

**TOWARDS THE DEVELOPMENT OF DUAL PHASE
CONSTITUTIVE RELATIONS FOR TI-6AL-4V BASED ON THE
MECHANICAL THRESHOLD STRESS MODEL**

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**TOWARDS THE DEVELOPMENT OF DUAL PHASE
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MECHANICAL THRESHOLD STRESS MODEL**

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To Christina, Paul and Hartley

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SUMMARY

Common effects of high-speed machining processes are the development of residual stresses, the evolution of texture and change in mechanical properties, often to the detriment of the workpiece. High-speed machining of Ti-6Al-4V parts often subjects the workpiece surface to increased temperatures, high strains and strain-rates and can lead to phase transformations, recrystallization, growth and grain size gradients. The description of the mechanical behavior of dynamic processes depends greatly on a constitutive model being able to account accurately for changes in the flow stress with variations in strain-rate and temperature that occur during processing. The Mechanical Threshold Stress (MTS) model is a physical-based internal state variable model that accounts for this behavior remarkably well. While much work has been invested in parameterizing the MTS model for various material systems, relatively little attention has been given to dual or multiphase systems. Additionally, most applications of the MTS model have been used to describe bulk material behavior without regard to the constitutive behavior at the slip system level.

In this work single-crystal MTS models for the α - and β -phases of the Ti-6Al-4V system were developed at the slip system level for use within the Viscoplastic Self Consistent (VPSC) crystal plasticity model to describe the stress-strain behavior of polycrystalline dual-phase Ti-6Al-4V undergoing high strain-rate compression over a wide range of temperatures. To properly model the constitutive behavior, modifications were made to the MTS model to 1) extend applicability to high-strain rate behavior where thermal dislocation activation transitions to dislocation drag mechanism and 2) more accurately model the initial work-hardening at the onset of plastic deformation. The results

were found to match reported experimental data to within 5%.

Simulations were also carried out to model the surface texture evolution of the Ti-6Al-4V α - and β -phases undergoing high-speed machining processes. X-ray diffraction (XRD) and electron backscatter diffraction (EBSD) measurements were made on as-received Ti-6Al-4V samples to provide input texture data as an initial state for simulations while measurements made on post-machined samples were used to validate simulated texture results. Because experimental measurements provide texture information at the surface as well as below the surface, novel methods were devised to subtract out the sub-surface texture information and better represent the experimental texture at the surface. High-speed machining simulation texture results showed good qualitative agreement with this method.

CHAPTER 1. INTRODUCTION

1.1 Motivation

Titanium alloys are attractive in aerospace applications owing to their corrosion resistance, low weight and high strength. One of the most actively studied and used alloys of titanium is Ti-6Al-4V, which was developed in 1954 at the Illinois Institute of Technology and is commonly used in aerospace applications where material reliability is essential [1]. Examples of applications using Ti-6Al-4V are structural materials, fastener bolts and engine intake fan blades and casings [2]. While many parts used in aerospace applications are forged, others are machined to specification; it is also not uncommon that forged parts may also go through machining as a finishing process to meet design specifications or to improve surface properties. Regardless, high-speed machining processes, such as planing, milling or turning, are often necessary to form a workpiece to final specified dimension. This process, however, often subjects the workpiece surface to increased and highly variable temperatures, strains and strain-rates [3]. In complex alloy systems, the dynamic environment often changes the near-surface microstructure and affects the materials properties through the introduction of texture evolution, recrystallization, growth, grain size gradients, etc., which may be detrimental or beneficial to the workpiece [4, 5].

To capture the stress-strain response under dynamic processing conditions a constitutive model must be able to account for changes in processing path history. The Mechanical Threshold Stress (MTS) model is a physical based internal state variable model that describes the flow stress behavior of a material and is based on the initial work of Mecking and Kocks and later extended by Follansbee and Kocks [6, 7]. The novelty of this

model is that it can account for the flow stress behavior under changes in processing conditions (e.g. strain-rate, temperature) by evaluating the flow stress against the mechanical threshold stress; that is, the flow stress at 0 K where the material structure is considered a constant. Initially formulated for single-phase materials to model the averaged flow stress response of polycrystalline copper at low temperatures (<300 K) and a broad range of strain-rates (10^{-4} s^{-1} to 10^4 s^{-1}), the MTS model has in recent years been extended to a variety of materials (Ti-6Al-4V, aluminum alloys and austenitic stainless steels) and extended to account for a variety of effects (static strain aging and dynamic strain aging) [8, 9, 10].

Though the MTS model has been applied to the Ti-6Al-4V system and to cases of high-speed machining, the results have been quite mixed and several problems persist. Follansbee and Gray first parameterized the MTS model for Ti-6Al-4V based on compression test experiments with a wide range of strain-rates (between 0.001 and 3000 s^{-1}) and a limited temperature range (76 – 495 K) [11]. While the fit with experimental data is quite remarkable, stress predictions tend towards negative values as the temperatures are increased. Follansbee and Gray's model was later extended by Pan et al. based on the work of Kotkunde et al. in an attempt to capture the constitutive behavior at a wider temperature (77 – 673 K) and strain-rate (10^{-5} – 3000 s^{-1}) range [3,12]. Their model was implemented within finite element codes in an attempt to model the constitutive behavior of Ti-6Al-4V under machining conditions. In Pan et al.'s work, the stress-strain response was not directly modeled, but rather translated into terms of machining forces. Finite element results were compared against experimental machining forces and errors were within anywhere from a few percent to as high as $\sim 41\%$. While good flow stress results post yielding have been

shown, it would appear that the MTS model over predicts the constitutive response at yielding and immediately thereafter and does not accurately capture the Stage II - III work-hardening behavior. Additionally, if the strain-rates used for these models were extended to higher and higher values, the MTS model would continue to predict a linear increase in the yield stress values in contradiction to experimental results that find an exponential increase as the deformation controlling mechanism transitions from thermal activation to drag mechanisms [13]. These issues are inherent problems with the MTS model in general.

To model the anisotropic constitutive behavior of dual-phase alloys and provide a means for testing constitutive models at the single crystal level, a crystal plasticity simulation program is used to simulate dual-phase Ti-6Al-4V undergoing high-speed turning operations. The Viscoplastic Self Consistent Model (VPSC), a program developed at Los Alamos National Laboratories will be used to model the texture and material property evolution under various temperatures and strain-rates; to clarify, VPSC is not only a crystal plasticity program, but also a specific crystal plasticity model. In order to model the mechanical response under dynamic conditions, the Mechanical Threshold Stress (MTS) constitutive model will be utilized as the flow stress model within the VPSC framework. This is also the core area of focus for this work as there has been much less work focused on formulating single-crystal MTS constitutive relations for use within crystal plasticity models as compared to models developed around bulk, or macroscopic, polycrystalline behavior; and little to no work has focused on using the MTS model with multiphase materials within crystal plasticity models.

While there is no shortage of experimental stress-strain data for Ti-6Al-4V over wide ranges of temperatures and strain-rates, there is a shortage of consistent data. Ti-6Al-

4V is indeed a complex alloy and the stress-strain behavior is affected by solute concentration [14], solution treatment and aging [11], morphology (lamellar, equiaxed, or bimodal) [15, 16], texture/preferred orientation [17], phase composition [18], among other factors. Experimental results from the same researchers for similar Ti-6Al-4V specimens have been shown to yield widely varying results [19, 20, 21]. This variety of data really highlights the fact that in most cases, a constitutive model and its parameters are not unique to a material system and caution should be exercised when applying such parameterized model to experimental results. In this work, results from Lee and Lin are used as it provides the necessary data to extend the limits of the MTS model [20]. First, their results are quite comprehensive and provide the yield stress and flow stress values up to a strain of 0.2. Secondly, their results show the signs of deviations from linearity in the yield stress with increasing strain-rates. Though, their reported experimental flow stress results are lower than that of Follansbee and Gray's original work, their work is sufficient to develop the concepts presented herein, which can be applied more generally.

1.2 Objectives

The main goal of this work is to develop dual-phase constitutive relations for the Ti-6Al-4V system using the Mechanical Threshold Stress model that can be used within crystal plasticity simulations to provide an accurate stress-strain response and description of the texture evolution. To achieve this goal, modeling and simulation efforts are utilized and rely heavily on validation through experimental stress-strain data reported from the literature and measured texture from high-speed machining experiments. The specific objectives for this work are as follows:

1. Development of modifications to the MTS model to extend applicability to high-strain rate behavior and better model the initial work-hardening behavior post yield of Ti-6Al-4V.
2. Extension of the MTS model and modifications to a single-crystal model for use within the VPSC program to model the stress-strain behavior of Ti-6Al-4V at high strain-rates over a wide range of temperatures.
3. Extension of the MTS model within the VPSC program to simulate the stress-strain behavior at high strain-rates over a wide range of temperatures and the texture evolution under high-speed machining conditions for dual-phase Ti-6Al-4V.

This dissertation is divided into seven chapters and is designed to provide a cohesive flow to the development of the dual-phase constitutive relations. Chapter 2 provides a theoretical background on the models used within this work starting with a discussion of the MTS model and associated equations. The VPSC model is also discussed at length to promote understanding of the connections between the material constitutive description at the microscopic and macroscopic level. In Chapter 3, the modifications to the MTS model and their rationale are discussed at length and model predictions are compared to experimental high strain-rate compression data reported in the literature. Chapter 4 examines the modification of this model to the single-crystal level and its use within the VPSC program. Simulations are run modeling high strain-rate compression to generate stress-strain curves at various temperatures and strain-rates and are compared to experimental data. In Chapter 5, experimentally measured textures are computed using x-ray diffraction and electron backscatter data acquired for as-received and post-machined Ti-6Al-4V samples. Novel methods are then developed to calculate more accurate

representations of texture at and near the machined surface. Chapter 6 presents the development of the full two-phase constitutive relations. The VPSC program using the two-phase constitutive relations is then used to model the stress-strain response of high strain-rate compression and the texture evolution of high-speed machining. Finally, Chapter 7 will provide a summary of results and discuss the extension of this work into future projects.

CHAPTER 2. BACKGROUND

2.1 MTS Model

The MTS model is typically presented in a form that consists of a summation of contributions to the flow stress [7, 11]:

$$\frac{\sigma}{\mu} = \frac{\sigma_a}{\mu} + S_i(\dot{\epsilon}, T) \frac{\hat{\sigma}_i}{\mu_0} + S_d(\dot{\epsilon}, T) \frac{\hat{\sigma}_d}{\mu_0} \quad (1)$$

where σ_a , $\hat{\sigma}_i$ and $\hat{\sigma}_d$ are the athermal, mechanical threshold stress and strain hardening contributions of the flow stress, respectively, $\dot{\epsilon}$ is the strain-rate, T is the temperature, μ_0 is the shear modulus at 0 K, and μ is the temperature dependent shear modulus (often called the Varshni Equation), given here as [22]:

$$\mu = \mu_0 - \frac{a}{\exp\left(\frac{T_0}{T}\right) - 1} \quad (2)$$

where μ_0 , a and T_0 are constants and T is the temperature.

The athermal contribution, σ_a , is rate independent and is taken as the contribution of the flow stress with grain boundaries or other long-range barriers while the mechanical threshold stress, $\hat{\sigma}_i$, is taken as a strain-rate and temperature dependent contribution due to short range barriers, such as thermally activated dislocations [7, 11]. Together, these terms within Equation 1 can be taken as the yield strength of the material as a function of temperature and strain-rate and will be the main focus of this work. The strain hardening contribution, $\hat{\sigma}_d$, is taken as a strain-rate and temperature dependent contribution due to

dislocation interaction and dislocation density increases and provides the plastic deformation (flow stress) post yielding [7, 11]. Though the athermal and mechanical threshold stress are (typically) constant for a given temperature and strain-rate, the strain hardening component evolves as a function of the current material state. The shear modulus (and its value at 0 K) is included in the formula as a means of factoring out contributions to thermal activation due to temperature dependencies of the shear modulus. It should be noted that in some treatments, the stress may be given in terms of a shear stress, τ . This is taken as the application of the MTS model to a single crystal system whereas the formulation in terms of the symbol σ is taken as the application to a macroscopic polycrystalline system.

The scaling factors, $S_i(\dot{\epsilon}, T)$ and $S_d(\dot{\epsilon}, T)$, are a ratio of the applied stress to the mechanical threshold stress and can loosely be thought of as the fractional measure of the stress required to move dislocations past an obstacle at specific temperatures and strain-rates relative to the stress required at 0 K. The scaling factors are a function of temperature and strain-rates and are given by the following equations [7, 11]:

$$S_i(\dot{\epsilon}, T) = \left\{ 1 - \left[\frac{kT}{\mu b^3 g_{oi}} \ln \left(\frac{\dot{\epsilon}_{0i}}{\dot{\epsilon}} \right) \right]^{1/q_i} \right\}^{1/p_i} \quad (3)$$

$$S_d(\dot{\epsilon}, T) = \left\{ 1 - \left[\frac{kT}{\mu b^3 g_{od}} \ln \left(\frac{\dot{\epsilon}_{0d}}{\dot{\epsilon}} \right) \right]^{1/q_d} \right\}^{1/p_d} \quad (4)$$

where k is Boltzmann's constant (1.38062×10^{-23} J/K), b the magnitude of the Burgers vector (here taken as 2.96×10^{-10} m for Ti-6Al-4V), g_{oi} and g_{od} normalized barrier activation energies, $\dot{\epsilon}_{0i}$ and $\dot{\epsilon}_{0d}$ constant reference strain-rates and p_i , q_i , p_d and q_d are

constants that model the shape of the energy barrier. With the exception of k and b , all other constants are fit to the material system under investigation. Though Equation (1) as presented lists only one mechanical threshold component to the MTS model, other components may be added in order to model dislocation interactions with substitutional atoms, interstitial atoms, precipitates, etc.

