0$) are fixed. All other surfaces have free boundary conditions. The loading axis (y) is assigned the crystal orientation [7 8 0] to match the experiments.

The crystal plasticity parameters specified in Table 4.1 correspond to a solution-ized Ti-50.6at.\%Ni alloy [1]. The parameters specifying the Landau polynomial for transformation are reasonable, but not specifically calibrated to a specific Ni-Ti alloy. This choice of the material parameters can be justified as follows - The relative values of the transformation and plasticity parameters (e.g. the critical stresses for transformation and that for plasticity) are more likely to determine the magnitude of the transformed volume and the plastic strain, rather than the interaction between the two mechanisms. E.g. changing the yield stress is unlikely to change whether the slip activity is concentrated in front of a growing martensite plate or a receding one. Since the aim of this study is to qualitatively study the interaction between phase transformation and plasticity, rather than quantify the two mechanisms, a model
set of parameters is chosen for the two mechanisms. A key feature of the Landau polynomial is that, it involves an activation barrier. The plasticity law incorporates hardening through a set of parameters, phenomenologically representing the latent and the kinematic hardening.

Figure 4.1: Micropillar model schematic.

Previous experimental works on compression of [780] oriented micropillar have shown the activation of a single martensite invariant plane with CV 1 and 4 (See Table 4.3 of Bhattacharya [8] for the notation and [40, 43] for the experimental evidence). Based on this information, only CV 1 and 4 are included in the simulations. The
<table>
<thead>
<tr>
<th>Elastic and thermal</th>
<th>Elastic constants (GPa): $C_{11(A)} = 130$; $C_{22(A)} = 98$; $C_{44(A)} = 21$; $C_M = C(A/2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Thermal expansion coefficients ($10^{-6}$/K): $\alpha_A = 11$; $\alpha_M = 6.6$</td>
</tr>
<tr>
<td>Phase transformation</td>
<td>Equil. transf. temp. (K): $\theta_T = 250$</td>
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<tr>
<td></td>
<td>Latent heat of transf./unit vol. (MPa): $\lambda_T = 20$</td>
</tr>
<tr>
<td></td>
<td>Landau polynomial coefficients in Eqn. 2.37: $p = 0.5$, $q = -0.25$, $b = 1.0$, $d = -2.0$, $f = 1.0$</td>
</tr>
<tr>
<td></td>
<td>Mobility in Eqn. 2.5 (/s): $M = 2.0$</td>
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<tr>
<td></td>
<td>Number of martensite CVs: $N_T = 2$</td>
</tr>
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<td></td>
<td>Transformation strains for CVs: Listed in Eqn. 4.1</td>
</tr>
<tr>
<td></td>
<td>Interface energy term in Eqn 2.23, $K_{tu} = 0.0$</td>
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<tr>
<td>Austenite plasticity</td>
<td>Reference shear strain rate (1/s): $\dot{\gamma}_0 = 0.02$</td>
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<tr>
<td></td>
<td>Strain rate exponent: $m = 0.1$</td>
</tr>
<tr>
<td></td>
<td>Initial slip system flow shear strength (MPa): $g^0_s = 130$</td>
</tr>
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<td></td>
<td>Self-hardening coefficient (MPa): $h_0 = 1250$</td>
</tr>
<tr>
<td></td>
<td>Ratio of self to latent hardening: $Q = 1.4$</td>
</tr>
<tr>
<td></td>
<td>Hardening exponent: $a = 0.1$</td>
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<td></td>
<td>Saturation shear strength (MPa): $g_{sat} = 1000$</td>
</tr>
<tr>
<td></td>
<td>Number of slip systems: $N_S = 6$</td>
</tr>
</tbody>
</table>

Table 4.1: Material values for the simulations used to model NiTi pillar compression.

Transformation strains for CV 1 and 4 are listed in Equation 4.1. Twelve FCC slip systems with slip planes of $\{100\}$ and $\{110\}$ family are modeled. The transformation and slip systems are listed in Table 4.2. Modeling of two CVs, rather than twelve, allow the micro-compression scenario to be simulated in a reasonable amount of time.

$$E_1 = \begin{bmatrix} 3.1 & -4 & -7.2 \\ -4 & -4.5 & 1.7 \\ -7.2 & 1.7 & 2.7 \end{bmatrix} \quad (4.1a)$$

$$E_4 = \begin{bmatrix} 3.1 & -4 & 7.2 \\ -4 & -4.5 & -1.7 \\ 7.2 & -1.7 & 2.7 \end{bmatrix} \quad (4.1b)$$
<table>
<thead>
<tr>
<th>Slip plane ( (m_{\text{slip}}) )</th>
<th>Burger’s vector ( (b_{\text{slip}}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (0 1 0)</td>
<td>[1 0 0]</td>
</tr>
<tr>
<td>2 (0 0 1)</td>
<td>[1 0 0]</td>
</tr>
<tr>
<td>3 (1 0 0)</td>
<td>[0 1 0]</td>
</tr>
<tr>
<td>4 (0 0 1)</td>
<td>[0 1 0]</td>
</tr>
<tr>
<td>5 (1 0 0)</td>
<td>[0 0 1]</td>
</tr>
<tr>
<td>6 (0 1 0)</td>
<td>[0 0 1]</td>
</tr>
<tr>
<td>7 (0 1 1)</td>
<td>[1 0 0]</td>
</tr>
<tr>
<td>8 (0 1 \bar{1})</td>
<td>[1 0 0]</td>
</tr>
<tr>
<td>9 (1 0 1)</td>
<td>[0 1 0]</td>
</tr>
<tr>
<td>10 (1 0 \bar{1})</td>
<td>[0 1 0]</td>
</tr>
<tr>
<td>11 (1 1 0)</td>
<td>[0 0 1]</td>
</tr>
<tr>
<td>12 (\bar{1} \bar{1} 0)</td>
<td>[0 0 1]</td>
</tr>
</tbody>
</table>

Table 4.2: Austenite slip systems implemented in the simulations in Chapter 4.

### 4.1.2 Micropillar compression experiments

Experimental data for micropillar compression was obtained from the state-of-the-art tests performed at The Ohio State University. Micropillars with 5 \( \mu m \) diameter were machined from single crystals of Ti-50.7at.%Ni. [7 8 0] crystal direction of the pillars was oriented along the loading axis (Y). The pillars were compressed at ambient temperature at which austenite is the stable phase. TEM samples were prepared from the pillars after the compression loading-unloading was performed. The foil normal was \([0 0 \bar{1}]\). For the details of the experimental work, the reader is referred to Norfleet et al [40] and Bowers et al [43].
4.2 Results

4.2.1 Modeling Results

The stress-strain response of the pillar for two compression cycles is shown in Figure 4.2. During the first cycle, phase transformation starts to occur as soon as the platen comes into contact with the top of the pillar. This is due to gradual stabilization of martensite in the presence of external stress as shown in Figure 2.1(b). The instability (sudden reduction in the magnitude of stress) occurs when the homogeneously grown martensite CV mixture separates into alternating bands of martensite variants. The shape of the instability mimics the drop in the Landau polynomial after the activation barrier is crossed. During unloading, the stress is small in magnitude and fairly constant. At the end of unloading, the stress-strain response shows unstable behavior. This is potentially due to inertial effects when the platen is not in contact with the top of the pillar. During the second cycle, the stress for transformation is lower. Potentially because of formation of martensite plate at the very beginning of the cycle. During unloading in the second cycle, the stress magnitude is gradually decreasing, rather than being constant as in the first cycle. The stress-strain response is averaged over the entire volume of the pillar, including the base. However, microstructural changes occur only in the stem of the pillar.

A single martensite plate is formed during each of the stress cycles. Figure 4.3 shows the plate geometry at an intermediate stage in each loading cycle. During the first cycle, the plate nucleates on the right surface of the pillar. It continues to grow horizontally across the width of the pillar. However, during this stage the orientation of the austenite-martensite (A-M) interface is transient. During the unloading part of the 1st cycle, the A-M interface is stabilized to the orientation shown in Figure
Figure 4.2: Simulated stress-strain response of Ni-Ti pillar under compression. The instability during the first cycle corresponds to the formation of martensite plate. The stress for transformation during the second cycle is lower. Due in part by plasticity mediated nucleation of martensite and potentially an effect of retained martensite.

4.1(a). During the second cycle, the plate nucleates at the top right corner of the pillar. This is the point where the platen comes into contact with the pillar surface. Similar to the first cycle, the A-M interface changes orientation during the loading half of the second cycle and stabilizes during the unloading part. Orientations of the A-M and martensite-martensite (M-M) interfaces during the two cycles are shown in Figure 4.3. In this figure, martensite volume fraction is plotted on the undeformed shape. However, the pillar bends in the X direction when loaded. The martensite bands produce local stress field at the A-M interface, which can potentially lead to activation of slip systems in austenite.

Plastic deformation in the pillar is observed to be localized in two regions- at the pillar surfaces near the bottom of the pillar and along bands in the center of the
Figure 4.3: Martensite plate formed during the 1st and the 2nd cycle. A (0 0 1) cut of the model is shown.

pillar. Figure 4.4 shows the equivalent plastic strain in the pillar at the end of the first and second cycle. The bands of plastic strain in the center correspond to the M-M interface orientation of the martensite plate formed. After the sample is unloaded, the bands of plasticity match exactly to the M-M interfaces that were formed in the stressed state. The contribution of different slip systems to the total plastic strain is not the same. There is a dominant slip system.

(1 1 0)[0 0 1] slip system dominates among the twelve FCC slip systems modeled, in terms of slip activity. Among the material points that have larger than 0.1% equivalent plastic strain at the end of the first cycle, 47% material points have the largest slip activity on (1 1 0)[0 0 1] slip system. During the second cycle, this number increases to 54%. Figure 4.5 shows the distribution of the dominant slip system at
the end of the first and the second cycle. Near the free surfaces \{100\} type of slip systems are dominant.

### 4.2.2 Experimental Results

Dislocations were indexed on the \((1\overline{1}0)[010]\) slip system in the post-mortem TEM analysis of compressed micropillars performed by Norfleet et al [40]. The remnant dislocations loops were localized in bands in across the width of the micropillar. The bands were nearly oriented with the \([780]\) loading axis. The dislocation content after the second cycle was significantly higher than that after the first cycle. Bowers et al observed dislocations of the \((\overline{1}10)[001]\) system [43]. Further the sign of the dislocation Burgers vector was observed to change sign in different regions. These loops were elongated in the same direction as reported by Norfleet et al.
Figure 4.5: Dominant slip system based on the slip activity at the end of the 1\textsuperscript{st} and the 2\textsuperscript{nd} cycle. A (001) cut of the model is shown. The plot is on the undeformed shape of the pillar.

4.3 Discussion

M-M interfaces predicted by the simulations correspond to Mode B Type II twins in the notation of Bhattacharys [8]. Crystallographic theory of martensite based calculations predict a Mode B Type II twin interface between CV 1 and CV 4 with shear direction \( a = [0.0198, 0.0044, 0.2890] \) and twin plane normal \( n = [0.9736, 0.2281, 0.0000] \) in the global coordinate system. The trace of the twin plane \( n \) projected onto (001) plane makes an angle of 13.2° with the loading axis (Y). This matches well with the modeling prediction of 12°. Previous experimental studies on NiTi micropillars had inferred the formation of the same M-M interface based on the orientation of the resultant dislocation bands [43, 40].
A-M interface predicted by simulation in the first cycle corresponds to the maximum Schmid factor martensite plate that CV1 and CV4 pair can form. Crystallography-based calculations predict the highest Schmid factor martensite plate to have plane normal, \( m_1 = [0.1690, 0.8167, 0.5517] \). This plate produces -5.2% strain along the loading direction. Trace of \( m_1 \) on the \((0 0 1)\) plane makes an angle of 63.4° with the loading axis \( Y \). This matches well with the simulation prediction of 62°. The A-M interface predicted by simulations during the second cycle has a lower Schmid factor. Crystallographic calculations predict a lower Schmid factor plate involving Mode B Type II twins to have \( m_2 = [0.7682, 0.4306, 0.4737] \). This plate produces -4.8% strain along the loading direction. Trace of \( m_2 \) projected on \((0 0 1)\) plane projects an angle of 27.3° with the loading axis. This matches with the simulation prediction of 32°. Further, the micro-compression experiments inferred the formation of martensite plate with invariant plane normal \( n_2 \) based on the hypothesis that the remnant dislocation structure is localized around the martensite plate formed.

Widespread plastic deformation may be thought of as the reason behind the prediction of different A-M interface forming during first and second cycle of the simulations. During the first cycle, when there is no plastic deformation, the martensite plate that does the maximum mechanical work is formed. However, the plastic strain accumulated during the first cycle, affects nucleation of the plate during the second cycle. The discrepancy between the TEM observation and the simulation prediction in the first cycle could be due to features of the experiments not included in the model e.g. surface roughness, exact platen misalignment, rounded contact between pillar vertical surfaces and the base.
The A-M interface is transient during the loading half the stress cycle potentially because there are three competing regions of stress concentration in the pillar: the corners on the right and on the left where the vertical surface of the pillar joins the base, and the top surface where misaligned platen comes into contact with the pillar. The stress concentration near the contact with the base and transient A-M interface might be seen as the cause behind plastic strain localization on the two sides of the pillar.

The observed dominant slip system \((110)[001]\) can be rationalized in terms of the strains generated by the two martensite variants. Equation 4.1 shows the strain generated by CV 1 and CV 4 in the global coordinate system. The shear strains in the Z direction \((\epsilon_{xz} \text{ and } \epsilon_{yz})\) alternate sign between CV 1 and CV 4. This alternating distortion in Z direction must be locally accommodated by austenite at the A-M interface. Dislocations with Burgers vector along [001] can achieve this. The mechanism for accommodation of deformation at the A-M interface is discussed in the following Section.

4.3.1 Accommodation of deformation at A-M interface by slip activity

The slip system observed in the micro-compression experimental work [43] is referred to as Bowers (B) slip system (\((110)[001]\) in austenite crystal basis). The dominant slip system in the simulations is referred to as the H slip system \((110)[001]\) in austenite crystal basis). Note that, in the global coordinates, these slip systems become: \(B = (\overline{1}00)[001]\) and \(H = (010)[001]\).

Since CV 1 and CV 4 form a Type II twin, they create an alternating shear in the Z direction. A 2D schematic of the distortion created by the twins is shown below in
Figure 4.6. Note that the twin plane (oriented at 12° to Y) is essentially a direction along which deformation is zero.

Figure 4.6: Schematic of the distortion created by the twinned martensite. Global axes XYZ have the same orientation as in Figure 1. Twin interface is shown by black dotted line inclined to Y axis by 9°. As you move along the X direction from one twin interface to another, either +7.2% or -7.2% shear in the Z direction is created. The resultant displacement is shown by u (along +Z) and d (along -Z). Similarly moving along Y direction results in either an up or down movement of 1.7%. At the twin interface, there is no distortion produced along Z. At 90° to the twin interface, there exists a direction along which maximum distortion is produced along the Z direction.

Since the austenite needs to maintain compatibility with twinned martensite at the invariant plane, the deformation due to martensite is accommodated in austenite by
Figure 4.7: A schematic of Z-distortion created by martensite twins and its accommodation in austenite. There is a transition region in austenite, along the invariant plane, in which the Z-displacement rapidly drops to zero. The displacement gradient at different locations is shown by dashed arrows. It is hypothesized that, this accommodation is achieved through plastic deformation in austenite.

local plastic deformation. A schematic of compatibility at the austenite-martensite interface is shown in Figure 4.7. The distortion due to martensite is not accommodated by matching homogeneous deformation in austenite. Rather, there is a transition region in austenite where a tent-like deformation gradient is generated which matches the distortion due to martensite. Due to this, the slip system that produces the same shear as martensite need not be the one to activate.
We are looking for a slip system that can produce

\[ u_{z,x} = 7\% \] at A-M interface \hspace{1cm} (4.2a)

\[ u_{z,x} = 0 \] in autenite \hspace{1cm} (4.2b)

\[ (u_{z,x})_y = u_{z,xy} = (u_{z,y})_x = 7\% \] \hspace{1cm} (4.2c)

\[ (u_{z,x})_y \Rightarrow \text{ B slip system produces such gradient} \hspace{1cm} (4.2d) \]

\[ (u_{z,y})_x \Rightarrow \text{ H slip system produces such gradient} \hspace{1cm} (4.2e) \]

This can be achieved by activating either B or H slip system. Hence we have a choice. The only other requirement is that the remnant dislocation structure after growth and decay of martensite should match the TEM observation. Note that calculating \( n_i E_{ij} b_j \) gives us the slip system that produces the same homogeneous shear as the transformation strain \( E_{ij}^{tr} \). We do not want that.

Figure 4.8 shows two possible arrangements that produce the required Z-deformation gradient. The dislocations appearing as segments are in reality loops either on the Y or the X plane. This is the dislocation structure, potentially generated during the growth and decay of martensite. Two mechanisms for the evolution of this dislocation structure are discussed. For each case, the dislocation content left behind after evolution is discussed as well, allowing comparison with TEM observations.

**B dislocations**

As the martensite front grows or shrinks along Y direction, B loops can translate on their slip plane until they encounter oppositely signed stress from the neighboring twin regions. This will leave B_{edge}:B_{screw} content in ratio of approximately 6:1. \((1/\tan(9^\circ) = 6.3)\). Further, the bands of dislocations will have opposite signs. If TEM observation reports far larger edge content than screw, then this scenario is likely.
Figure 4.8: Dislocation loops accommodating the distortion created by martensite at the invariant plane. The dislocations appearing as segments are actually loops in the Y or the X plane.

**H dislocations**

If H dislocations are formed in front of the interface, then they can evolve in two ways.

**H dislocations translate:** Assuming that the edge components of the H dislocations run out; the H screws can cross-slip and translate along the Y direction. They will leave edge content of B type behind until they encounter oppositely signed stress field of an adjacent twin. They will also leave behind some edge content of H type. In this case $B_{edge}:H_{edge}$ will be 6:1. There will be no screws left behind.

**H dislocations renucleate:** The second possibility is that H dislocations renucleate as the martensite front is moving. This will leave large H screw content behind. There will be no edge content. H dislocations may need to renucleate if propagation due to cross slip is not feasible.
The mechanisms for deformation accommodation along with the remnant dislocation content are summarized in Figure 4.9. These mechanisms propose two ways in which the deformation due to martensite can be accommodated by slip in austenite. However, they do not justify why H slip system is predicted in the simulations rather than B slip system. Activation of H slip system is rather surprising because the shear strain produced by martensite is larger in the $\epsilon_{xz}$ direction than in the $\epsilon_{yz}$ direction. Based on this, we would expect to have larger $\sigma_{xz}$ shear stress component. However, activation of the H slip system can be rationalized based on the dynamic nature of the simulations and higher constraint in the Y direction. Based on the St. Venant principle, one can argue that the elastic stress field of a martensite CV extends in austenite to a distance approximately equal to the width of the CV. In the Y direction, there is an additional effect of martensite front being in motion. This would compress the elastic zone during forward martensitic transformation and relax it during reverse transformation. This would lead to the width of the transition region in Figure 4.7 to change, consequently altering the yz component of shear stress. The constraint in Y direction is higher due to the fixed boundary condition at the bottom surface of the pillar and displacement boundary condition on the platen at the top. An additional effect not discussed here is the non-planar structure of the A-M interface. The interface may assume a non-planar structure to minimize the elastic energy [92]. The diffuse interfaces involved in the phase field formulation may add to this effect.

Another explanation for the observation of slip system B, rather than H in the TEM study may be given on the basis of the ability of the dislocation loops on each of those slip systems to propagate in front of a moving martensite interface.
When a martensite front is growing, slip system H cannot cross-slip or glide to keep up with the front movement. It needs to renucleate. However, the loops on slip system B can cross slip and keep up with the marching martensite front until they encounter an oppositely signed stress field of a neighboring martensite CV. At that point they stop moving and potentially remain embedded in the martensite region, once the martensite front sweeps through the sessile dislocation structure. Since the renucleation mechanism necessary for the movement of H loops is energetically unfavorable compared to B, perhaps B slip system is present in an overwhelming proportion compared to H in the experimental samples. At this time, the PF/FE framework does not capture the mechanism of nucleation of the loops.
Figure 4.9: A summary of the deformation accommodation and the remnant defect content of the two candidate slip systems considering in this study.