It was mentioned previously that the strain hardening contribution of the mechanical threshold stress is not a constant value and evolves as dislocation densities increase and the system hardens. The evolution of the strain hardening threshold stress is given by a modified Voce hardening law [23]:

$$\frac{d\hat{\sigma}_d}{d\varepsilon} = \theta_0 \left[1 - \frac{\hat{\sigma}_d}{\hat{\sigma}_{ds}(\dot{\varepsilon}, T)} \right]^\kappa \quad (5)$$

where $\hat{\sigma}_{ds}(\dot{\varepsilon}, T)$ is the temperature and strain-rate dependent saturation stress, κ is an empirically derived parameter, θ_0 is an empirically derived hardening rate parameter that may be constant or temperature and strain-rate dependent and ε is the strain. The strain-rate and temperature dependence of the saturation stress is given by the following [23]:

$$\ln \left(\frac{\hat{\sigma}_{ds}}{\hat{\sigma}_{ds0}} \right) = \frac{kT}{\mu b^3 g_{ds0}} \ln \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_{ds0}} \right) \quad (6)$$

where $\hat{\sigma}_{ds0}$ is the saturation stress at 0 K, g_{ds0} is normalized activation energy and $\dot{\varepsilon}_{ds0}$ is a constant reference strain-rate.

2.2 VPSC Model

The VPSC program was developed at Los Alamos National Laboratories in the early 1990's to simulate rolling processes of polycrystalline zirconium alloys to predict texture evolution and anisotropic plastic deformation [24]. It is based on Hill's self-consistent approach to the Eshelby inclusion problem whereby the macroscopic plastic strain and the plastic strain of a grain are taken as equal, or self-consistent [25, 26, 27]. Molinari et al. extended this model to large deformation of polycrystals where each grain is treated as viscoplastic ellipsoidal inclusions in a homogeneous but anisotropic viscoplastic medium [28]. It must be noted that the VPSC program does not treat the elastic contribution of deformation as the elastic response is fractionally small in plastic forming processes. While other crystal plasticity models exist, all subsequent discussion will focus on the VPSC model and is in no way intended to be a comprehensive treatment of its implementation. While it is not the intent of this section to provide an exhaustive overview of the VPSC model, it is intended to provide a theoretical background that promotes understanding of the connections between material constitutive description, local behavior (microscopic level) and global behavior (macroscopic level). These considerations will be discussed in more depth in the coming paragraphs. For the purposes of this work, the VPSC program allows the prediction of two very important features: the anisotropic mechanical response of the material and the evolution of texture.

Crystal plasticity models in general are used to model the anisotropic elastic-plastic mechanical response (or deformation) and texture evolution of polycrystalline metals, which are themselves typically anisotropic in nature. Single crystals comprising a polycrystalline material are inherently anisotropic in nature and the orientation dependence

of the mechanical response of such single crystals are well known [29]. This orientation dependence is due to the coupled behavior of external loading (i.e. work) and the slip activity due to dislocation motion on slip systems that are anisotropic in behavior because of the inherent anisotropy of the crystal lattice. Dislocations become active and glissile when the applied shear stress reaches a critical value (the Critically Resolved Shear Stress or CRSS) and, upon yielding, single grains tend to change shape due to dislocation motions through the crystal leading to gradual changes in the crystallographic orientation with increased deformation [30]. It should also be mentioned that twinning activity is also a very important mode of plastic deformation behavior, but will not be evaluated in this work. From a kinematical standpoint, this process can be mathematically modeled in two steps as shown in Equation (7):

$$F^c = R^c F_0^c \quad (7)$$

where F^c is the total deformation gradient of the crystal, F_0^c is the plastic contribution to the deformation gradient due to deformation via slip (the lattice orientations are preserved in this step) and R^c is the rotation contribution to the deformation gradient relative to an external frame of reference (the lattice orientations are likewise rotated relative to an external reference frame). This is shown schematically in Figure 1.

Additionally, single grains tend to harden due to an increase of dislocation pile-ups and networks, allowing for further yielding once enough energy has been introduced to overcome these obstacles [30]. When polycrystals are considered, interactions between grains must also be taken into account [31]. Polycrystalline metals also may be inherently textured; that is to say that there is an existing degree of preferred orientation of some

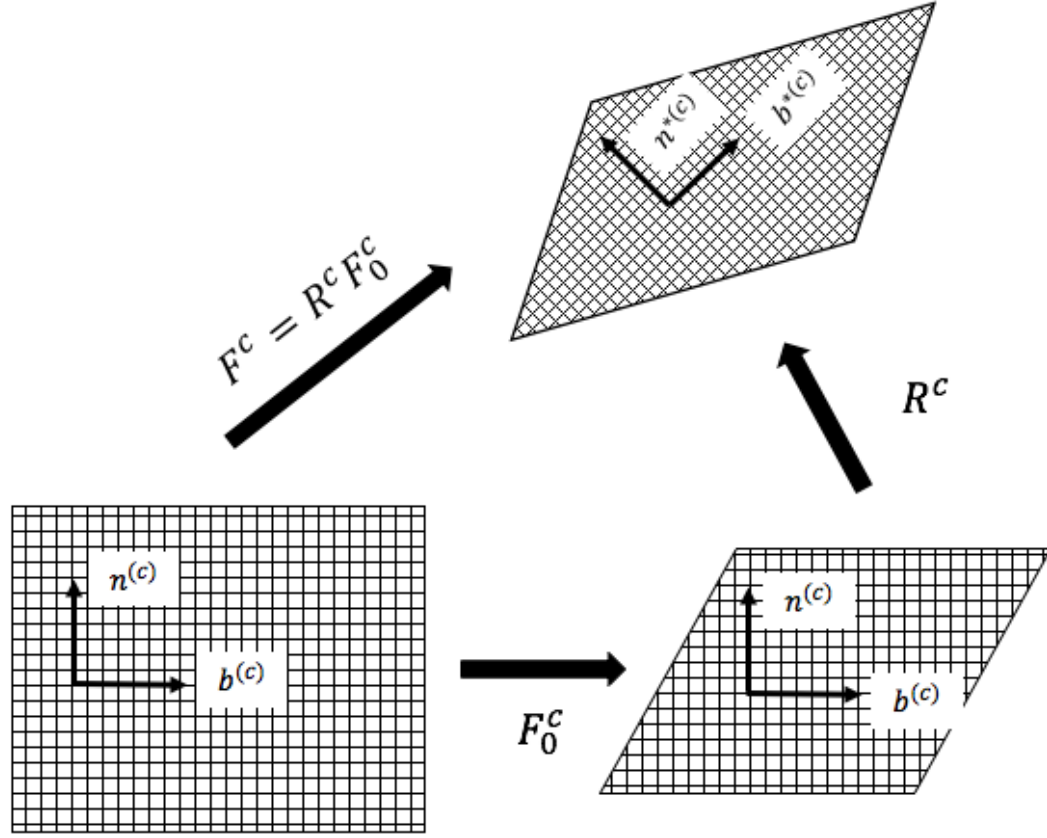


Figure 1: Schematic illustrating the two-step process for a crystal lattice deforming via slip and rotation. F^c is the total deformation gradient of the crystal, while F_0^c and R^c are the plastic and rotation contributions, respectively. Elastic deformation is not considered here. Figure adapted from Asaro [32].

crystals over others. This textured environment leads to an anisotropic composite behavior in the mechanical properties, which further leads to an anisotropic response in the deformation under applied loads and increase in texturing of the material.

2.2.1 Anisotropic Mechanical Response

The VPSC program represents a polycrystalline material in a way such that each grain is

treated as viscoplastic ellipsoidal inclusions in a homogeneous but anisotropic viscoplastic medium. To describe the constitutive behavior of each grain locally in terms of the strain-rate, the phenomenological non-linear rate-sensitively equation is used [24]:

$$\dot{\epsilon}_{ij}(\bar{x}) = \sum_s m_{ij}^s \dot{\gamma}^s(\bar{x}) = \dot{\gamma}_0 \sum_s m_{ij}^s \left(\frac{m_{kl}^s \sigma_{kl}(\bar{x})}{\tau_0^s} \right)^n \quad (8)$$

where $\dot{\gamma}^s(\bar{x})$ is the local shear (or slip) rate on slip system s , $\dot{\gamma}_0$ is a normalization factor, τ_0^s is the threshold stress in the crystal system (or slip resistance), $m_{ij}^s = \frac{1}{2}(n_i^s b_j^s + n_j^s b_i^s)$ is the Schmid tensor for slip system s , $\sigma_{kl}(\bar{x})$ is the applied stress and n is the inverse rate-sensitivity exponent; all values are independent for each crystal. Essentially, the rate of slip can be viewed as the ratio of the applied stress resolved on a specific slip system to the stress needed to activate the slip system to the power n , the inverse of the strain-rate sensitivity. This means that small resolved applied stresses would yield values < 1 and little to no slip activity while larger resolved applied stresses lead to an increase in slip activity for a specific slip system. Increasing values of the inverse of the strain-rate sensitivity parameter, n , magnifies this behavior.

Within the VPSC framework, the constitutive behavior in Equation (8) is linearized within grain (r) (here the viscoplastic ellipsoidal inclusion) as shown in Equation (9) [33, 34]:

$$\dot{\epsilon}_{ij}^{(r)} = M_{ijkl}^{(r)} \sigma_{kl}^{(r)} + \dot{\epsilon}_{ij}^{0(r)} \quad (9)$$

where $M_{ijkl}^{(r)}$ and $\dot{\varepsilon}_{ij}^{0(r)}$ are the crystal system viscoplastic compliance and the back-extrapolated strain-rate term of grain (r) and $\sigma_{kl}^{(r)}$ is the average stress in grain (r). A homogenization process is applied to each grain (r) along with a similar linearization scheme to develop an effective constitutive description of the homogeneous but anisotropic viscoplastic medium [33, 34]:

$$\dot{E}_{ij} = \bar{M}_{ijkl}\Sigma_{kl} + \dot{E}_{ij}^0 \quad (10)$$

where $\bar{M}_{ijkl}$ and $\dot{E}_{ij}^0$ are the macroscopic viscoplastic compliance and back extrapolated strain-rate term, respectively, while $\dot{E}_{ij}$ and Σ_{kl} are the macroscopic strain-rate and stress in the viscoplastic medium. It is this linearization method that ultimately leads to the self-consistency of the VPSC algorithm that relates the local and global constitutive behavior:

$$\bar{M}_{ijkl}\Sigma_{kl} + \dot{E}_{ij}^0 = \langle M_{ijkl}^{(r)} B_{klmn}^{(r)} \rangle \Sigma_{mn} + \langle M_{ijkl}^{(r)} b_{kl}^{(r)} + \dot{\varepsilon}_{ij}^{0(r)} \rangle \quad (11)$$

where $B_{klmn}^{(r)}$ and $b_{kl}^{(r)}$ are stress localization tensors and the brackets represent weighted average behavior over all individual grains. Various linearization schemes have been proposed (secant, tangent, affine and intermediate) that relate to the upper and lower bounds of composite theories, but this work will use the affine linearization scheme as it tends to yield results between the Sachs lower-bound approximation and the Taylor upper-bound approximation [33, 34, 35, 36]. A schematic illustrating the connection of the macro- and microscopic behavior is given in Figure 2.