4.4 Conclusion

1. Using a phase field/finite elements based modeling approach Mode B Type II twins are predicted to form in a [7 8 0] oriented Ti-50.7at.%Ni single crystal micropillar during compression loading.

2. Martensite plate that does the maximum mechanical work (maximum Schmid factor) is predicted to form during the first cycle. During the second cycle, a plate with lower Schmid factor is predicted, potentially due to widespread plasticity in the first cycle. This same plate is thought to be observed in the
micro-compression experiments. This is potentially due to aspects of the experiments like surface roughness not captured in the modeling.

3. Even though the A-M interface is compatible in an average sense, incompatible strain fields exist locally at the intersection between M-M and A-M interfaces. This incompatibility is accommodated by slip on \(\{1\ 1\ 0\}\) type of slip systems in the austenite.

4. \((1\ 1\ 0)[0\ 0\ 1]\) slip system is predicted to dominate in terms of slip activity in simulations. Activation of a slip system with \([0\ 0\ 1]\) Burgers vector is consistent with large shear strains \(\epsilon_{xz}\) and \(\epsilon_{yz}\) of opposite sign produced by the martensite variants 1 and 4. Post-mortem TEM analysis on the micro-pillar samples has observed remnant \((\bar{1}\ 1\ 0)[0\ 0\ 1]\) edge dislocation structure.

5. A mechanism is proposed by which the strain incompatibility at the A-M interface can be accommodated by slip on either \((\bar{1}\ 1\ 0)[0\ 0\ 1]\) or \((1\ 1\ 0)[0\ 0\ 1]\) slip systems in austenite. Analysis of remnant screw dislocation content in the experimental samples can reveal which mechanism is operational.
Chapter 5: Texture and Grain Neighborhood Effects on Ni-Ti Shape Memory Alloy Performance

The discussion in the previous three chapters of this thesis was focused on studying performance degradation in SMA due to plasticity at martensite c.v. (nanometer) length scale. At a higher length scale, the performance is determined by how an individual grain performs and how it interacts with its neighbors. And this, in turn, determines the performance of polycrystalline aggregate. In this chapter, the performance of SMA is studied at the grain scale.

The present work employs for the first time a micromechanical model to study in detail the effects of polycrystalline constraint on the statistics of grain performance. This is achieved by capturing the micron-scale distribution of phase transformation and plasticity at the granular scale. The details of fine (nm) scale intragranular plasticity within grains are not captured presently and pose a formidable computational challenge to cover such disparate length scales. However, in principle, nm-scale plasticity could be studied using phase-field simulations described in the previous three chapters.

A physical model for grain interaction should account for the redistribution of stress when more favorably oriented grains transform before others. As depicted in Figure 5.1, a grain that undergoes a positive axial transformation strain ($\varepsilon_{T(az)} > 0$)
sheds tensile axial stress ($\sigma_{zz} > 0$) to in-plane (IP) neighbors and compressive axial stress ($\sigma_{zz} < 0$) to out-of-plane (OP) neighbors. Quantitative estimates of the stress redistribution are provided by the Eshelby solution for an ellipsoidal inclusion in an elastic matrix [93]. For a space-filling, cuboidal grain arrangement as in Figure 5.1a, a solution by Li and Anderson [94] furnishes the change $\Delta \sigma$ in average axial stress in a parent grain caused by axial transformation strains $\epsilon_T$, $\epsilon_{T(IP)}$, and $\epsilon_{T(OP)}$ within the parent, in-plane, and out-of-plane neighbor grains, respectively,

$$\frac{\Delta \sigma}{E} = g_{\text{parent}} \epsilon_T + 4g_{\text{IP}} \epsilon_{T(IP)} + 2g_{\text{OP}} \epsilon_{T(OP)} \quad (5.1a)$$

$$g_{\text{parent}} = -0.59, g_{\text{IP}} = 0.08, g_{\text{OP}} = -0.24 \quad (5.1b)$$

The homogeneous, isotropic elastic modulus is $E$ and the factors of 4 and 2 account for the 4 IP and 2 OP neighbors to each grain, as shown in Figure 5.1b. Thus, the constraint between grains manifests in terms of stress redistribution, which can advance or retard the driving force for transformation. Similar to transformation, plastic deformation also redistributes stress. However the two processes transformation vs. plasticity are dependent on different Schmid factors. Thus, the competition (and stress redistribution) depends on the grain orientations in a polycrystalline neighborhood [8].

This study simulates the grain to grain variation in performance in polycrystalline NiTi and then offers an explanation for this variation in terms of the stress redistribution among neighboring grains. A predictive performance function for the parent grain is proposed in terms of the Schmid factors for transformation in the parent and neighboring grains. This is done initially for pristine material that is stress-free prior
to testing. The results are then extended to polycrystals that have been plastically pre-deformed in the austenite state (at $T \gg \theta_{AF}$), as to impart a residual stress state prior to testing. Variation in performance that is not captured by the performance function is rationalized in terms of the effect of crystal symmetry on the martensitic transformation. These simulations use a finite element method with constitutive parameters calibrated to a Ti-50.9at.%Ni alloy that has been homogenized to remove precipitates. However, the trends are expected to apply to other shape memory alloys.
Figure 5.1: Microstructural finite element model of a 729 grain polycrystal under pseudoelastic loading to 640 MPa at room temperature. (a) Predicted grain-to-grain variation in axial transformation strain $\varepsilon_T$ at peak stress. Maximum, minimum and intermediate values are shown at three grains, where $x$ is the grain coordinate. (b) The grain neighborhoods for four representative grains A, B, C, D inside the polycrystal. Values of $x$ and $\varepsilon_T$ are reported, along with the transformation Schmid factors for: the grain ($S_T$); the average over the 4 in-plane neighbors ($S_T(IP)$); the average over the 2 out-of-plane neighbors ($S_T(OP)$).

max($\varepsilon_T$) = 6.1% @ $x$ = 1, 6, 9
min($\varepsilon_T$) = 1.9% @ $x$ = 2, 1, 6

2.5% @ $x$ = 7, 9, 1
4.0% @ $x$ = 5, 9, 7
6.0% @ $x$ = 7, 4, 9

$\epsilon_T$ ( นาย )
5.1 Methods

A microstructural finite element (FE) model is used to simulate the thermo-mechanical response of polycrystalline NiTi SMA samples, the full details of which are in [1]. The model incorporates anisotropic elastic deformation in austenite and martensite, as well as the deformation due to crystal-based phase transformation and austenitic plasticity. A unique feature is that the mechanisms of plasticity and phase transformation are coupled in a large strain formalism. The constitutive relation determines the deformation increment at a material point given the local microstructure, stress and stress history as input quantities. A material point is viewed as an aggregate of austenite and martensite, with volume fraction $\nu_A$, anisotropic elastic constants $C_A$, and coefficient of thermal expansion $\alpha_A$ for the austenite (A) phase. The corresponding properties are $\nu_t$, $C_M$, and $\alpha_M$ for the 24 habit plane variants ($t = 1$ to 24) of martensite. The effective elastic constants and thermal expansion coefficients of the aggregate are approximated by a rule of mixtures.

A large deformation formulation is employed where the total deformation gradient in the aggregate is the product of the elastic ($F^e$) and inelastic ($F^\text{inel}$) deformation gradients, and where the inelastic velocity gradient is the sum of the velocity gradients arising from (i) rate-dependent crystal plasticity [80] in austenite and (ii) phase transformation from austenite to martensite or vice-versa [38]. In particular, the energetic driving force to transform a unit volume of austenite to martensite plate type $t$ is given in terms of the current volume fraction $\nu_t$ of plate type $t$, the Piola-Kirchoff stress $T^*$, and temperature $\theta$

$$f_t(\nu_t, T, \theta) = b_t \cdot (F^{eT} F^{eT} T^*) m_t - \frac{\lambda_t}{\theta_T} (\theta_T - \theta_T) - \sum_{u=1}^{N_T} h_{tu} \nu_u$$  \hspace{1cm} (5.2)
where the crystallographic normal \( m_t \) to the habit plane and the transformation direction \( b_t \) for habit plane variant \( t \) are furnished by the crystallographic theory of martensite [38]. Transformation from austenite to martensite occurs when \( f_t \) exceeds \( f_c \), a critical material value representing the nucleation threshold for transformation. Likewise, the reverse transformation occurs when \( f_t < -f_c \). Other alloy-specific transformation properties include \( \lambda_T \), the latent heat of transformation per unit volume and \( \theta_T \), the equilibrium transformation temperature at which the free energy of the austenite and martensite phases are equal, in the absence of stress. This is calibrated to the average of the martensite start \((\theta_{MS})\) and austenite start \((\theta_{AS})\) temperatures from differential scanning calorimetry measurements of stress-free single crystals. Substitution into Equation 5.2 and applying the transformation conditions yields \( \theta_{MS} = \theta_T(1 - f_c/\lambda_T) \) and \( \theta_{AS} = \theta_T(1 + f_c/\lambda_T) \) for a stress-free single crystal.

The hardening matrix \( h_{tu} \) between habit plane variants \( t \) and \( u \) reflects the decrease in driving force due to interaction between compatible \( (h_{comp}) \) and incompatible \( (h_{incomp}) \) habit plane variants. Material values are obtained from extensive validation to experimental data [30] for homogenized single crystals of Ti-50.9 at%Ni. Manchiraju and Anderson document the successful capture of pseudoelastic polycrystalline macro stress-strain response based on calibration to single crystal data [1]. The resulting material values are reported in Table 5.1.

The constitutive relation for crystal plasticity specifies the rate of slip on slip system \( s \)

\[
\dot{\gamma}_s = \dot{\gamma}_0 (\tau_s/g_s)^{1/m} \text{sgn}(\tau_s) \tag{5.3a}
\]

\[
\tau_s = b_s^{\text{slip}} : (F^{eT}F^{eT^*})m_s^{\text{slip}} \tag{5.3b}
\]
### Elastic and thermal

Elastic constants (GPa): $C_{11(A)} = 130; C_{22(A)} = 98; C_{44(A)} = 34; C_M = C(A/2)$

Thermal expansion coefficients ($10^{-6}$/K): $\alpha_A = 11; \alpha_M = 6.6$

### Phase transformation

Equil. transf. temp. (K): $\theta_T = 257$

Latent heat of transf./unit vol. (MPa): $\lambda_T = 130$

Hardening matrix $h_{tu}$:
- $h_{\text{com}} = C_{44(A)}/16000$
- $h_{\text{incom}} = C_{44(A)}/4000$

Critical driving force force for transformation (MPa): $f_c = 8.4$

Number of martensite plate types: $N_T = 24$

Habit plane variant normal $m_t$ and shear direction $b_t$ from [38]

### Austenite plasticity

Reference shear strain rate ($1/s$): $\dot{\gamma}_0 = 0.002$

Strain rate exponent: $m = 0.02$

Initial slip system flow shear strength (MPa): $g_0^s = 320$

Self-hardening coefficient (MPa): $h_0 = 500$

Ratio of self to latent hardening: $Q = 1.4$

Hardening exponent: $a = 0.125$

Saturation shear strength (MPa): $g_{\text{sat}} = 900$

Number of slip systems: $N_S = 12$

Table 5.1: Material values for the constitutive model.

Where $\dot{\gamma}_0$ is a reference slip rate, $m$ is the strain rate activity, and $\tau_s$ is the resolved shear stress on slip system $s$ with slip plane normal $m_s^{\text{slip}}$ and Burgers vector $b_s^{\text{slip}}$. The flow stress for slip system $s$ is

$$
\dot{g}_s = \sum_{r=1}^{N_s} h_r [Q + (1 - Q)\delta_{sr} |\dot{\gamma}_r|] \quad (5.4a)
$$

$$
h_r = h_0(1 - g_r / g_{\text{sat}})^a \quad (5.4b)
$$

An implicit time integration scheme is used to implement the governing constitutive relations (Eqs. 5.2, 5.3, 5.4) in a large deformation framework. An advantage of implicit time integration is that the numerical approach is stable irrespective of the time step. However, this approach requires the Jacobian matrices ($\partial T/\partial E$ and
\( \partial T/\partial \theta \). The detailed implementation of the numerical scheme and derivation of the Jacobian matrices are provided in [1]. The numerical scheme is implemented as a User Material Subroutine (UMAT) in ABAQUS FE software [77]. Typical simulations in this work take approximately 5 hours to run on an eight core 2.5GHz Opteron processor at the Ohio Supercomputer Center.

Figure 5.1 shows the finite element geometry. A 3D polycrystal is modeled as a 9x9x9 assembly of cuboidal grains, where each grain is represented by one or more hexahedral elements (C3D8 in ABAQUS finite element software), each containing eight integration points. A crystallographic orientation in the austenite basis is assigned to each grain according to a random texture. A simple cuboidal grain shape is used since the focus of this work is to study the effect of compatibility on average grain performance in a statistical sense. This captures the average response of the core interior of more complex grain shapes. More complex grain shapes are important to correlate with experimental studies of strain distributions and stress concentrations within grains (e.g., [72, 73]). However, the focus of this portion of the work is on average grain performance. For isothermal analyses, two boundary conditions are prescribed. The normal displacement \( u_z = 0 \) on the bottom face and \( du_z/dt = 10^{-4}/s \) on the top face. All other degrees of freedom are unconstrained except those required to prevent rigid body motion.

The Schmid factor for transformation \( S_T \) for the most favored habit plane variant in a grain is the maximum value of \( S_T(t) = b(t)z m(t)z \) among all possible \( t = 1 \) to 24 habit plane variants, where \( b(t) \) and \( m(t) \) are furnished by the Crystallographic Theory of Martensite and are reported by Thamburaja and Anand [38]. The subscript \( z \) denotes the component along the loading axis. Corresponding quantities are identified
in neighboring grains, with $S_{T(IP)}$ and $S_{T(OP)}$ denoting average values among the in-plane (IP) and out-of-plane (OP) neighbors. Equating the work of transformation at the macroscopic and local scale reveals that the axial transformation strain induced by the most preferred habit plane variant is directly proportional to $S_T$. In this work, martensite plates with $S_{T(t)}$ equal to or close to $S_T$ are referred to as efficient plates, since they are capable of producing the largest possible transformation strain.

Four simulations are carried out to study the effect of grain neighborhood and plastic pre-deformation on the isothermal stress-strain performance. All involve polycrystals of 729 randomly oriented grains. Simulations with more grains do not significantly change the macroscopic pseudoelastic response of the polycrystal [1] nor do they significantly alter the statistical nature of the grain level performance. Continuity of tractions and displacements is enforced across grain boundaries, corresponding to no opening or large-scale relative shear across grain boundaries. This is consistent with the absence of creep during room temperature deformation [40]. The 0% plastic prestrain case has no prior plastic strain and thus no residual stress state a priori. A macro uniaxial tensile stress loops from 0 to 640 MPa and back. It is imposed for two cycles at $\theta = 277$ K. This maximum stress is sufficient to induce a complete A$\rightarrow$M transformation in nearly all grains. The case +2% plastic prestrain pre-deforms the polycrystal at $\theta = 1000$ K to a macro plastic strain of +2%. The elevated deformation temperature imposes plastic deformation of the austenite phase with no transformation. The sample is then cooled during which martensite may form due to internal residual stress from prior plastic deformation. The macro stress loop to 640 MPa is then imposed for two cycles at $\theta = 277$ K. The case -2% plastic prestrain is similar but imposes a plastic prestrain of -2%. Finally, a bamboo case is considered to capture
a linear array of grains with minimal constraint from neighbors. The corresponding macrostrain is computed analytically from an isostress approach. For simplicity, the bamboo case uses isotropic elastic moduli with values reported in Table 5.1, compared to the anisotropic moduli used in the other cases.

The performance $P$ is introduced to quantify the recoverable strain generated during an isothermal loading/unloading cycle. At the macroscopic scale, $P$ is defined as the total macroscopic axial strain at the peak macro stress (640 MPa). $p$ is defined as the counterpart at the grain scale, so that $P$ is the average of $p$ within the polycrystal. The performance at the grain scale is partitioned into transformation and elastic components,

$$ p = p_T + p_e $$

(5.5)

where $p_T$ and $p_e$ are the respective transformation and elastic axial strains in a grain at 640 MPa. The transformation performance is obtained as

$$ p_T = \sum_{t=1}^{24} v_t p_T(t) $$

(5.6a)

$$ p_T(t) = b(t)z m(t)z $$

(5.6b)

where $b(t)$ and $m(t)$ are obtained from the Crystallographic Theory of Martensite (see Table 5.1). Formally, the average value of $p_T$ within a grain is reported as the average over all integration points within the grain. The ideal and relative transformation performances in a grain are

$$ p_T(\text{ideal}) = bS_T $$

(5.7a)

$$ p_R = p_T/p_T(\text{ideal}) $$

(5.7b)

where $b = 0.1308$ for this alloy system [38]. $p_T(\text{ideal})$ is thus the maximum possible axial transformation strain in a grain, obtained if the grain completely transforms to
the most favored habit plane variant. \( p_R \) is the ratio of the actual transformation strain to the ideal value.

### 5.2 Results

Figure 5.1a shows the grain-to-grain distribution of the transformation performance \( p_T \) for the 0% plastic prestrain case. It varies from 1.9 to 6.1%, with the extreme values at surface grains with positions \([x, y, z] = [2, 1, 6]\) and \([1, 6, 9]\) respectively. The respective \( p_T(\text{ideal}) \) values are 3.6% and 6.4%, underscoring the deleterious effect of constraint by neighboring grains. The results in Figure 5.1a are for the second cycle of tension, but the displayed spatial variation in \( p_T \) is typical for the first cycle as well as other cases involving plastic prestrain. The polycrystalline performance \( P_T = 4.7\% \) is shifted toward the upper end of the 1.9 to 6.1% range. This is consistent with a random distribution of grain orientations, for which the \( p_T \) distribution is skewed toward higher values. The discussion of Figure 5.2c elaborates on this feature.

Figure 5.1b shows that grains with the same \( p_T(\text{ideal}) \) perform differently due to their neighborhood. Consider grains A and B which both have a relatively small \( p_T(\text{ideal}) \) (3.9%) compared to the polycrystalline average. Here, \( p_T(A) = 3.6\% \) and \( p_T(B) = 3.0\% \). The neighborhoods in Figure 5.1b offer qualitative insight to this difference. Both A and B are surrounded by neighbors with higher \( S_T \), on average. However, A has IP neighbors with larger \( S_T \) compared to B. These larger \( S_T(\text{IP}) \) neighbors are expected to transform at a lower applied stress and provide a larger transformation strain than the parent grain. According to the Eshelby solution (Eq. 5.1), this will shed axial stress onto the parent. This beneficial effect is more pronounced for grain
A, since $S_{T(IP)}$ is larger for the A neighborhood. Grains A and B have OP neighbors with a relatively high $S_{T(OP)}$. These higher $S_{T(OP)}$ neighbors are expected to have a larger transformation strain than the parent. According to the Eshelby solution, this will reduce the axial stress on the parent grain, thereby lowering performance. Overall, the superior performance of A compared to B might be rationalized on A having higher $S_{T(IP)}$ neighbors, with both grains having deleterious (higher) $S_{T(OP)}$ neighborhoods.

Figure 5.1b also shows the results for grains C and D, which have a relatively large $p_{T(ideal)}$ (6.1%). Again, there is a spread in performance, with $p_{T(C)} = 5.9\%$ and $p_{T(D)} = 4.7\%$. These relative values cannot be rationalized entirely by the simple Eshelby model. The result $p_{T(C)} > p_{T(D)}$ might imply that C has a larger $S_{T(IP)}$ and smaller $S_{T(OP)}$. While the latter is true, the former isn’t. Might the beneficial effects of a smaller $S_{T(OP)}$ offset the negative effects of a smaller $S_{T(IP)}$? This is possible in theory because $|g_{OP}| > |g_{IP}|$ in Eq. 5.1, indicating that stress redistribution from OP neighbors is more potent. Overall, neighborhood descriptions in terms of $S_{T(IP)}$ and $S_{T(OP)}$ may be qualitatively useful but not definitive on a case by case basis.