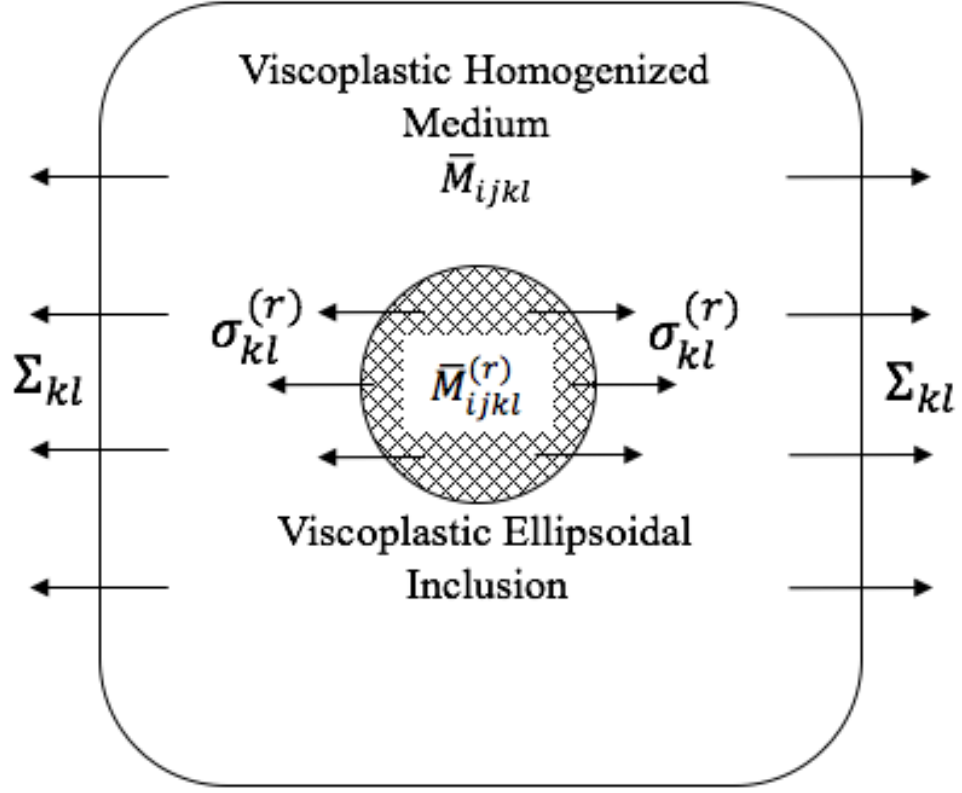


Figure 2: Schematic illustrating a viscoplastic ellipsoidal inclusion (a single crystal grain (r)) embedded in a viscoplastic homogenized medium (a bulk polycrystal). The linearized constitutive behavior of the inclusion is modeled using equation (9) where $\sigma_{kl}^{(r)}$ is the average stress in grain (r) and $\bar{M}_{ijkl}^{(r)}$ is the viscoplastic compliance. The linearized constitutive behavior of the medium is modeled using equation (10) where Σ_{kl} is the macroscopic stress and $\bar{M}_{ijkl}$ is the macroscopic viscoplastic compliance and represents the homogenized, or averaged, behavior of all grains. This averaged medium then affects each grain locally by activating slip modes causing local deformation in each grain. The deformed behavior and stress/strain of each grain is updated leading to a new state of the medium. The entire process is repeated many times. Figure adapted from Hutchinson [34].

A brief description of the core mechanism of the process that leads to the form of Equation (11) is in order and involves the method of eigen-strains [37]. This method equates the microscopic and macroscopic behaviors of Equations (9) and (10) and lumps

the differences into an eigen-strain-rate (sometimes called a polarization or residual) field, allowing for the formation of field equations, the solutions of which are given by convolution integrals using the Green's Function method. A more accurate statement regarding the field equations is that they are no longer a function of the microscopic and macroscopic strain-rates and stresses, but rather they are now a function of the deviations of the microscopic behavior from that of the macroscopic behavior (i.e., the difference). These Green Interaction tensors can be decomposed into symmetric and skew-symmetric components (also called Eshelby Tensors) that relate the eigen-strain-rates to the local deviations in strain-rates within a given grain and rotation-rate deviations of a given grain [24]. These solutions are also intricately tied to $B_{klmn}^{(r)}$ and $b_{kl}^{(r)}$, the stress localization tensors given in Equation (11), and establish the connections between Equations (9) and (10).

To model the hardening behavior, the VPSC program typically uses an extended Voce hardening law to model the evolution of the threshold stress, τ_0^s , in Equation (8) [38]. However, due to the dynamic processing conditions (variable temperatures and strain-rates) and process history dependent behavior that occurs in high-speed machining processes, the Mechanical Threshold Stress model was identified as an alternative constitutive model to the non-linear rate-sensitively equation. Kok et al. developed a MTS based polycrystal plasticity model which is implemented within VPSC and essentially replaces the non-linear rate-sensitively equation [39]. The MTS based polycrystal model is typically presented in the form of Equation (12) that consists of a summation of contributions to the flow stress and is similar in presentation to Equation (1) [7, 11]:

$$\frac{\tau}{\mu} = \frac{\tau_a}{\mu} + S_i(\dot{\epsilon}, T) \frac{\hat{\tau}_i}{\mu_0} + S_d(\dot{\epsilon}, T) \frac{\hat{\tau}_d}{\mu_0} \quad (12)$$

where τ_a , $\hat{\tau}_i$ and $\hat{\tau}_d$ are now the athermal contribution to the flow stress and the mechanical threshold stress and strain hardening contributions of the mechanical threshold stress at the single crystal level, respectively, and all other factors retain their previous definitions. As the MTS based polycrystal model only modifies the constitutive description and threshold stress evolution, the previously discussed homogenization and self-consistent approach remains unaltered.

2.2.2 Texture Evolution

Continuum mechanics treats the displacement of a crystal as a two-step sequential process (c.f. Figure 2 above): a plastic stretch (or distortion) of the crystal followed by a rigid roagation (again, the elastic deformation is not considered here). The VPSC program uses the same process to calculate both grain rotations and grain shape changes. Both processes are dependent on the values of the velocity gradient input into the program which are decomposed into a strain-rate and a rotation rate. For the purposes of texture evolution in the VPSC program, this discussion shall be limited to the rotation tensor, R^c , from Equation (7). To determine the rate of change of the crystal orientation matrix, ultimately leading to an update orientation of the crystal, the VPSC program uses the following equation [40]:

$$\dot{R}^c = (W^c - W_0^{c,R})R^c = \dot{\Omega}R^c \quad (13)$$

where $\dot{R}^c$ is the rate of change of the crystal orientation matrix, R^c is the rotation orientation tensor, W^c is the rotation rate (rather, the skew symmetric component of the velocity

gradient) in the current frame, $W_0^{c,R}$ is the rotation rate within the crystal frame, and $\dot{\Omega}$ can be thought of as a lattice spin. An assumption is made regarding the tensor $\dot{\Omega}$, namely that it is constant within small time increments, leading to (upon a non-trivial integration of Equation (13)):

$$R^c(t + \Delta t) = R^c(t) \exp(\Omega) \quad (14)$$

where $\exp(\Omega)$ is the Rodrigues' equation and is used to transform the current crystal orientation at step (t) to a new orientation at step $(t + \Delta t)$. Rodrigues' equation is used within the VPSC program in the form [41]:

$$\exp(\Omega) = I + \hat{\Omega} \sin \omega + \hat{\Omega}^2 (1 - \cos \omega) \quad (15)$$

where ω is a finite angle of rotation around a rotation axis $\hat{\Omega}$, which itself is a skew symmetric tensor comprised of the normalized vector components of the finite angle of rotation. At this point, it is worth noting that the skew-symmetric component of the Green Interaction tensor discussed in the previous section is the deviation of the rotation-rate, which is used to determine ω . Thus, the VPSC program, uses an iterative approach to update the rotation of each crystal through the calculation of ω at each step of the simulation. [33].

CHAPTER 3. MODIFICATION OF THE MTS MODEL

In this work, some of the parameters derived by Follansbee and Gray are retained, but modifications will be made to the others as necessary to fit the experimental data by Lee and Lin; specifically, the athermal stress component $\sigma_a = 100$ MPa and mechanical threshold stress constant reference strain-rate $\dot{\epsilon}_{0i} = 10^{10} \text{ s}^{-1}$ are kept [11]. Follansbee and Gray also implemented an approach to separate the mechanical threshold stress terms into one term which addresses short range dislocation interactions and an additional term to address dislocation-solute interactions. This approach is not taken here and one mechanical threshold stress term is utilized. Additionally, Follansbee and Gray's parameters for Equation (2) above are utilized as well: $\mu_0 = 49,020$ MPa, $a = 4355$ MPa and $T_0 = 198$ K [11]. The first step towards calibrating the MTS model to the experimental data entails plotting the experimental yield stress data as a function of strain-rate and temperature using Equation (3) with a rearranged version of Equation (1):

$$\left(\frac{\sigma - \sigma_a}{\mu}\right)^{p_i} = \left(\frac{\hat{\sigma}_i}{\mu_0}\right)^{p_i} - \left(\frac{\hat{\sigma}_i}{\mu_0}\right)^{p_i} \cdot \left(\frac{1}{g_{oi}}\right)^{1/q_i} \cdot \left[\frac{kT}{\mu b^3} \ln\left(\frac{\dot{\epsilon}_{0i}}{\dot{\epsilon}}\right)\right]^{1/q_i} \quad (16)$$

This initial step does not include the hardening parameters and only seeks to linearize the experimental yield stress data in order to find the mechanical threshold stress, $\hat{\sigma}_i$, and the mechanical threshold stress normalized barrier activation energy, g_{oi} , using the plot intercept and slope, respectively. Ideally, all of the experimental yield data would fall on a single linear plot, where the mechanical threshold stress would be found via an extrapolation back to a temperature of 0 K (i.e., the intercept with the ordinate axis).

However, in this particular data set, the mechanical threshold stress constant reference strain-rate, $\dot{\epsilon}_{0i}$, needs to be on the order of 10^4 - 10^5 s⁻¹ to properly linearize the data. This is undesirable as small $\dot{\epsilon}_{0i}$ values can set a lower bound on the strain-rates that can be used within the MTS model, especially at higher temperatures.

Because Equation (7) is a function of temperature and strain-rate, there are two approaches that can be taken going forward. The first would plot the experimental yield stress as a function of strain-rate at constant temperatures while the second approach would plot the data as a function of temperature at constant strain-rates. Figure 1 (a) shows the plot of the experimental yield stress data for the first approach, while Figure 1 (b) shows the plot for the second approach; the data for strain-rates of 400, 450, 2700 and 3300 s⁻¹ where not included in Figure 1 (b) as only one data point exists for each of these strain-rates. From both figures, it is obvious that the yield stress data shifts either as a function of temperature or strain-rate, leading to values of $\hat{\sigma}_i$ and g_{oi} that are dependent on temperature or strain-rate (or both). In this work, the second approach is utilized as it allows for the extrapolation of the mechanical threshold stress term to a temperature of 0 K for each strain-rate. For a discussion regarding the thermally activated flow stress, the reader is referred to Nemat-Nasser et al. [42]. Additionally, values of $p_i = 2/3$ and $q_i = 1$ are used to model the mechanical threshold stress barrier shape.

Plotting the experimental yield stress for constant strain-rate leads to Figures 2 (a)-(e) where a linear fit of each plot yields the slope and intercept and subsequently a value of $\hat{\sigma}_i$ and g_{oi} . From Equation (7) the value of $\hat{\sigma}_i$ is found from:

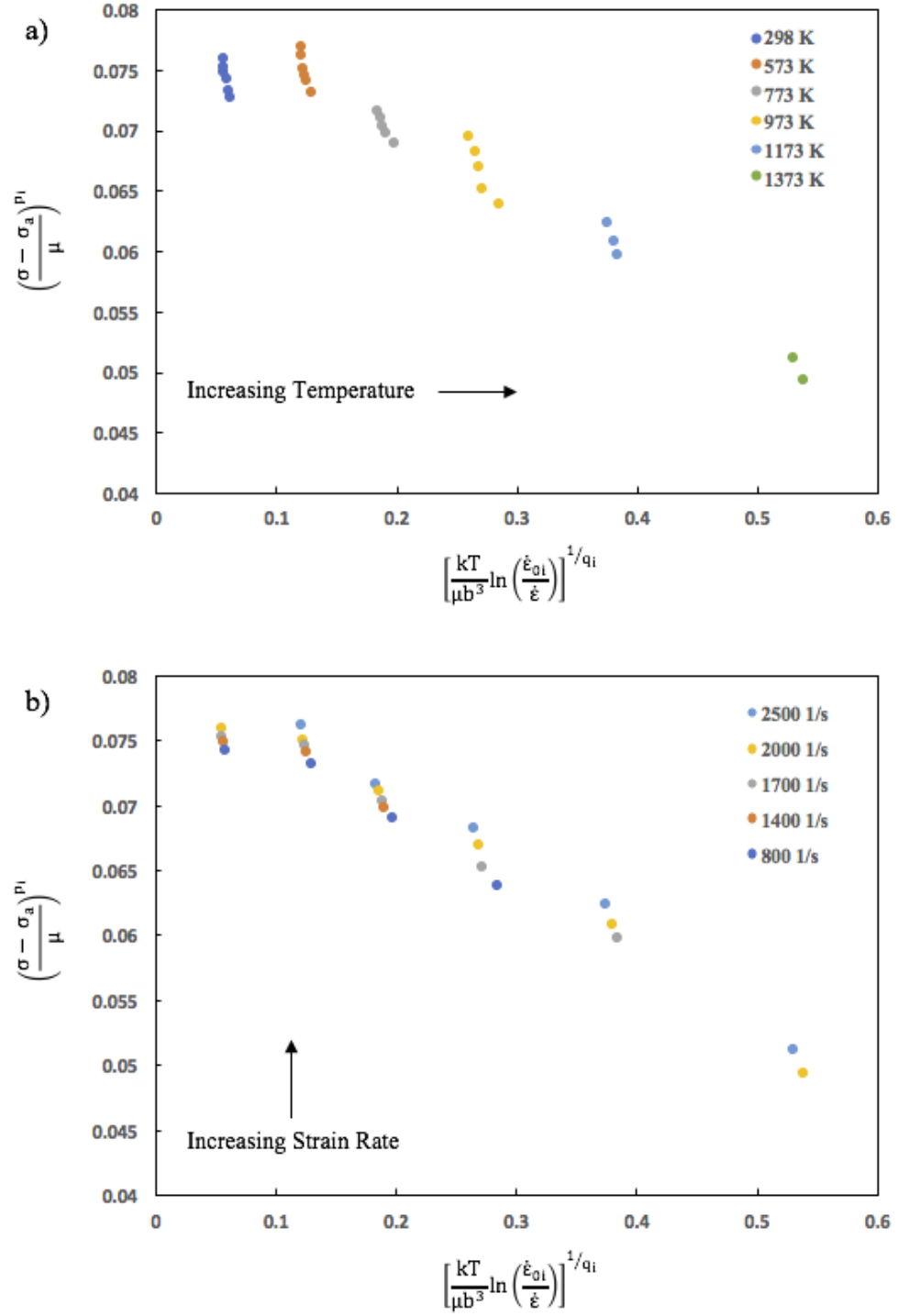


Figure 3: Experimental yield stress data plotted using Equation (7) for a) constant temperature and b) constant strain-rate.