Figure 5.2a shows the total performance $p$ (Eq. 5.5) vs. $S_T$ for the 729 grains in the 0% plastic prestrain case. Overall, $p$ increases with $S_T$. However, the data is scattered due to neighborhood effects and elastic anisotropy. Superimposed on the plot is a solid line for $p_{T(ideal)}$ as given by the first of Eqs. (5.7). Figure 5.2b shows that the elastic contribution $p_e$ tends to decrease with $S_T$. The large magnitude of elastic strain (> 3%) occurs since after complete transformation to martensite, grains continue to deform elastically, without reorientation and detwinning. For this reason,
Figure 5.2: Statistical results from the 729 grain model in Figure 5.1, showing: (a) \( p \) vs. \( S_T \), where \( p \) (Eq. 5.5) is the axial total strain in a grain at 640 MPa macro stress and \( S_T \) is the Schmid factor for transformation in the grain. The colors divide the grains into three equal groups based on \( S_T \) values. The solid line is the ideal axial transformation strain \( p_T(\text{ideal}) \) (Eq. 5.7); (b) the axial elastic strain \( p_e \) vs. \( S_T \); (c) the axial transformation strain \( p_T \) vs. \( S_T \); (d) \( S_T \) vs. crystallographic axis of tensile loading. The orientations of grains A, B, C, D in Figure 5.1b are shown.

Subsequent results focus on the transformation performance \( p_T \) as a more realistic output of performance rather than the total \( p \).

Figure 5.2c shows that \( p_T \) increases with \( S_T \) as expected from theory [8], with less scatter than for \( p \). Lower performing grains such as B and D operate at 65% of \( p_T(\text{ideal}) \) while the best performing grains such as A and C operate at 80 to 87% of \( p_T(\text{ideal}) \). Figure 5.2d shows an inverse pole figure with contours of \( S_T \) relative to the...
[001], [101], and [111] crystallographic directions. Based on the results in Figure 5.2c, the contours of $S_T$ in Figure 5.2d represent approximate contours of $p_T$. Moreover, the correlations shown here for the second stress cycle are also prevalent for the first cycle and they persist for the plastic prestrain cases.

Figure 5.3a shows the effects of 0, +2%, and -2% plastic prestrain on the 2nd cycle tensile macrostress-strain ($\Sigma - E$) polycrystalline response. The inset table in Figure 5.3a shows that plastic prestrain degrades polycrystalline performance, from $P = 6.5\%$ (0% prestrain) to 5.3% (+2% prestrain) and 4.6% (-2% prestrain). These 2nd cycle curves begin at nonzero macrostrain due to accumulated strain during the first cycle. The inset table in Figure 5.3a shows starting martensite volume fractions of 0.01, 0.25, and 0.34 for 0%, +2% and -2% plastic prestrain cases respectively. Thus, inhomogeneous internal stress generated by plastic prestrain is predicted to stabilize large fractions of remnant martensite, by augmenting the local driving force for transformation (Eq. 5.2). The tabular results also show that the martensite volume fraction $\nu_M$ at the peak macrostress ($\sim 640$ MPa) decreases modestly with plastic prestrain. Thus, $P$ decreases with plastic prestrain primarily from a reduction in the volume fraction of available austenite for the $A \rightarrow M$ transformation. Figure 5.3b helps to inform the dependence of plastic prestrain on grain orientation. Grains near [1 1 1] and [1 1 0] such as C and D have relatively large Schmid factors for plasticity ($S_p$) and thus are plastically soft. Figure 5.2d shows that these grains also have larger Schmid factors for transformation ($S_T$) and thus are expected to transform at smaller tensile applied stress. Compressive prestrain puts these grains in residual tension. This drives the production of remnant martensite and lowers the required macrostress for onset of transformation. Conversely, tensile prestrain puts
these grains in residual compression, increasing the required macrostress for onset of transformation. The reverse is true for grains A and B, which have relatively small $S_P$.

![Figure 5.3: Results from the 729 grain model in Figure 5.1 showing (a) the macroscopic pseudoelastic stress-strain response at room temperature, following tensile prestraining at elevated temperature ($T \gg \theta_{AF}$) to plastic strains of 0%, +2%, and -2%. The response for the second cycle of pseudoelastic loading is shown; (b) Schmid factor for plasticity ($S_P$) vs. crystallographic axis of tensile loading.](image)

Figure 5.4 shows the effect of removing all intergranular constraint, by comparing the analytical response for the bamboo case and 2$^{nd}$ cycle simulation response for
the 0% plastic prestrain case. Both have the same distribution of randomly oriented grains, but in 1D vs. 3D arrangements (see the inset figures). The latter case is modified slightly from that in Figure 5.3a to make the hardening matrix $h_{tu} = 0$ (Eq. 5.2). This allows for a more equivalent comparison to the analytic bamboo case, which also assumes zero hardening. Overall, the bamboo case requires a consistently smaller macroscopic stress for transformation and it achieves a larger $P$ (8.2%). The lower $P$ (6.6%) for the 3D case is consistent with constrained transformation, where inefficient habit plane variants must form to maintain compatibility between grains. Although the macrostress for the onset of transformation is similar (300 MPa), the 3D geometry displays a rounded transition, consistent with shedding of stress from early-transforming (high $S_T$) grains to late-transforming (low $S_T$) grains. The stress state becomes inhomogeneous, unlike the idealized bamboo case, which has sharp forward and backward transitions. The effective elastic moduli are slightly different for the two cases, where the bamboo case assumes isotropic elasticity. This simplification does not affect the key trends.
Figure 5.4: Macro stress-strain response vs. the arrangement of grains in a random textured polycrystal. The bamboo arrangement (right inset) consists of the same grains as in the random polycrystal (left inset). However, in the bamboo case, the grains are arranged in an isostress configuration. The bamboo case is characterized by a sharp onset of transformation and larger net strain at peak stress.

5.3 Discussion

5.3.1 Transformation Performance Function

The polycrystalline data for $p_T$ in Figure 5.2c is approximated by a new four-parameter performance function

$$p_{T*} = c_0 + c_P S_T + c_{IP} S_{T(IP)} + c_{OP} S_{T(OP)} \quad (5.8)$$

The motivation for the first two terms stems from the approximate linear dependence of $p_T$ on the transformation Schmid factor $S_T$ of the parent grain. The last two terms are inspired by the Eshelby solution (Eq. 5.1), whereby the change in stress $\Delta \sigma$ in the parent grain is linearly dependent on the transformation strains $\epsilon_{IP}$ and $\epsilon_{OP}$ in in-plane and out-of-plane neighboring grains (see Figure 5.1 geometry for IP and OP
notation). In turn, \( \epsilon_{IP} \propto S_{T(IP)} \), the average Schmid factor for transformation in the in-plane neighbors. A parallel assumption \( \epsilon_{OP} \propto S_{T(OP)} \) is made for out-of-plane neighbors. Thus, \( \Delta \sigma \propto S_{T(IP)} \) and \( S_{T(OP)} \). A final assumption is that \( \Delta \sigma \) directly affects \( p_T \).

Figure 5.5a shows \( p_T \) vs. \( p_T^* \) using the data in Figure 5.2c, where the values \( c_0 = -0.0141, c_P = 0.1291, c_{IP} = 0.0220, \) and \( c_{OP} = -0.0045 \) are determined by a least-squared-error fit, yielding \( R^2 = 0.89 \). In this case, \( S_{T(IP)} \) and \( S_{T(OP)} \) for each grain are averaged among the four in-plane and two out-of-plane grains, respectively. The relatively large \( c_P \) indicates that \( p_T \) is most dependent on the parent grain orientation. The oppositely signed \( c_{IP} \) and \( c_{OP} \) indicate that \( p_T \) is increased when in-plane neighbors have a large \( S_T \) and out-of-plane neighbors have a small \( S_T \). This is consistent with the oppositely signed \( g_{IP} \) and \( g_{OP} \) terms in the Eshelby model (Eq. 5.1) and the fit affirms the underlying assumption that stress redistribution to the parent grain increases \( p_T \).

Figure 5.5b shows \( p_e \) vs. \( p_e^* \) for the elastic strain in the parent, using the data in Figure 5.2b. Here, \( p_e^* \) is a fitted performance function of the same form in Eq. 5.8. A least-squared-error fit yields coefficients \( c_{0e} = 0.0428, c_{Pe} = -0.0878, c_{IPe} = 0.0312, \) and \( c_{OPe} = -0.0047 \). Thus, \( p_e \) is most dependent on \( S_T \). The negative value of \( c_{Pe} \) affirms that a large \( S_T \) shifts stress away from the parent grain, thereby decreasing elastic strain. Similarly, a high \( S_{T(IP)} \) shifts stress to the parent while a high \( S_{T(OP)} \) does the opposite. The effect on total strain is given by adding \( p_T \) and \( p_e \) as noted in Eq. 5.5. Thus, the net effect of the parent Schmid factor \( S_T \) is given by adding the oppositely signed coefficients \( c_P \) and \( c_{Pe} \). The sum is positive (0.0413), indicating total strain increases with \( S_T \). But the correlation is weaker, as observed in Figure
5.2a. For comparison, \( c_{IP} \) and \( c_{IPe} \) sum to 0.0532 and \( c_{OP} \) and \( c_{OPe} \) sum to -0.0092. Thus, it is interesting that the total strain is most dependent on \( S_{T(IP)} \) while the transformation strain and elastic strain are most dependent on \( S_T \).

### 5.3.2 Dominance of a Single Plate Type Within Grains

Figure 5.2c clearly indicates that \( p_T \) falls short of the ideal performance exhibited by a counterpart single crystal under the same tensile stress. In the single crystal case, the martensite plate type with the largest \( S_T \) is expected to transform before other plate types. This most-favored plate type will consume the entire crystal, achieving a volume fraction of 1 below a tensile stress of 640 MPa. The only exceptions are tensile axes along the perimeter of the stereographic triangle in Figure 5.2d, where multiple plate types have equal values of \( S_T \). In contrast, Figure 5.6 shows that among the 729 grains in the polycrystalline model (0% prestrain case as in Figure
5.2), no martensite plate type ever reaches a volume fraction of 1, regardless of grain orientation. Rather, the largest volume fraction of a single plate type is $\nu_{\text{M}*} \sim 0.8$ at $S_T \sim 0.47$. A least-squared-error fit gives the dashed line $\nu_{\text{M}*} \propto S_T$, but the statistical deviation is large.

Figure 5.6: Statistical predictions from the model in Figure 5.1 showing the volume fraction of the dominant martensite plate type within a grain vs. the transformation Schmid factor $S_T$ for that grain, at a macroscopic stress of 640 MPa. In the model, 24 martensite plate types compete within each grain. Grains with a larger $S_T$ tend to have a larger volume fraction of a dominant plate, indicating the grain has fewer plates and strongly textured martensite. Grains with a smaller $S_T$ activate more plate types owing to the complex stress history caused by transformation in neighboring grains.

The trend $\nu_{\text{M}*} \propto S_T$ in Figure 5.6 can be rationalized in that grains with a larger $S_T$ tend to transform earlier, at smaller macrostress. This can establish a dominant plate type in the grain, even prior to the onset of transformation in neighboring
grains. A larger $S_T$ grain redistributes stress to neighbors. However, this stress is multiaxial in nature and may favor plate types different than that from the applied stress. Thus, grains with a lower $S_T$ tend to inherit complex stress states prior to the onset of transformation. The large deviation in Figure 5.6 can be rationalized in terms of constraints imposed by compatibility. The local stress state is not equal to the macroscopic tensile stress, in part due to elastic anisotropy, but also due to complex stress histories related to inhomogeneous transformation. Lower $S_T$ grains experience these complex stress histories prior to the onset of transformation. Also, $S_T$ values for primary, secondary, and tertiary plate types tend to be more similar in value in lower $S_T$ grains. This leads to less dominance by one plate type in low $S_T$ grains.

5.3.3 Effect of Predeformation at the Grain Scale

The tabular data in Figure 5.3a clearly indicate that the macroscopic performance $P$ of polycrystals is reduced by plastic predeformation, achieved in this case by 2% axial extension or compression in the austenite state. These results are for the second stress cycle following predeformation. The reduced $P$ is attributed to a nonzero martensite volume fraction $\nu_M$ at the start of the cycle. Presumably, this leaves less available austenite to transform, thus limiting the transformation contribution to macrostrain. This hypothesis for why $P$ is reduced is examined in Figure 5.7, where the local tensile stress-strain response during the second cycle is shown for the representative grain A in Figure 5.1. In the no pre-deformation case, a small residual strain exists at the start of the cycle (pt. $n_0$) due to small amounts of plasticity during the first cycle. Compared to the counterpart isolated crystal response
(dashed curve), the transition at pt. \( n_1 \) is rounded, substantial hardening occurs from pt. \( n_1 \) to pt. \( n_2 \), and the relatively large angle \( \phi \) at pt. \( n_2 \) signifies incompletion transformation. For the tensile predeformation case, tensile residual stress stabilizes martensite at the start of the cycle. This causes the transformation to complete early in the cycle (near pt. \( t_2 \)) because there is less available austenite to transform. Thus, the hypothesis is substantiated. For the compressive pre-deformation case, the hypothesis is not substantiated. Although martensite is stabilized by compressive stress at the start of the cycle, this martensite is removed during loading and a different plate type forms. The hardening from pt. \( c_1 \) to \( c_2 \) is so large that the transformation never completes and \( \nu_M \) does not reach 1. Thus, \( p_T \) is small not because of a reduced amount of available austenite to transform but rather, the inability to complete the transformation. In all three cases, the local tension required for the onset of transformation varies from \( \sim 200 \) MPa to \( \sim 600 \) MPa - a manifestation of multiaxial residual stress states within polycrystals.

5.3.4 Effects of Packing and Texture

It is evident from Figure 5.5a that the fitted function \( p_T^* \) does not completely capture the neighborhood effect, because \( p_T \) can vary by \( \sim 1.5\% \) among grains that have the same \( p_T^* \). The source of such scatter is studied using three idealized grain packings containing a bimodal texture. These bimodal textured polycrystals are depicted in 5.8a and are denoted isotress (ISO\( \sigma \)), isostrain (ISO\( \epsilon \)), and checkerboard (CHEQ). In the ISO\( \sigma \) packing, each grain sustains the same applied tensile stress along the loading (z) axis. For the ISO\( \epsilon \) packing, each grain sustains the same direct strain along the z axis. In the CHEQ packing, neither isostrain nor isostress conditions
Figure 5.7: Predictions from the model in Figure 5.1 showing the average axial stress vs. average axial strain in grain A during the second macroscopic pseudoelastic stress cycle from 0 to 640 MPa and back. The results are shown for 0%, +2%, and -2% plastic predeformation of the polycrystal at elevated temperature in the austenitic state, before cooling to room temperature and conducting the pseudoelastic stress cycling. The predeformation generates remnant plastic and transformation strain at the start of the cycle and increased hardening during transformation.

prevail along the z axis. The bimodal texture is specified by selecting two grain orientations with lower vs. higher Schmid factors ($S_T$). Dark-shaded “L grains” have a lower $S_T$ (0.2), corresponding to a cube-oriented crystal with [0 0 1] $\parallel$ z axis, [1 0 0] $\parallel$ x, and [0 1 0] $\parallel$ y. The stereographic triangle in Figure 5.8b confirms a [0 0 1] tensile axis creates the lowest possible Schmid factor for transformation. Light-shaded “H grains” have a higher ST (0.41). This is achieved by picking either ●[1 1 1], ■[4 4 13], or ♦ [18 1 18] $\parallel$ z. 5.8b confirms a similar high $S_T$ for all three H grain orientations.

5.8a shows the performance $p_{T(L)}$ for the L grains in the lower left (solid) square and performance $p_{T(H)}$ for the H grains in the upper right (dashed) square. The nine
simulations are generated by analyzing the ISO$\sigma$ packing for the three •, ■, and ♦ textures, and then doing the same for the ISO$\epsilon$ and CHEQ packings. Mirror boundary conditions are applied to the x, y, and z faces of the finite element model. Thus, the ISO$\sigma$ packing corresponds to tension perpendicular to a sandwich of alternating L and H layers. The ISO$\epsilon$ packing corresponds to tension parallel to a sandwich of alternating L and H layers. Finally, the CHEQ packing corresponds to tension perpendicular to alternating L and H rods. In all cases, the samples were loaded along the z axis to a peak stress of $\sim$640 MPa for two cycles, and the resulting $p_T$ values are based on the second cycle.

Table 5.2 lists the orientations of boundaries between L and H grains for each of the packings. For the ISO$\sigma$ packing, the L/H boundaries have a normal $n_z$ and for the ISO$\epsilon$ packing, it is $n_y$. The CHEQ packing has L/H boundary normals along both $n_z$ and $n_y$. Table 5.3 lists the orientation relations between the L and H grains for the three textures. Only the • texture involves high symmetry orientations in both L and H grains.

<table>
<thead>
<tr>
<th>Packing</th>
<th>L/H Interface Normal</th>
</tr>
</thead>
<tbody>
<tr>
<td>ISO$\sigma$</td>
<td>$n_z$ only</td>
</tr>
<tr>
<td>ISO$\epsilon$</td>
<td>$n_y$ only</td>
</tr>
<tr>
<td>CHEQ</td>
<td>$n_y$ and $n_z$</td>
</tr>
</tbody>
</table>

Table 5.2: Interface normals for different grain packings

Observations about texture are drawn from the simulations. First, the • texture tends to produce the highest $p_{T(L)}$ and $p_{T(H)}$ values, regardless of the packing (ISO$\sigma$, ISO$\epsilon$, CHEQ). This can be rationalized in that the • texture employs loading along
<table>
<thead>
<tr>
<th>Texture</th>
<th>Axis</th>
<th>L Grain</th>
<th>H Grain</th>
</tr>
</thead>
<tbody>
<tr>
<td>• High Symmetry</td>
<td>x</td>
<td>[1 0 0]</td>
<td>[1 0 1]</td>
</tr>
<tr>
<td></td>
<td>y</td>
<td>[0 1 0]</td>
<td>[1 0 1]</td>
</tr>
<tr>
<td></td>
<td>z</td>
<td>[0 0 1]</td>
<td>[1 1 1]</td>
</tr>
<tr>
<td>■ Low Symmetry</td>
<td>x</td>
<td>[1 0 0]</td>
<td>[11 35 14]</td>
</tr>
<tr>
<td></td>
<td>y</td>
<td>[0 1 0]</td>
<td>≈[5 2 1]</td>
</tr>
<tr>
<td></td>
<td>z</td>
<td>[0 0 1]</td>
<td>[4 4 1]</td>
</tr>
<tr>
<td>♦ Low Symmetry</td>
<td>x</td>
<td>[1 0 0]</td>
<td>[139 18 138]</td>
</tr>
<tr>
<td></td>
<td>y</td>
<td>[0 1 0]</td>
<td>≈[7 200 18]</td>
</tr>
<tr>
<td></td>
<td>z</td>
<td>[0 0 1]</td>
<td>[18 1 18]</td>
</tr>
</tbody>
</table>

Table 5.3: Orientation relations for different textures

high symmetry axes and also high symmetry boundary normals. In particular, Figure 5.8b shows that tension along ⟨1 1 1⟩, ⟨1 0 1⟩, and ⟨1 1 2⟩ in the cubic B2 parent phase produces equal driving forces on 6, 4, and 4 martensite plate types, respectively. These correspond to the z, x, and y directions of the H grain in the • texture. In principle, such high symmetry axes permit more arbitrary transformation strain paths at a given stress, akin to vertices in yield surfaces. Such arbitrary paths are needed to satisfy compatibility across L/H interfaces. Conversely, the H grain has low symmetry axes in the ■, and ♦ textures and $p_{T(H)}$ is correspondingly lower. The poor $p_{T(H)}$ in the ♦ texture occurs even though the H grain has a tensile axis [18 1 18] that is close to [1 0 1] (Figure 5.8b). The transverse axes are not high symmetry, however.

Observations about packing show that the CHEQ case consistently has lower $p_{T(L)}$ and $p_{T(H)}$. This can be rationalized in terms of CHEQ packing having both nz and ny boundaries and thus increased constraint. The CHEQ packing also is most sensitive to texture, where $p_{T(H)}$ is maximum for the high symmetry • texture. However, $p_{T(L)}$
for CHEQ packing is poor regardless of the texture. The ISO$\epsilon$ packing is predicted to be high performing and relatively insensitive to texture.

The approximate function $p_T*$ that was fit to random polycrystalline data captures the coarse trend that $p_{T(H)}* > p_{T(L)}*$, regardless of packing or texture. However, it does not capture the dependence of $p_{T(H)}$ and $p_{T(L)}$ on packing. In particular, $p_T*$ predicts that performance is greatest for ISO$\epsilon$ packing, followed by CHEQ, then ISO$\sigma$. Rather, the simulations show that ISO$\epsilon$ and ISO$\sigma$ values are quite comparable and CHEQ is consistently lower. $p_T*$ also predicts that performance should be independent of the • vs. ■ vs. ♦ textures. Rather, the simulations show texture can be important, particularly for CHEQ packing.