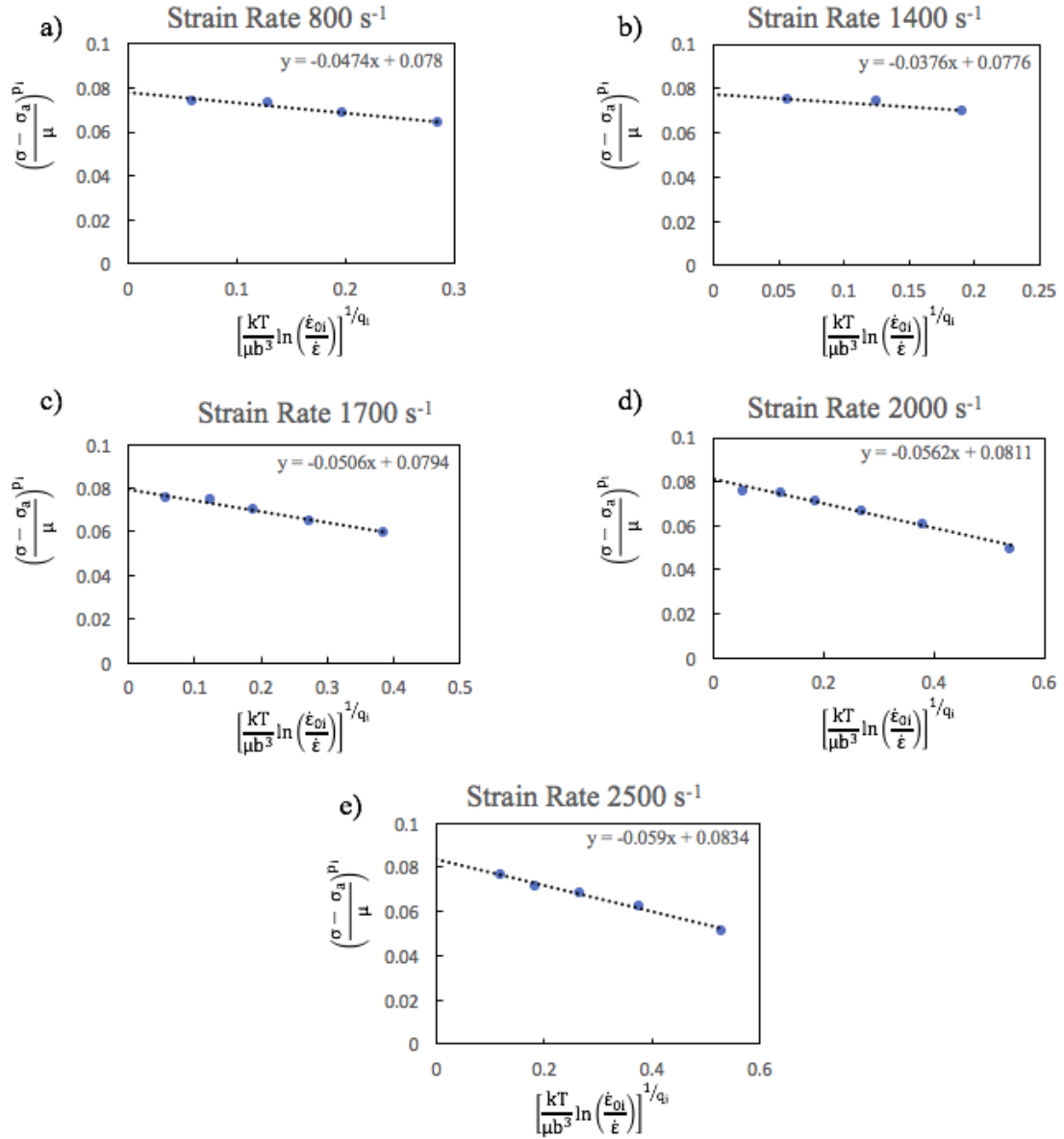


Figure 4: Experimental yield stress data plotted using Equation (7) for each individual strain-rate with linear fit. The intercepts allow for the calculation of the mechanical threshold stress, $\hat{\sigma}_i$, while the slope allows for the calculation of the mechanical threshold stress normalized barrier activation energy, g_{oi} .

$$\hat{\sigma}_i = \mu_0 \cdot (intercept)^{1/p_i} \quad (17)$$

and the value of g_{oi} is found from:

$$g_{oi} = \left(\left(\frac{-1}{slope} \right) \cdot \left(\frac{\hat{\sigma}_i}{\mu_0} \right)^{p_i} \right)^{q_i} \quad (18)$$

The calculated values for $\hat{\sigma}_i$ and g_{oi} are given in Table 1 and are plotted on a semi-log plot of the strain-rates in Figures 3 and 4. From the calculated values of $\hat{\sigma}_i$ and g_{oi} , two trends are found.

Table 1: Calculated values of $\hat{\sigma}_i$ and g_{oi} obtained from Equations (17) and (18)

Strain-rate (s ⁻¹)	$\hat{\sigma}_i$ (MPa)	g_{oi} (J)
800	1067.86	1.65
1400	1059.66	2.06
1700	1096.74	1.57
2000	1132.15	1.44
2500	1180.65	1.41

First, as the strain-rate increases, the value of g_{oi} appears to linearly decrease (slightly), with the exception of the point at a strain-rate of 1400 s⁻¹. The experimental data at 1400 s⁻¹ is limited (c.f. Figure 3 (b)) and it is believed that the data available does not provide as reliable a trend with respect to measurements made at other strain-rates. Indeed,

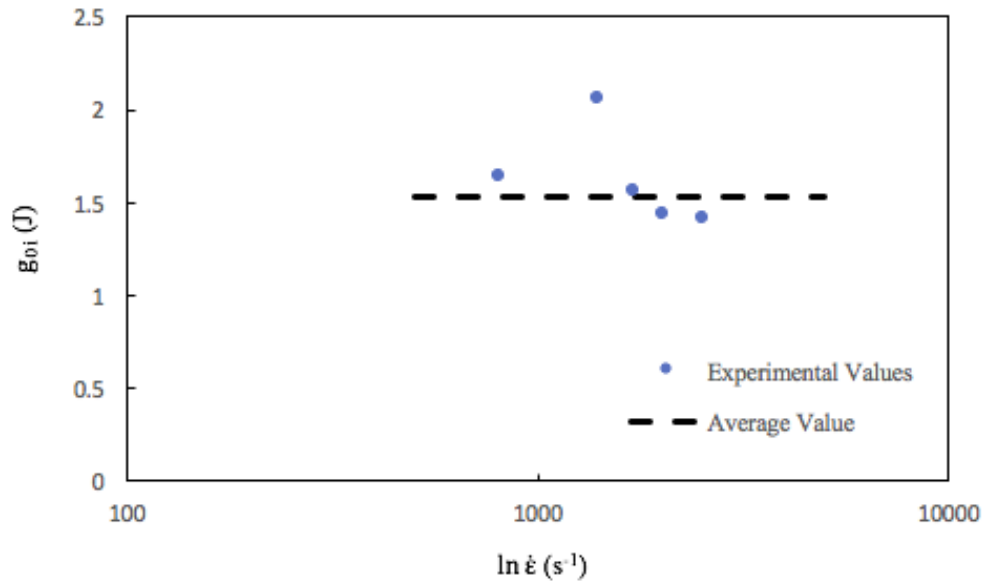


Figure 5: Plot of the mechanical threshold stress normalized barrier activation energy as a function of the natural-log of the strain-rate. With the exception of the value at 1400 s^{-1} , the values are found to slightly decrease as a function of strain-rate, but can be approximated as a constant of the average value.

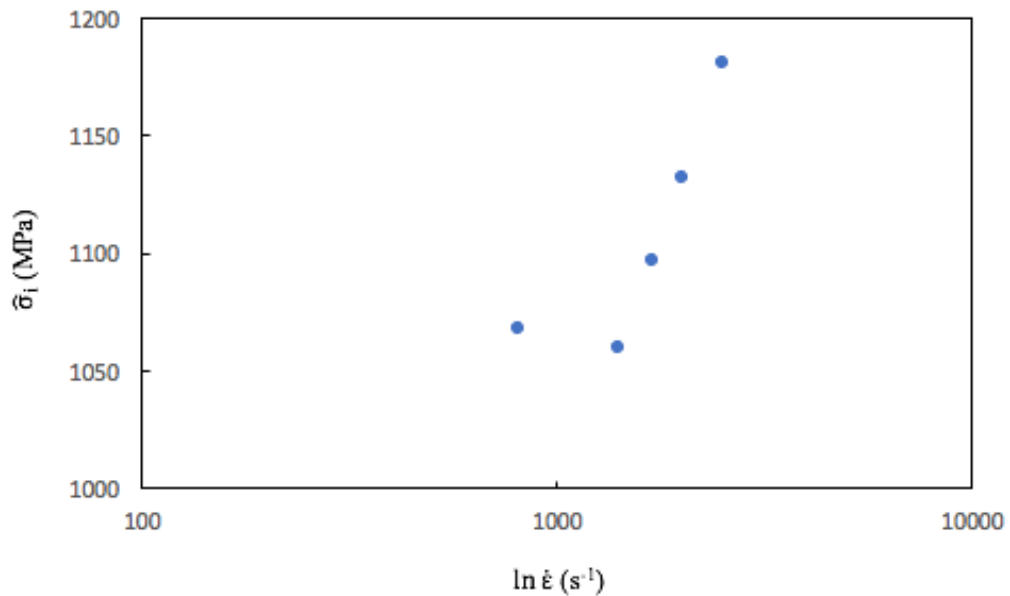


Figure 6: Plot of the mechanical threshold stress as a function of the natural-log of the strain-rate. The results show signs of an increasingly strong dependence on strain-rate such as found in high strain-rate experiments.

it appears to over predict a value of g_{oi} and under predict a value of $\hat{\sigma}_i$. Because of this, and because the decrease in g_{oi} with increasing strain-rate is only slight, an average value is taken over the values of g_{oi} (disregarding the value at 1400 s^{-1}) yielding $\sim 1.53 \text{ J}$. Figure 3 shows this constant value relative to the calculated values of g_{oi} and appears to be a good fit.

Secondly, as the strain-rate increases, the value of $\hat{\sigma}_i$ appears to increase at an increasing rate. This type of behavior (“hockey-stick” behavior for lack of a better term), has been well documented in high strain-rate measurements of the yield (and flow) stress as a function of strain-rate where the deformation controlling mechanism transitions from thermal activation to drag mechanisms [13]. However, from the definition of the threshold stress (i.e. the flow stress at 0 K), a dependency of the threshold stress on strain-rate should be taboo. The MTS model does well modeling the flow stress behavior over a wide range of temperatures and strain-rates, but in its current form, with a constant mechanical threshold stress, it is unable to model the behavior at high strain-rates where drag mechanisms begin; the current formulation would continue forward with a linear increase, greatly under predicting the flow stress behavior at higher strain-rates.