### 5.3.5 Local Effects Near Interfaces

Figure 5.9 explores the spatial variation in performance $p_T$ around L/H boundaries. CHEQ packing is chosen because it provides both $n_z$ and $n_y$ interfaces. Distributions of $p_T$ are shown for the three textures (•, ■, and ♦) along the $x = 0$ plane. For the high symmetry • texture, the interior core (dark red) region of the H grain performs near that of a single crystal. Yet, for the lower symmetry ■ and ♦ textures, all regions of the H grain lose performance, including the core. This is attributed to the activation of inefficient martensite plate types to satisfy compatibility across H/L boundaries. The penetration occurs in both the $z$ and $y$ directions, indicating the $n_z$ and $n_y$ interfaces are both potent generators of constraint due to compatibility. A net effect is the degradation in the average performance $p_{T(H)}$ from 5 to 4.5 to 3.5%, respectively, for the three textures. $p_{T(L)}$ degrades in the same manner, even though the L grain orientation is fixed among the three textures. For the high symmetry •
texture, the L grain performance is enhanced nearly everywhere except at the core. Presumably, this enhancement stems from the redistribution of stress from the H to L grain. The enhancement diminishes in the lower symmetry ■ and ♦ textures. Figure 5.9 summarizes this effect in terms of the width \( w \) of performance penetration normal to the \( n_y \) interface and the height \( h \) of penetration normal to the \( n_z \) interface. For the high symmetry ● texture, the values of \( w \) and \( h \) are smallest and the penetration is primarily into the L grains, enhancing their performance. For the lower symmetry ■ and ♦ textures, \( w \) and \( h \) are larger and the penetration is primarily into the H grains, decreasing their performance. This underscores the complex, but important role of texture and boundary orientation relationships on polycrystalline performance.

The dependence of \( p_{T(H)} \) on the orientation relationships at boundaries can be rationalized based on the need for multiple plate type activation to satisfy compatibility. This is somewhat similar to the need to activate at least five slip systems to accommodate arbitrary plastic strain. Consider an H grain with a high symmetry direction along the loading axis (e.g. in ●). Such a grain orientation would lie near the corners of the stereographic triangle in Figure 5.8(b). A high symmetry grain is capable of activating 4 to 8 equivalent plates with the largest Schmid factor for transformation. Such a grain is likely to satisfy compatibility across the boundary without activating inefficient plates. It is also expected to efficiently shed stress to L grains. Hence, the performance width is expected to penetrate beneficially into L grains but not detrimentally into H grains. Conversely, H grains with low symmetry directions are likely to activate less efficient plates to satisfy compatibility. Hence, the performance width is expected to penetrate detrimentally into H grains and not
beneficially into L grains. These features are reflected in the $p_{T(H)}$ distributions in Figure 5.9.

Having relatively few, high symmetry grain boundaries is demonstrated to improve the performance of both H and L grains. These can be viewed as two criteria for high macro performance. An extreme case satisfying these conditions would be a bamboo packing with a bimodal texture consisting of high symmetry orientations. Although the detailed $p_T$ distributions are not shown, Figure 5.4 shows that the polycrystalline bamboo arrangement has a superior performance to a 3D packing. It has been reported in the literature that such bamboo arrangement shows superior fatigue response compared to bulk polycrystal, in a Cu-Zn-Al shape memory alloy [74]. Combined with this work, the results suggest that systems with minimal constraint across grain boundaries may have higher performance and improved structural life.
Figure 5.8: (a) Predictions of the grain transformation performance $p_T$ vs. the performance function $p_T^*$ for isostress (ISO$\sigma$), isostrain (ISO$\epsilon$) and chequerboard (CHEQ) packing of bicrystals containing high $S_T$(H) and low $S_T$(L) grains. The geometry of each sample is shown in the inset sketches. Each face of the sample has mirror boundary conditions on it. For each packing, three textures are considered using three tensile axis orientations ($\circ \langle 1 \ 1 \ 1 \rangle$, $\blacksquare \langle 4 \ 4 \ 13 \rangle$, $\blacklozenge \langle 18 \ 1 \ 18 \rangle$ of the high $S_T$ grains (see upper inset). The tensile axis orientation of low $S_T$ grain is held fixed at $\langle 0 \ 0 \ 1 \rangle$. (b) Stereographic triangle showing the three tensile axis orientations used for high $S_T$ grains. The number of efficient plates types activated is listed next to each orientation.
Figure 5.9: Predictions of the microstructural finite element model at a macroscopic stress of 640 MPa, showing the distribution of transformation performance $p_T$ within grains of CHEQ samples. Three different CHEQ samples are shown, where the tensile axes of the H and L grains are (a) $\langle 1 1 1 \rangle$ and $\langle 0 0 1 \rangle$; (b) $\langle 4 4 13 \rangle$ and $\langle 0 0 1 \rangle$; (c) $\langle 18 1 18 \rangle$ and $\langle 0 0 1 \rangle$. Four grains are shown in each case. $p_T$ varies inside a grain, with its value close to $p_T(\text{ideal})$ near the center of each grain interior. The Schmid factors for transformation $S_T$ of the H and L grains are similar in each case. The grain averaged performance and H grain crystallographic orientation are listed in Figure 5.8.
5.4 Conclusions

The goal of this work is to predict the statistical nature of transformation performance $p_T$ of grains in a pseudoelastically stressed polycrystalline SMA. This is achieved using microstructural FE model simulations, where $p_T$ is defined as the transformation strain achieved in a grain at a large ($\sim$640 MPa) macrostress, sufficient to achieve 100\% transformation in free-standing single crystals of any orientation.

A key result is the development of a new predictive function (Eq. 5.8) for grain performance $p_T$ that takes into account the orientations of the parent grain and the nearest neighbors. It is inspired by the Eshelby solution for the stress field of a cuboidal region that undergoes an axial transformation strain. The predictive function captures the trend that transverse neighboring grains that are easy to transform will tend to increase $p_T$ of the parent grain, by shedding stress onto the parent grain. Conversely, axial neighboring grains that are easy to transform will tend to decrease $p_T$ of the parent grain, by reducing stress on the parent grain. The predictive "neighborhood" function captures the $p_T$ data from the simulations with a least-squared error fit $R^2 = 0.9$. An overall consequence is that grains typically operate from 65 to 85\% of the ideal single crystal performance. Easy to transform grains tend to have a higher percentage and greater texture of favorable martensite plates. Even then, no grain is observed to exceed 90\% of the ideal single crystal performance. Compared to an idealized, unconstrained bamboo geometry, a 3D polycrystal exhibits pronounced transformation hardening and reduced performance.

The results also highlight the deleterious effect of predeformation of an austenitic polycrystal at elevated temperature ($T \gg \theta_{AF}$), prior to pseudoelastic testing at lower temperature ($T > \theta_{AF}$). Polycrystalline performance $P$ is predicted to decrease
from 6.5% to 5.3% if +2% plastic predeformation is imposed. \( P \) decreases to 4.6% if -2% plastic predeformation is imposed. The reduced performance is attributed to the residual stress state, which can stabilize martensite. Depending on the sign of residual stress, it can leave less available austenite to transform or delay the start of the phase transformation.

A study of polycrystalline geometries predicts that isostrain geometries (e.g., tensile loading parallel to a layered set of grains) achieve superior performance. Isostress geometries are competitive, provided the grain boundaries involve grain boundary normals along high symmetry crystal directions (e.g., \( ⟨111⟩ \)). The rationale is that high symmetry directions can invoke multiple equivalent martensite plates, relaxing constraint.

The results connect to experimental investigations by Yuan and Yi [70] showing that accurate theoretical estimates of polycrystalline performance cannot be based on average texture measurements and values of idealized transformation strain in free-standing single crystals. The results also quantify the observations of constraint between hard and easy to transform grains by Daly et al [71]. Like the experimental observations of Mao et al [72], the predicted volume fraction of martensite can be vastly different for grains with similar Schmid factors for transformation. Further, the type and number of martensite plates activated in a grain depends on the neighborhood, as observed by Merzouki et al [73].

The microstructural FE simulations are state-of-the-art in the sense that they incorporate the coupled effects of anisotropic elasticity in the austenite and martensite phases, crystallographic descriptions of the phase transformation among 24 competing martensite plates in the B2 to B19 transformation system, and crystal-based
plasticity among 12 competing austenite slip systems. The austenite-martensite aggregate approach used here is expected to be reasonable when grain size $\gg$ martensite plate size. Otherwise, discrete martensite plate geometries and fine scale plasticity [14, 31, 40] gain in importance. The generic aspects of constraint explored here should apply to other shape memory systems in addition to the homogenized Ti-50.9 at%Ni explored here.
Chapter 6: Contributions and Future Work

This thesis has achieved twofold goals- First, a martensite CV scale modeling approach has been developed that captures interaction between phase transformation and plasticity in SMA. Second, a detailed analytical study of factors influencing statistics of pseudoelastic performance of a grain in a polycrystalline SMA is presented. The unique contributions of this work to the literature and their shortcomings are summarized in the next two Sections. Lastly, opportunities for future work based on these two studies are explored.

6.1 Assessment of the PF/FE Model

1. A comprehensive modeling approach for SMA is developed. This approach combines the deformation mechanisms of $A \leftrightarrow M$ phase transformation and re-orientation, plastic deformation in austenite, anisotropic elasticity and isotropic thermal expansion in asutenite and martensite. The transformation law is based on the phase field approach [55] and the plasticity law is from the well-known crystal plasticity framework of Peirce et al [80]. An efficient explicit time integration scheme is implemented. Gradient based interface energy term in the martensite evolution law is calculated on a non-uniform mesh by spatially interpolating the order parameter values. The finite element implementation makes
this approach versatile in modeling arbitrary loading and boundary conditions. The simulations can be run on parallel processing environments.