3.1 Extension to High Strain-Rate

A particularly nice solution to this problem is adapted from Follansbee and Kocks’ original work that is used to model the work-hardening rate as a function of strain-rate [7]. To model the behavior of the mechanical threshold stress, the following empirical formula is used:

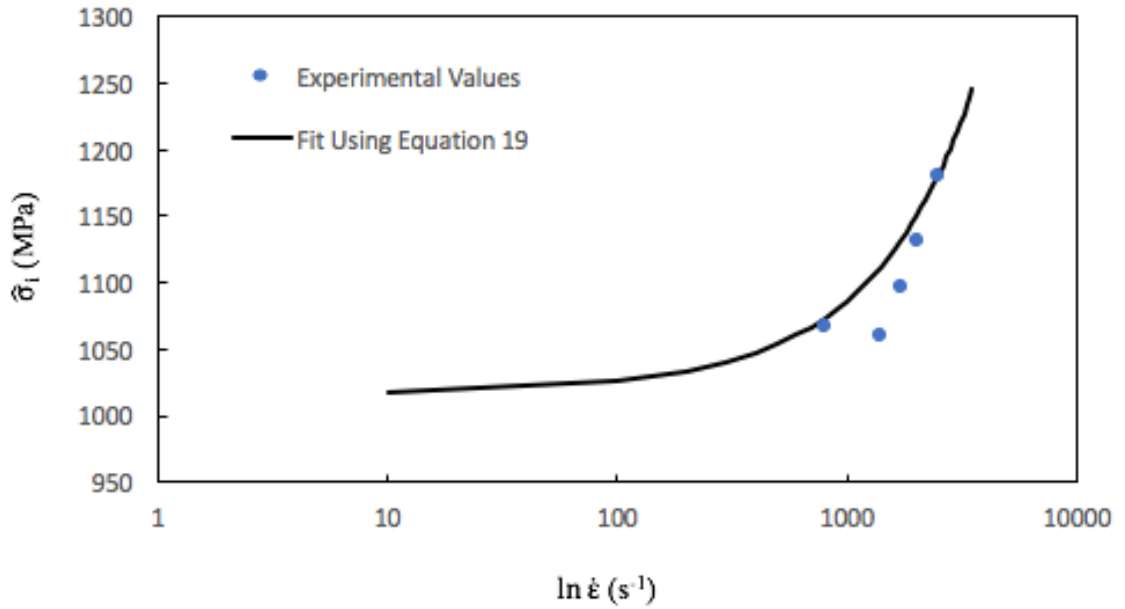


Figure 7: Plot of the mechanical threshold stress as a function of the natural-log of the strain-rate as compared with the model in Equation (19). The fit is quite remarkable and allows for a more accurate prediction of the yield stress behavior as a function of strain-rate.

$$\hat{\sigma}_i(MPa) = a + b \ln(\dot{\epsilon}) + c\dot{\epsilon} \quad (19)$$

where a , b and c are empirical constants and $\dot{\epsilon}$ is the strain-rate. Though not part of the current work, it is noted that these constants could also be a function of temperature to handle any temperature dependencies of the mechanical threshold stress. Indeed, this formulation gives the expected “hockey-stick” behavior with a linearly increasing value of $\hat{\sigma}_i$ at lower strain-rates and transitioning to an exponential increase at higher strain-rates. Figure 5 shows both the experimentally derived values of $\hat{\sigma}_i$ plotted using Equation (10) with values of $a = 1015$, $b = 1.2$ and $c = 0.063$. With the exception of the value of $\hat{\sigma}_i$ at 1400 s^{-1} , the fit works quite well.

While these parameters work well with the experimentally derived values of $\hat{\sigma}_i$, more optimized values were used to model the experimental yield stress behavior: $a = 1012$, $b = 0.94$ and $c = 0.04$. A comparison of the experimental yield stresses and the MTS model (sans hardening terms) with constant and modified mechanical threshold stress as a function of strain-rate is given in Figure 6. For the constant mechanical threshold stress, an averaged value of the values given in Table 1 is used: $\hat{\sigma}_i = 1107.41$ MPa. The MTS model using the modified mechanical threshold stress value yields a noticeably better fit for the experimental yield stress values and gives the expected “hockey-stick” behavior that has been noted in experimental literature [13]. It is also shown that without using a modified mechanical threshold stress, the MTS model would continue predicting a linear increase in yield stress behavior for higher strain-rates. Although the experimental data used is limited and other reported data may widely vary, this procedure should quite easily and reliably allow for (with appropriate experimental data in the transition range) the extension of the MTS model to the high strain-rate regime.

Such a modification of the mechanical threshold stress (temperature and strain-rate dependencies) would certainly appear to run afoul with its very definition. This may very well be true for pure substances or single-phase materials, but multiphase materials (such as Ti-6Al-4V) do often change volume fractions of phases or nucleate additional phases as a function of temperature (and pressure). It is possible that this behavior is purely a consequence of treating the system as a homogenized medium and a non-constant mechanical threshold stress manifests itself due to this homogenization. It is not the intent of this work to ascribe a physical interpretation or meaning to Equation (10), but to simply

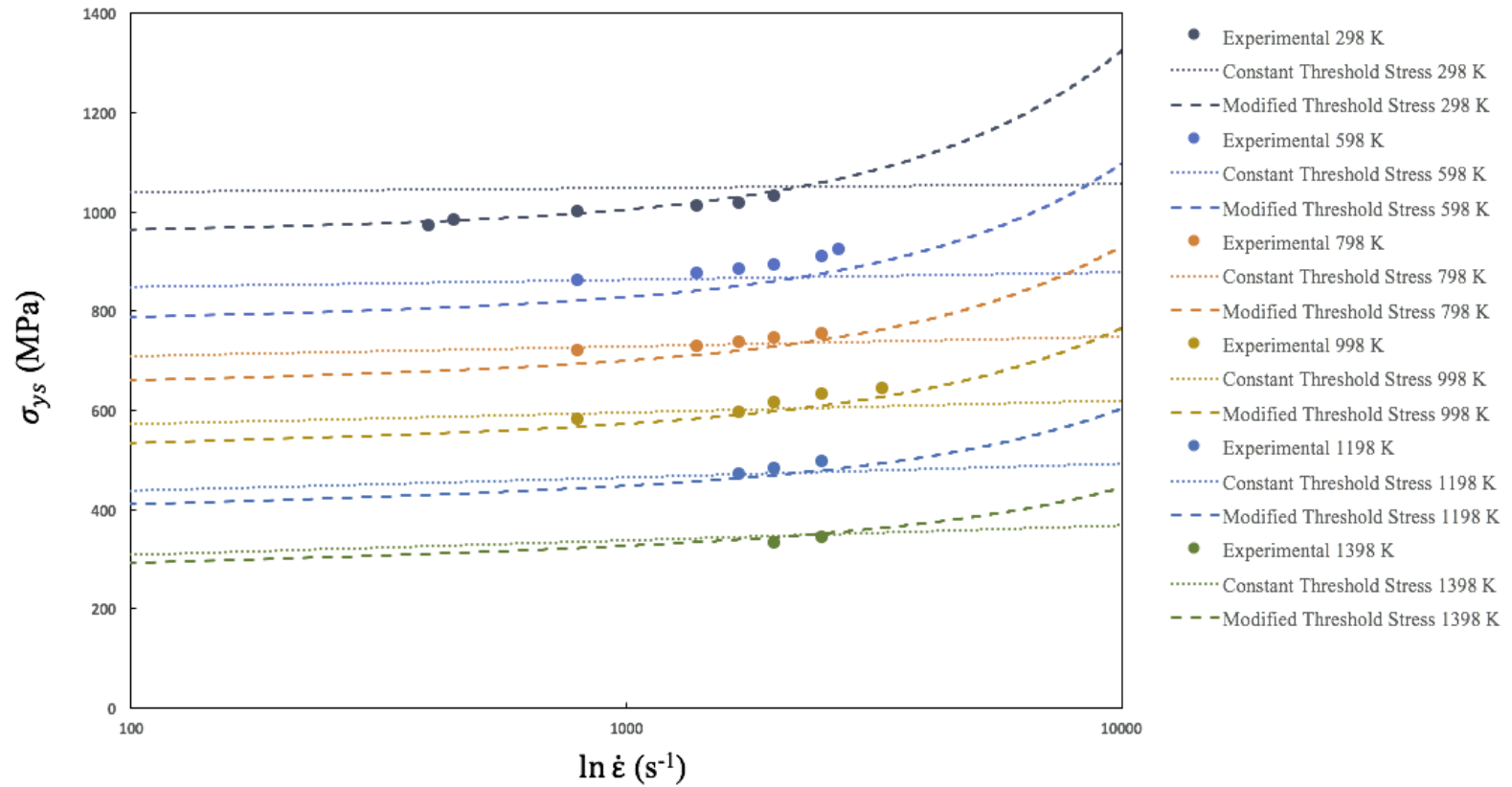


Figure 8: Plot of the experimental yield stress data and the MTS model with and without the modified threshold stress. The modified threshold stress yields the expected “hockey-stick” behavior that has been noted in experimental literature whereas the constant threshold stress yields only a linearly increasing behavior.

state that it is a convenient mathematical tool to extend the behavior of the MTS model to higher strain-rates.

3.2 Correction to Initial Work-Hardening Rate

To complete the MTS calibration, parameters for Equations (4)-(6) relating to the plastic deformation (flow stress evolution) portion of the model are needed. In this work, because limited data is available for fitting the hardening portion of the MTS model, the work-hardening rate parameter and saturation stress values are simply fitted to the experimental data using Equations (5) and (6). For practical purposes, Equation (6) is used in its integrated form where a value of 1 is used for κ :

$$\hat{\sigma}_d = \hat{\sigma}_{ds} \left[1 - \exp\left(\frac{-\theta_0 \cdot \varepsilon}{\hat{\sigma}_{ds}}\right) \right] \quad (20)$$

Typically, the work-hardening rate parameter, θ_0 , is taken as a constant value, though it has been modeled as a function of temperature and/or strain-rate [43]. In this work, the work-hardening rate parameter is modeled as an exponential function of strain in order to capture the rapid decay of an initially high work-hardening rate to one of a lower constant value as strain increases and is used as a post integrating factor in Equation (20). This has the benefit of better modeling the initial hardening region and transitioning to a constant work-hardening parameter that is more commonly used within the MTS model. The model used here is given by:

$$\theta_0(MPa) = l \cdot [\exp(-\varepsilon)]^n + m \quad (21)$$

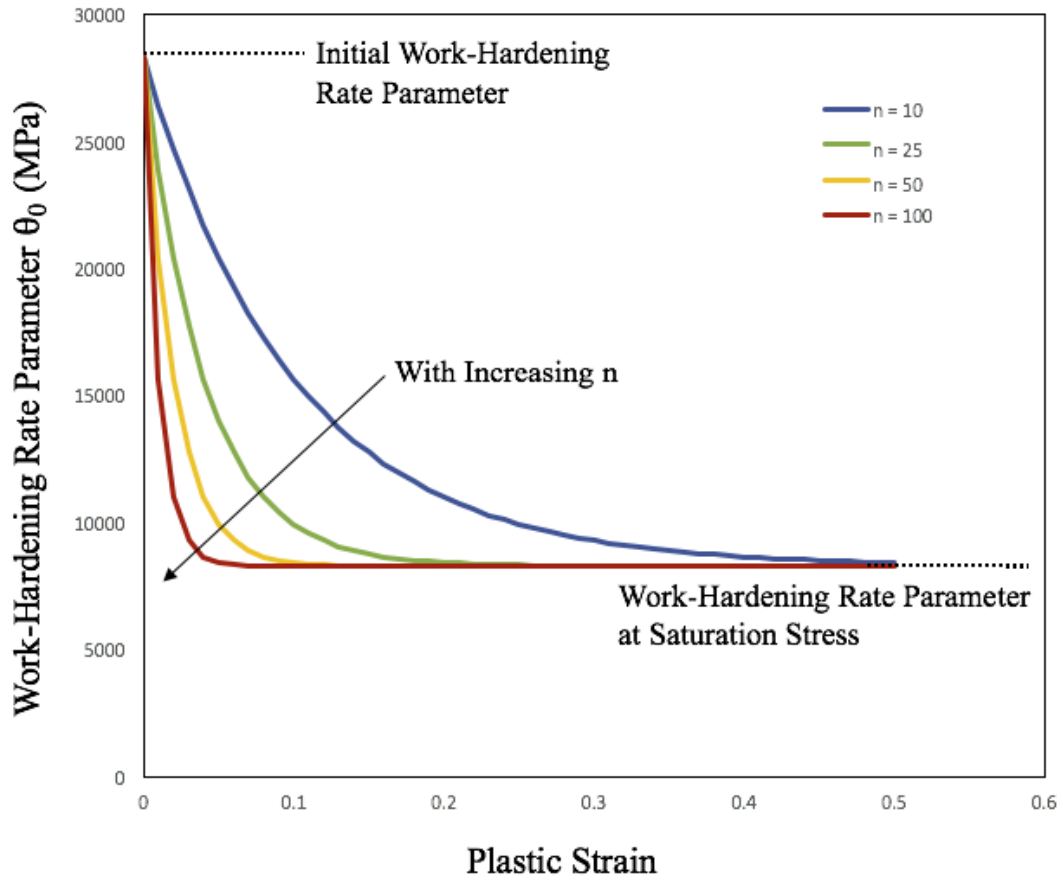


Figure 9: Plot of the work-hardening rate parameter, θ_0 , as a function of strain with $l = 20,000$ MPa and $m = 8300$ MPa for $n = 10, 25, 50$ and 100 . The initial parameter l is large and can approach values on the order of the Elastic Modulus while the value m represents the value of the work-hardening rate parameter when saturation stress is reached. The value n controls the rate of decay of the initial value to the value at saturation stress.

where l is the initial work-hardening rate parameter at yield, m is the constant work-hardening rate parameter in the Stage III region, n is a constant that fits the decay rate and ε is the plastic strain. In this model, $l = 20,000$ MPa, $m = 8300$ MPa (Follansbee and Gray's value is given as 2721 MPa), and $n = 30$ [11]. A plot of Equation (21) with $l = 20,000$ MPa and $m = 8300$ MPa for $n = 10, 25, 50$ and 100 is given in Figure 9.

A few comments are made regarding the hardening parameters to highlight differences between this work and the work of Follansbee and Gray. The work-hardening rate, θ_0 , presented in above is much higher than that used in Follansbee and Gray's work. Their approach uses a value based on the work of Kocks that finds that the initial work-hardening rate in the Stage III region should have a value between 1/20 to 1/15 of the shear modulus and is temperature and strain-rate independent [23]. Kocks' conclusions on the work-hardening rate treats the portion of the stress-strain curve dealing with a constant saturation stress for a given temperature and strain-rate, though he conjectures that adjustments to his model may be needed for alloys (or more complicated systems) [23]. This method, though physics based, tends to severely underestimate the initial work-hardening rate, post-yield, and does not capture the transient behavior towards a steady state work-hardening rate in the Stage III region. A review of Follansbee and Gray's MTS parameters for Ti-6Al-4V appears to follow suit and back extrapolate the flow stress to the point of yield using a constant work-hardening rate, thus over predicting the flow stress at yield and post yield up to the point of constant saturation stress [11].

The parameters for the modified work-hardening parameters are not derived and are merely fitted to the experimental data. All of the parameters for the macroscopic MTS model described thus far for the high strain-rate behavior of Ti-6Al-4V are given in Table 2 and span Equations (1), (2), (3), (4), (6), (19), (20) and (21). Experimental stress-strain data and the MTS model predictions are given in Figures 7, 8 and 9 for temperatures ranging from 298-1373 K and strain-rates from 1700-2500 s⁻¹ with the maximum percent error being ~4.53 % for a temperature of 1373 K and a strain-rate of 2000 s⁻¹; tables comparing all reported experimental data points with the macroscopic MTS results and

their associated percent errors are found in Appendix A.1. Although this improved work-hardening rate parameter captures the experimental behavior in the transient work-hardening region quite well (c.f. Lee and Lin [20]), it is still inadequate to fully describe the initial hardening post yield and shows that more work is needed in this area.

Table 2: Macroscopic MTS model parameters used for high strain-rate behavior of Ti-6Al-4V

σ_a	100 MPa	μ_0	49020 MPa
$\hat{\sigma}_i$	$1012 + 0.94 \ln(\dot{\epsilon}) + 0.04 \cdot \dot{\epsilon}$ MPa	a	4355 MPa
g_{oi}	1.53 J	T_0	198 K
$\dot{\epsilon}_{oi}$	$1 \times 10^{10} \text{ s}^{-1}$	θ_0	$20000(\exp(-\epsilon))^{30} + 8300$ MPa
p_i	2/3	σ_{ds0}	590 MPa
q_i	1.0	g_{ds0}	2 J
g_{od}	1.6 J	$\dot{\epsilon}_{ds0}$	$1 \times 10^7 \text{ s}^{-1}$
$\dot{\epsilon}_{od}$	$1 \times 10^7 \text{ s}^{-1}$	κ	1
p_d	2/3	k_b	$1.38062 \times 10^{-23} \text{ J/K}$
q_d	1.0	b	$2.96 \times 10^{-10} \text{ m}$

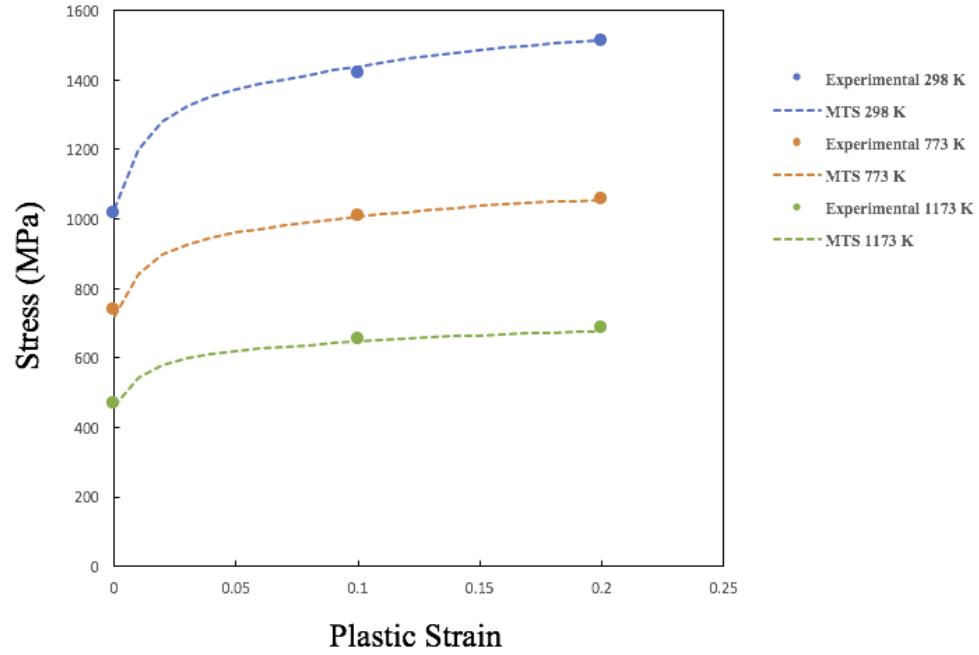


Figure 10: Comparison of the experimental flow stress behavior and the macroscopic MTS predicted behavior for a strain-rate of 1700 s^{-1} and temperatures ranging from 298–1173 K.

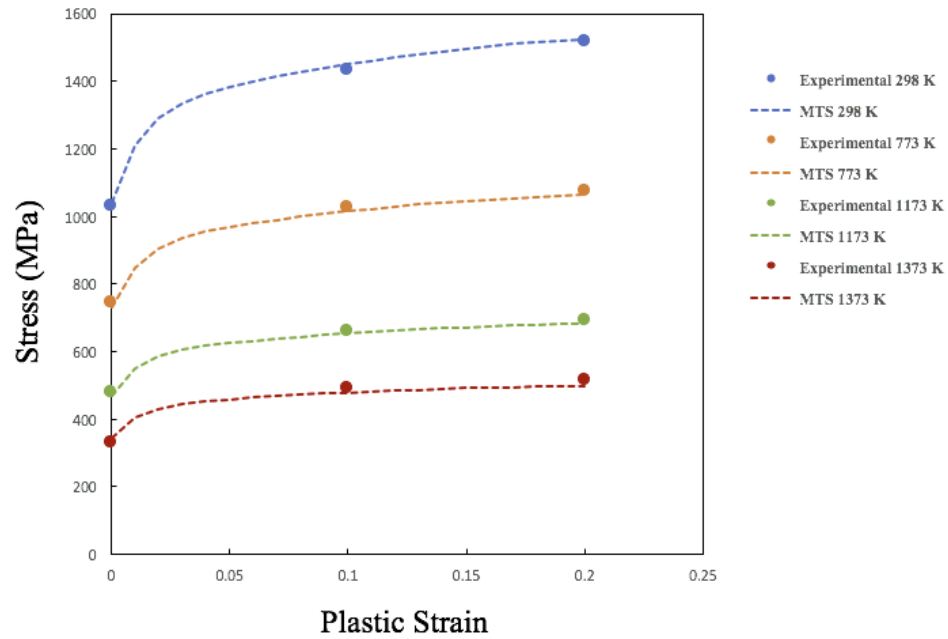


Figure 11: Comparison of the experimental flow stress behavior and the macroscopic MTS predicted behavior for a strain-rate of 2000 s^{-1} and temperatures ranging from 298–1373 K.

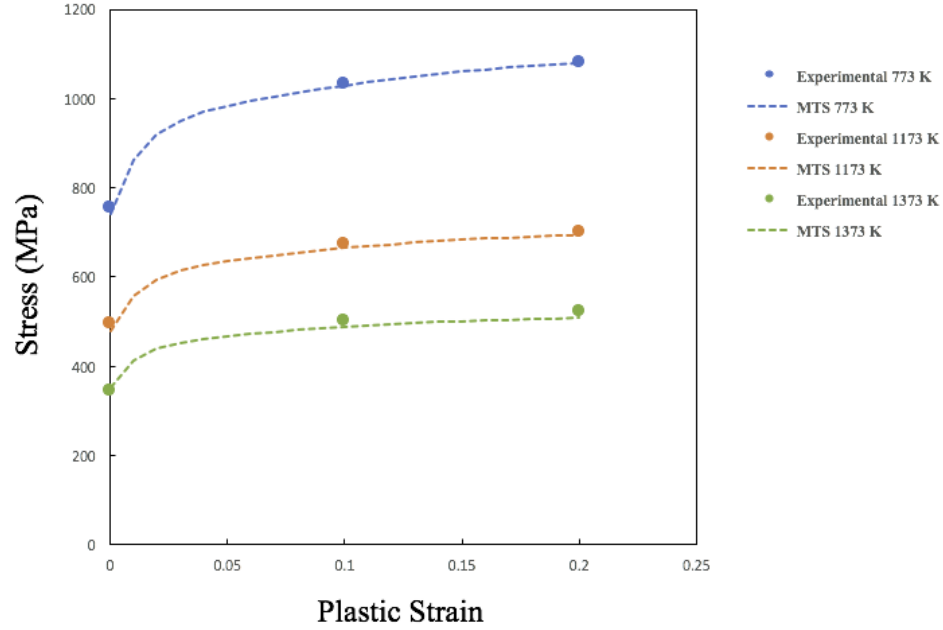


Figure 12: Comparison of the experimental flow stress behavior and the macroscopic MTS predicted behavior for a strain-rate of 2500 s^{-1} and temperatures ranging from 773–1373 K.

3.3 Summary

An alternative approach to fitting the mechanical threshold stress within the MTS model is examined using experimental data at the cusp of the transition region where the deformation controlling mechanism transitions from thermal activation to drag mechanisms. It is found that fitting the mechanical threshold stress as a function of strain-rate can lead to the “hockey-stick” behavior (linear behavior at low strain-rates and exponentially increasing behavior at high strain-rates) of the yield stress as a function of strain-rate typically found in many high strain-rate experiments. This approach, while having no physical basis, is a convenient mathematical tool to extend the MTS model to the high strain-rate regime, provided experimental data exists. Additionally, the work-hardening model developed by Kocks and used in conjunction with the MTS model is

critiqued and a strain dependent work-hardening rate is introduced. It is found that this mathematically fitted work-hardening rate provides a more realistic fit to the experimental data in the early stages of hardening post yield, though it is concluded that more work is necessary to model the transient work-hardening behavior. Finally, it is stressed that a constitutive model of this type (more generally any constitutive model) typically cannot be used universally due to variations in experimental data and microstructural features and should be applied to material systems on a case by case basis, though more universal applicability may occur in pure or single-phase systems.

CHAPTER 4. SINGLE-PHASE VPSC MTS MODEL

The VPSC model has shown great predictive capability for determining the stress-strain behavior of anisotropic single-phase polycrystalline materials using the non-linear rate-sensitivity equation in, Equation (8), in conjunction with a threshold stress modeled by an extended Voce hardening law [24, 44, 45]. Less work has been conducted on single-phase polycrystalline materials using the MTS to model the threshold stress, let alone work conducted on two-phase materials. In this section, the application of the VPSC model to the Ti-6Al-4V system is investigated using the previously modified MTS model as the constitutive hardening law. The work in this section is intended only as an intermediate step to test the robustness of the MTS model within the VPSC program before transitioning to a full two phase model.

To test the MTS model, the system is treated as a hypothetical single-phase hcp polycrystalline material, at all temperatures and strain-rates, where each crystal is treated as a separate grain with a unique orientation. While the specific type of slip systems to be used in plasticity simulations for hcp systems has been debated and various parameters have been given for Ti-6Al-4V, the $\{0001\}\langle 11\bar{2}0 \rangle$ Basal $\langle a \rangle$ (with 3 modes), $\{10\bar{1}0\}\langle 11\bar{2}0 \rangle$ Prismatic $\langle a \rangle$ (with 3 modes), $\{10\bar{1}1\}\langle 11\bar{2}0 \rangle$ 1st order Pyramidal $\langle a \rangle$ (with 6 modes), $\{10\bar{1}1\}\langle 11\bar{2}3 \rangle$ 1st order Pyramidal $\langle c+a \rangle$ (with 12 modes) and $\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$ 2nd order Pyramidal $\langle c+a \rangle$ (with 6 modes) slip systems are used here [46, 47, 48]. A schematic of the various hcp slip systems used is given in Figure 13. Another item to note is that, for the hypothetical single-phase model, the same MTS parameters are used for each slip system and homothetic hardening (or, the same hardening rate) is used