2. The A-M and M-M interface parameters are the output of this model, rather than an input. The effect of crystallographic orientation is captured as shown in the micropillar simulations of Chapter 4. The only crystallographic inputs to the model are the local crystal orientation at a material point and the Bain strain matrices for the martensite CVs. However, the interfaces predicted by the model are diffuse. Experimentally, the interfaces in SMAs are sharp. One of the reasons for the prediction of diffuse interfaces is the Ginzburg-Landau kinetic relation used in the martensite evolution law. It allows the order parameter to gradually evolve once the driving force becomes positive. This happens, for example, in the thermal cycling simulations when the temperature drops just below the transformation temperature. The gradient based interface energy term can enhance the diffuse nature of the interface as well. This is because, a sharp interface has larger spatial gradient in the order parameter compared to a diffuse interface. The local approach on calculating the energy of the interface does not take into account the interface width. The only penalty for a diffuse interface is the activation barrier in the Landau polynomial based chemical free energy term, which penalizes $0 < \nu_t < 1$.

3. The model is able to capture the hysteretic response during thermal cycling. However the flag-shaped stress-strain response during pseudoelastic loading of single crystals is not accurately captured. This is because, phase transformation begins to occur as soon as a non zero favorably aligned stress is applied - leading
to a gradual elastic + transformation right at the beginning of the stressing instead of a steep elastic only region in the stress-strain curve.

4. Transformation induced plasticity is captured as shown in the simulations in Chapters 3 and 4. Two types of transformation induced plasticity is identified. The first is in the austenite that is trapped between martensite bands (Chapter 3) and the second is in front of an advancing or retracting martensite front (Chapter 4). The latter has been reported in the micron scale experiments on NiTi SMAs [44, 15, 40, 13, 43]. However, the plastic deformation due to local stress field of martensite twins may be underestimated due to diffuse nature of the interfaces.

6.2 Assessment of Grain Performance Statistics Study

1. A systematic analytical study of the effect of local grain neighborhood on the pseudoelastic performance of grains in a polycrystalline SMA is carried out. This study is unique in the sense that it addresses the statistics of grain performance. This is achieved using a grain-scale microstructural FEM model calibrated to Ti-50.9at.%Ni SMA [1].

2. Grain performance $p_T$ is quantified as the local transformation strain along the loading direction at the maximum macro stress.

3. Three factors are identified that introduce variation in $p_T$ in a polycrystal - the grain crystal orientation, orientation of the neighbors and the symmetry of the interface between the grain and the neighbors.
4. A key outcome of this work is a predictive function for $p_T$ based on the Schmid factor for transformation of the parent grain and the neighbors. This function is based on the idea of stress transfer between differently deformed parent and neighbor grains and it is inspired by the Eshelby solution for the stress field of an inclusion in an elastic medium [93].

5. Plastic predeformation in the austenitic state, whether tensile or compressive, has deleterious effect on $p_T$. The reduction in $p_T$ being 20-30% compared to a pristine sample.

6. When isostress, isostrain and chequerboard arrangements of grains are considered in terms of resultant $p_T$, the isostrain geometries are most efficient. Another desirable feature to improve $p_T$ is to have high symmetry interfaces that are capable of activating multiple equivalent martensite plates.

7. The results of this work pertaining to the grain level constraint and its effect of grain performance suggest that- full field simulations are necessary to predict features of grain-scale performance and aggregate based homogenization approaches may not be sufficient.

8. Grain shape and size is one factor that can influence the transfer of stresses between the grains. The discussion in Section 5.3.5 indirectly addressed this by considering the variation in $p_T$ inside a grain. However, this factor is not considered in detail. For example, the effect of stress concentration due to grain shape may lead to $p_T$ variation that is not considered by the fitting function.
6.3 Future Work

The PF/FE approach developed in this dissertation is a tool for studying martensite microstructure evolution and the interaction between phase transformation and plasticity. Three potential applications of this model are suggested.

1. **Nanoindentation of SMA:** Several recent experimental works have studied nanoindentation of Ni-Ti SMA at a temperature where stress induced martensite is stabilized [95, 26] and in the pseudoelastic regime [25]. The experiments with stabilized martensite show indentation surface patterns that can be rationalized on the basis of Schmid factor type arguments. However, for the indentation work of Pfetzing-Micklich et al [25], the hardness data is apparently does not follow the Schmid law for transformation. Further, the dislocations observed under the indenter are proposed to be on the martensite slip systems. The PF/FE model can provide about the active deformation mechanisms during nanoindentation. Further, these results can be compared with the pillar type microcompression experiments to assess the effect of confined volumes.

2. **Load-biased thermal cycling of NiTi:** Recent experimental work has shown that the load-biased thermal cycling of NiTi single crystals leads to substantial changes in the local crystal orientation of the sample. These observations are not well understood. The PF/FE approach can be used to study this. Specifically, the model can predict whether the martensite microstructure continuously evolves cycle after cycle or a fixed pattern emerges, leading to large localized plastic deformation. Such localized plastic deformation can lead to lattice rotation.
3. A library of martensite plates and austenite slip systems activated:

Simulations of pseudoelastic loading similar to ones shown in Chapter 4 can be carried out with different single crystal orientations. Each crystal orientation can be chosen to activate a specific and unique martensite plate. The results can yield a library of martensite plates and the corresponding austenite slip systems that are activated due to the local stress of the plate. This will be useful in interpreting future micron scale experiments on Ni-Ti.

The grain neighborhood study presented in Chapter 5 connects well with the upcoming X-ray based tomography techniques. These experiments are capable of providing grain center of mass, martensite volume fraction and elastic strain tensor data. The predictive function presented in this dissertation (equation 5.8) can be used in interpreting those results.
Appendix A: ABAQUS User Subroutine Algorithm

Inputs:

1. The time at the previous increment: $t$
2. The time at the current increment: $\tau = t + \Delta t$
3. The total deformation gradient at the time $t$: $F(t)$
4. An imposed total deformation gradient at the time $\tau$: $F(\tau)$
5. The inelastic component of the deformation gradient at the time $t$: $F^{\text{inel}}(t)$
6. The temperature at the previous increment: $\theta(t)$
7. The temperature at the current increment: $\theta(\tau)$
8. The martensite volume fractions at the time $t$: $\nu(t)$
9. The local crystallographic orientation
10. Various material properties (Bain strains, stiffness tensor, thermal expansion coefficient etc.)

Outputs:
1. The Cauchy stress at the current increment: \( T(\tau) \)

2. The martensite volume fractions at the time \( \tau \): \( \nu(\tau) \)

3. The slip rate at the time \( \tau \): \( \dot{\gamma}(\tau) \)

4. The inelastic component of the deformation gradient at the time \( \tau \): \( F^{\text{inel}}(\tau) \)

**Step 1:** Assume a trial value of the inelastic deformation gradient \( (F^{\text{trial}})^{\text{inel}} \) at \( \tau \) equal to that calculated at \( t \). Calculate a trial value of the elastic deformation gradient through a multiplicative decomposition.

\[
F^{\text{trial}}_e = FF^{\text{inel}}_{\text{trial}}^{-1}
\]

From the trial elastic deformation gradient, calculate the local elastic strain.

\[
E^{e}_{\text{trial}} = \frac{1}{2}(F^{eT}F^{e} - I)
\]

**Step 2:** Calculate an effective elastic stiffness and a thermal expansion coefficient using a rule-of-mixtures approach

\[
C = \nu_A(t)C_A + \nu_M(t)C_M \quad \text{and} \quad A_{\text{therm}} = \nu_A(t)A_{A-\text{therm}} + \nu_M(t)A_{M-\text{therm}}
\]

**Step 3:** Calculate a trial stress

\[
T^{*}_{\text{trial}} = C(E^e - A_{\text{therm}}\Delta\theta)
\]

**Step 4:** Calculate the stress work component of the driving force for transformation

\[
\tau^{\text{trans}}_i = F^{eT}F^{e}T^{*} \cdot S^{\text{trans}}_i
\]

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Step 5: Calculate the resolved stress on the slip systems

\[ \tau_{\text{slip}}^i = F^e T^e T^* \cdot S_{\text{slip}}^i \]

Step 6: Calculate the total driving force for transformation

\[ f_t^{\text{trans}} = K_{tu} \nabla^2 \nu_t + F^e T^e T^* S_t^{\text{trans}} - \frac{\partial f_{\text{LP}}(\nu_t, \theta)}{\partial \nu_t} \]

Step 7: Calculate the increment in the martensite volume fractions from the Ginzburg-Landau kinetic law

\[ \dot{\nu}_t = M_{tu} f_t^{\text{trans}} \]

Step 8: Calculate the slip rate from the crystal plasticity law

\[ \dot{\gamma}_s = \dot{\gamma}_0 \left( \frac{\tau_s}{g_s} \right)^{\frac{1}{m}} \text{sign}(\tau_s) \]

Step 9: Based on the values of \( \Delta \nu_t(\tau) \) and \( \dot{\gamma}_s(\tau) \), calculate an updated value of the inelastic deformation gradient.

\[ F^{\text{inel}}(\tau) = \left( 1 + \sum_{t=1}^{N_P} \dot{\nu}_t S_t^{\text{trans}} + \nu_A \sum_{t=1}^{N_P} \dot{\gamma}_t S_t^{\text{slip}} \right) F^{\text{inel}}_{\text{trial}} \]

Step 10: Update the effective elastic stiffness constant and the thermal expansion coefficient.

\[ C = \nu_A(t) C_A + \nu_M(t) C_M \quad \text{and} \]
\[ A_{\text{therm}} = \nu_A(t) A_{A\text{-therm}} + \nu_M(t) A_{M\text{-therm}} \]

Step 11: Update the slip system hardness.

\[ \dot{g}_s = \sum_{r=1}^{N_s} = h_r (Q + (1 - Q) \delta_{sr}) |\dot{\gamma}_r| \]
\[ h_r = h_0 \left( a - \frac{g_r}{g_{\text{sat}}} \right)^a \]

$$
F^e(\tau) = FF^\text{inel}(\tau)^{-1}
$$

$$
E^e = \frac{1}{2}(F^e(\tau)^T F^e(\tau) - I)
$$

$$
T^*(\tau) = C(E^e - A_{\text{therm}} \Delta \theta)
$$

Step 13: Calculate the Cauchy stress

$$
\mathbf{T}(\tau) = F^e(\tau) \cdot \left[ \frac{T^*(\tau)}{\det F^e(\tau)} \right] F^{eT}(\tau)
$$
Bibliography


National Laboratory for Sustainable Energy, Technical University of Denmark, January 2011.