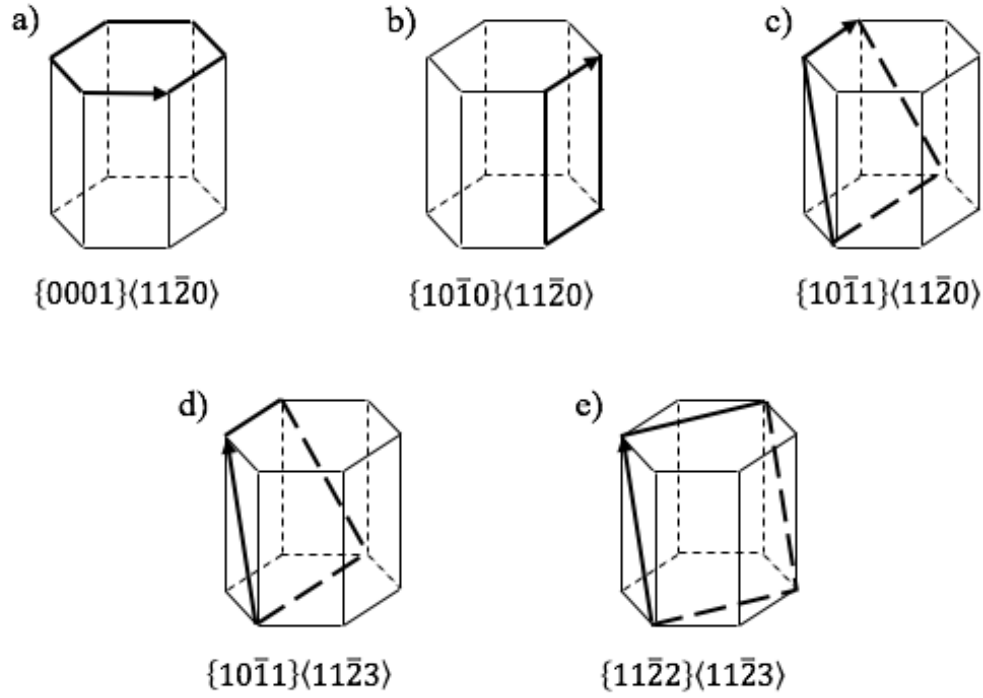


Figure 13: Representation of five common slip systems found in hcp materials: a) the $\{0001\}\{11\bar{2}0\}$ Basal $\langle a \rangle$ (with 3 modes), b) $\{10\bar{1}0\}\{11\bar{2}0\}$ Prismatic $\langle a \rangle$ (with 3 modes), c) $\{10\bar{1}1\}\{11\bar{2}0\}$ 1st order Pyramidal $\langle a \rangle$ (with 6 modes), d) $\{10\bar{1}1\}\{11\bar{2}3\}$ 1st order Pyramidal $\langle c+a \rangle$ (with 12 modes) and e) $\{11\bar{2}2\}\{11\bar{2}3\}$ 2nd order Pyramidal $\langle c+a \rangle$ (with 6 modes) slip systems.

throughout to 1) ease the calibration process and 2) because of the lack of single crystal stress-strain data surrounding each individual slip system. While it is well established that the critical resolved shear stress (CRSS) varies with the different slip systems, the procedure used here is solely to develop a single crystal MTS model that will be later extended [49].

The first step in this process requires the re-scaling of the macroscopic MTS model into a shear stress model at the single crystal level; a reminder that here that the symbol σ is taken as the application to a macroscopic polycrystalline system whereas the symbol τ is taken as the application to a single crystal system. To do this, VPSC was run using 10,000

randomly generated orientations (random texture) and the macroscopic MTS parameters listed in Table 2 to determine the scaling difference between the two models. Simulations were carried out in compression using an equivalent Von Mises strain measure and an average scaling factor (Taylor Factor) of ~ 2.17 was found between the yield strengths of the VPSC simulations and those of their respective input MTS models. This value appears to be close to values reported in the literature for hcp systems [50, 51, 52]. The MTS model, as shown in Equation (1), along with the integrated form of the modified Voce hardening law in Equation (20) scale quite easily with only the athermal stress σ_a , the mechanical threshold stress $\hat{\sigma}_i$ and the saturation stress $\sigma_{\varepsilon s0}$ needing to be divided by the scaling factor. The work-hardening rate parameter was also adjusted to account for the difference in hardening rates between the macroscopic and single crystal models, and was fitted as it is

Table 3: Single crystal MTS model parameters used within the VPSC program for high strain-rate behavior of a hypothetical single-phase HCP Ti-6Al-4V system

τ_a	46.1 MPa	μ_0	49020 MPa
$\hat{\tau}_i$	$466.4 + 0.43 \ln(\dot{\varepsilon}) + 0.018 \cdot \varepsilon$ MPa	a	4355 MPa
g_{oi}	1.53 J	T_0	198 K
$\dot{\varepsilon}_{0i}$	$1 \times 10^{10} \text{ s}^{-1}$	θ_0	$12000(\exp(-\varepsilon))^{50} + 1300$ MPa
p_i	2/3	τ_{ds0}	272.88 MPa
q_i	1.0	g_{ds0}	2 J
g_{od}	1.6 J	$\dot{\varepsilon}_{ds0}$	$1 \times 10^7 \text{ s}^{-1}$
$\dot{\varepsilon}_{0d}$	$1 \times 10^7 \text{ s}^{-1}$	κ	1
p_d	2/3	k_b	$1.38062 \times 10^{-23} \text{ J/K}$
q_d	1.0	b	$2.96 \times 10^{-10} \text{ m}$

within a non-linear relation and is unaffected by the scaling factor. The parameters for the single crystal MTS model are given in Table 3 below.

4.1 Results

With the single crystal MTS model calibrated, VPSC was then re-run under the various compression loading conditions (temperatures and strain-rates) specified in Lee and Lin's work [20]. Again, the system is treated as a single-phase hcp polycrystalline using the Basal, Prismatic, 1st order Pyramidal $\langle a \rangle$, 1st order Pyramidal $\langle c+a \rangle$ and 2nd order Pyramidal $\langle c+a \rangle$ slip systems, with each slip system using the same single crystal MTS model and homothetic hardening. Figure 14 shows the results of the single-phase VPSC model using the single crystal MTS model along with the results of the macroscopic MTS model and the experimental data under compression conditions at 298 K and a strain-rate of 2000 s^{-1} ; the single crystal MTS model is also plotted independently for reference. The

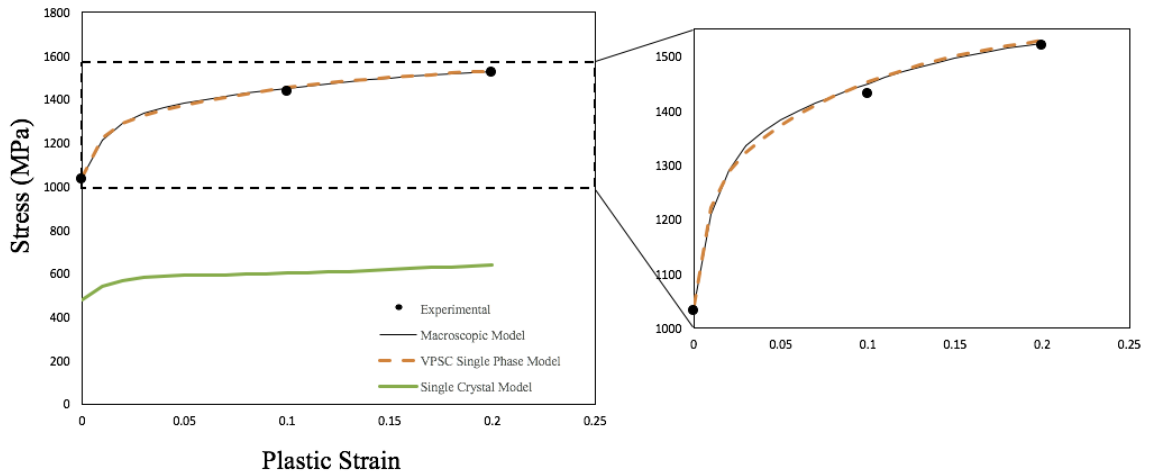


Figure 14: Results of the single-phase VPSC model using the single crystal MTS model along with the results of the macroscopic MTS model and the experimental data under compression conditions at 298 K and a strain-rate of 2000 s^{-1} ; the single crystal MTS model is also plotted independently for reference.

results are in excellent agreement with the Macroscopic model and experimental data with the maximum percent error being $\sim 1.48\%$.

Experimental stress-strain data and the single-phase VPSC predictions are given in Figures 15, 16 and 17 for temperatures ranging from 298-1373 K and strain-rates from $1700\text{-}2500\text{ s}^{-1}$ with the maximum percent error being $\sim 4.50\%$ for a temperature of 1373 K and a strain-rate of 2000 s^{-1} ; tables comparing all reported experimental data points with the single-phase VPSC results and their associated percent errors are found in Appendix A.2. There is a slight, but noticeable trend in that the percent error appears to increase with increasing temperature and that the VPSC single-phase model (as well as the macroscopic MTS model) appears to under predict the stress-strain response. This is attributed to the fact that the Ti-6Al-4V system is a two-phase material where the volume fraction of the hcp α -phase decreases with increasing temperature and that of the bcc β -phase increases. In the models thus far considered, the materials systems have been treated as a single hcp α -phase system without regard for the bcc β -phase; topic to be addressed in Chapter 6.

4.2 Summary

In this chapter, the previously calibrated macroscopic MTS model was adapted to a single crystal system and incorporated within the VPSC program to simulate the stress-strain response of a hypothetical single-phase hcp Ti-6Al-4V system undergoing high strain-rate compression. The hcp $\{0001\}\{11\bar{2}0\}$ Basal $\langle a \rangle$, $\{10\bar{1}0\}\{11\bar{2}0\}$ Prismatic $\langle a \rangle$, $\{10\bar{1}1\}\{11\bar{2}0\}$ 1st order Pyramidal $\langle a \rangle$, $\{10\bar{1}1\}\{11\bar{2}3\}$ 1st order Pyramidal $\langle c+a \rangle$ and $\{11\bar{2}2\}\{11\bar{2}3\}$ 2nd order Pyramidal $\langle c+a \rangle$ slip systems were used with each slip system utilizing the same constitutive model and model parameters with homothetic hardening.

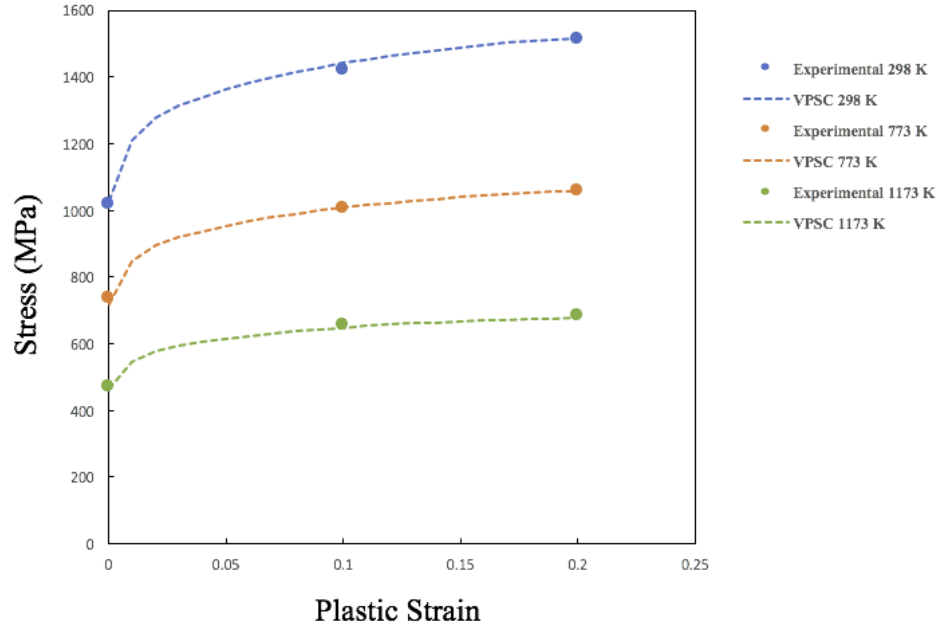


Figure 15: Comparison of the experimental flow stress behavior and single-phase VPSC predicted behavior for a strain-rate of 1700 s⁻¹ and temperatures ranging from 298–1173 K.

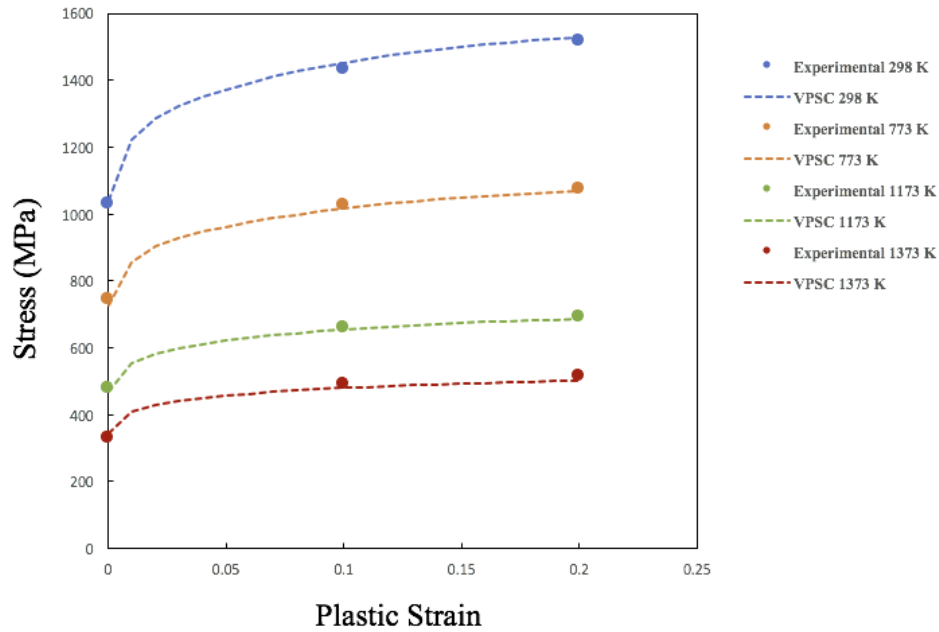


Figure 16: Comparison of the experimental flow stress behavior and single-phase VPSC predicted behavior for a strain-rate of 2000 s⁻¹ and temperatures ranging from 298–1373 K.

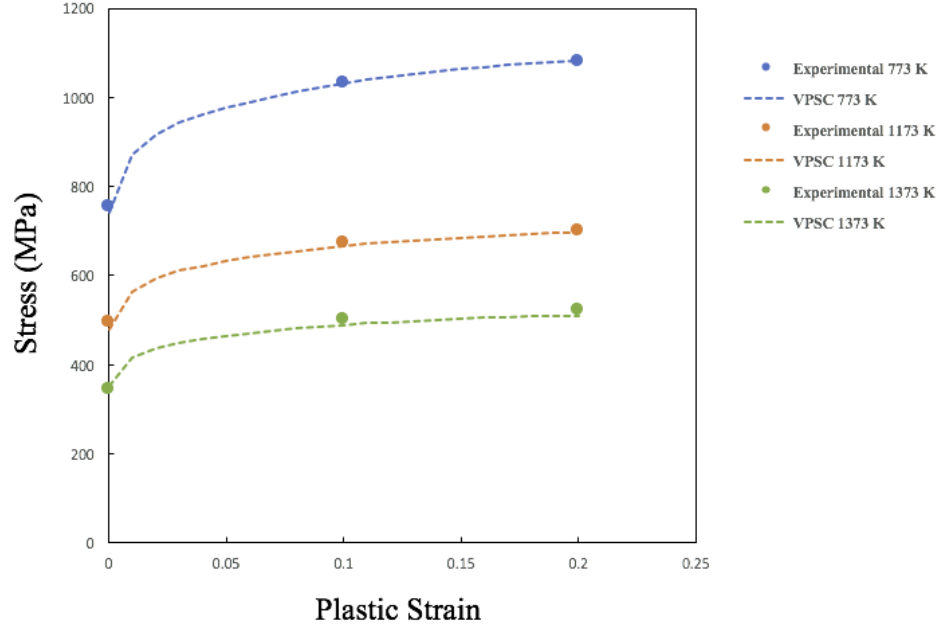


Figure 17: Comparison of the experimental flow stress behavior and single-phase VPSC predicted behavior for a strain-rate of 2500 s^{-1} and temperatures ranging from 773–1373 K.

hardening. Simulations were carried out in compression using an equivalent Von Mises strain measure with the initial material state having 10,000 random orientations (individual grains).

The VPSC program was first run using the macroscopic MTS model in order to obtain a scaling factor for the ratio of the yield stress between the two models. This scaling factor (or Taylor Factor) was found to be equal to ~ 2.17 and was used to re-scale the macroscopic MTS model to a single crystal model. Due to its non-linearity within the modified Voce hardening law, the work-hardening rate parameter was fitted until the desired stress-strain response was achieved. While the stress-strain results for the macroscopic MTS and the single-phase VPSC models are in excellent agreement with each other, there are two items that limit the applicability to model the evolution of texture. Firstly, using the same MTS

parameters for each slip system prohibit a realistic texture evolution of the α -phase as it is well established that the critical resolved shear stress (CRSS) varies with the different slip systems. Secondly, the lack of a model for the β -phase prohibits the modeling of the full evolution of texture for the dual-phase Ti-6Al-4V system. Additionally, it is noted that as the temperature increases, the simulated stress-strain response begins to deviate from the experimental data, though only slightly. This is due to the lack of a constitutive model for the β -phase and will be addressed in Chapter 6.

CHAPTER 5. MICROSTRUCTURE AND TEXTURE DATA

Before proceeding to the full multiphase VPSC model, experimental texture data is needed to properly simulate the high-speed machining texture evolution of dual-phase Ti-6Al-4V. In Chapter 4, it was seen that the VPSC program relies on crystallographic orientation data as an input for each grain and 10,000 random orientations were used to model the single-phase stress-strain response of a high strain-rate compression process. To model the high-speed machining process, random texture data is insufficient and two sets of experimental texture data are required. First, the texture from a virgin non-machined sample is needed. This data will be used as the input and initial state of the simulation and the texture for both the hcp α -phase and bcc β -phase is required. Secondly, the α -phase and β -phase texture data for the post-machined sample is required to compare against simulation results. In this chapter, x-ray diffraction (XRD) and electron backscatter diffraction (EBSD) measurements of virgin and post-machined samples are analyzed and texture for α - and β -phases constructed in a manner that best approximates the orientations of grains within the machining affected region.

It is well known that high-speed machining mostly affects the near surface microstructure within ~50-100 micrometers of the surface due to the high temperatures and strain-rates experienced during the cutting process [53, 54, 55]. For this reason, X-Ray Diffraction (XRD) and Electron Backscatter Diffraction (EBSD) methods are used to determine macro- and micro-texture, respectively, of the near surface microstructure. The first sample consists of pre-formed rods of Ti-6Al-4V provided by the Boeing Company and is designated as the as-received sample. The second sample consists of an as-received

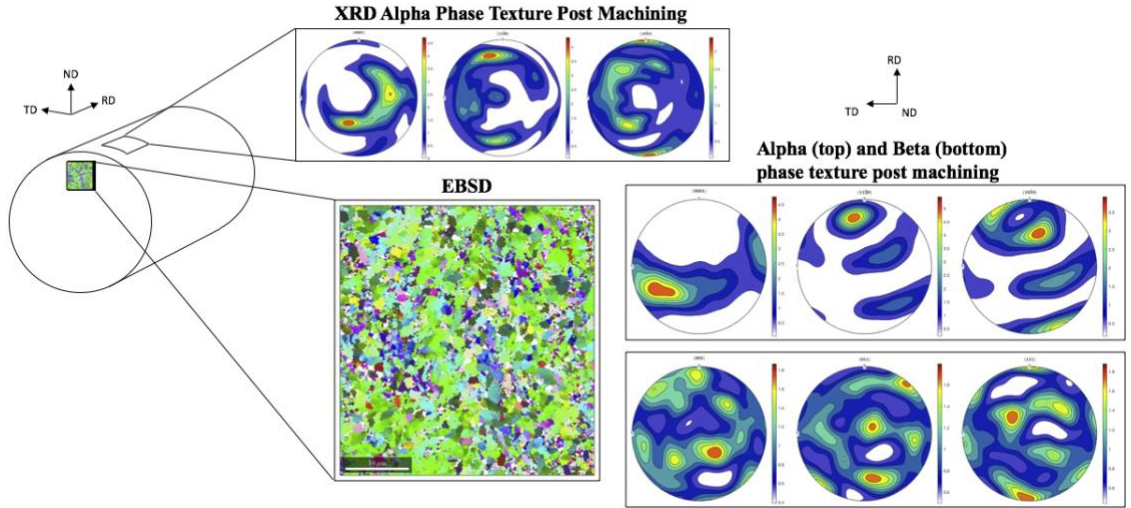


Figure 18: Location of XRD and EBSD measurements relative to the sample work piece. Machining occurred on the curved surface in the transverse direction. XRD measurements were taken directly on the machined surface while EBSD measurements were taken on a plane orthogonal to the cutting plane.

sample that underwent a high-speed turning operation using a Kennametal TPG322 type ceramic cutting tool piece at a Rake angle of 0° with a cutting speed of 100 m/min, a depth of cut of 0.2 mm and a feed rate of 0.0508 mm/revolution. Figure 18 shows the positions that XRD and EBSD measurements were taken with respect to the machined surface; here, the curved surface represents the machined surface with the tool piece traversing across the surface in the transverse direction (TD).

5.1 XRD Results

XRD measurements for each sample were obtained using a PANalytical X'Pert Pro MRD diffractometer with a Proportional Detector XE and a CuK-alpha source. Absolute scans were first made to determine appropriate peaks for texture scans, the results of which are given in Figure 19. Correlations between the peak locations (2θ) and diffraction planes are given in Equation (22):

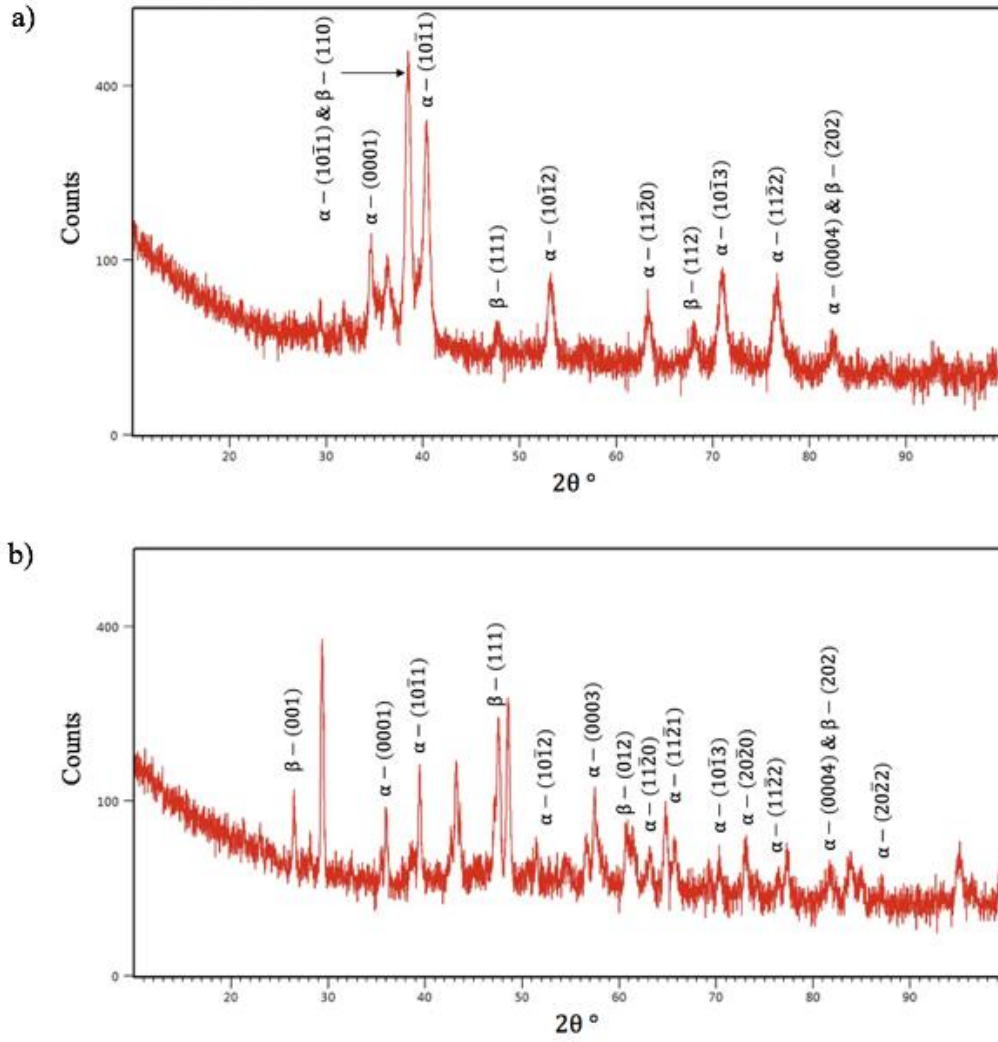


Figure 19: Absolute XRD scans for a) as-received sample and b) post-machined sample.

$$\lambda = 2d \cdot \sin(\theta) \quad (22)$$

where λ is the wavelength of the x-ray source ($\sim 1.54 \text{ \AA}$ for a CuK-alpha source) and d is the interplanar spacing (d-spacing) between families of parallel planes. The d-spacing for hcp crystals is given in Equation (23):

$$\frac{1}{d_{hcp}^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a_{hcp}^2} \right) + \frac{l^2}{c_{hcp}^2} \quad (23)$$

where h , k and l are the miller indices of the hcp system (in the three-index notation) and a_{hcp} and c_{hcp} are the lattice parameters given as 2.95 Å and 4.686 Å respectively. The d-spacing for cubic crystals is given in Equation (24):

$$\frac{1}{d_{cubic}^2} = \left(\frac{h^2 + k^2 + l^2}{a_{hcp}^2} \right) \quad (24)$$

where h , k and l are the miller indices of the bcc system and a_{hcp} is the lattice parameter given as 3.3174 Å. Analysis of the absolute XRD scans indicate that peaks located at 2θ values of 40.1698°, 52.9864°, 62.9648°, 70.6227° and 76.2100° belong to the α -phase and are of sufficient fidelity for use in texture measurements. Analysis of the peaks associated with the β -phase yield several problems. First, there is only one shared peak between the two samples, the peak located at a 2θ value of 47.4293°. While this problem is not insurmountable, it can have a bearing on accuracy when trying to compare texture between multiple samples. Second, and more importantly, for the as-received sample, two of the four measured peaks associated with the β -phase are coincident with peaks from the α -phase, thus not providing enough peaks to properly reconstruct the β -phase texture.

Texture measurements were also made using the PANalytical X'Pert Pro MRD and were performed only for the α -phase at the 2θ values mentioned above representing the (10 $\bar{1}$ 1), (10 $\bar{1}$ 2), (11 $\bar{2}$ 0), (10 $\bar{1}$ 3) and (11 $\bar{2}$ 2) families of planes, here given in the four-

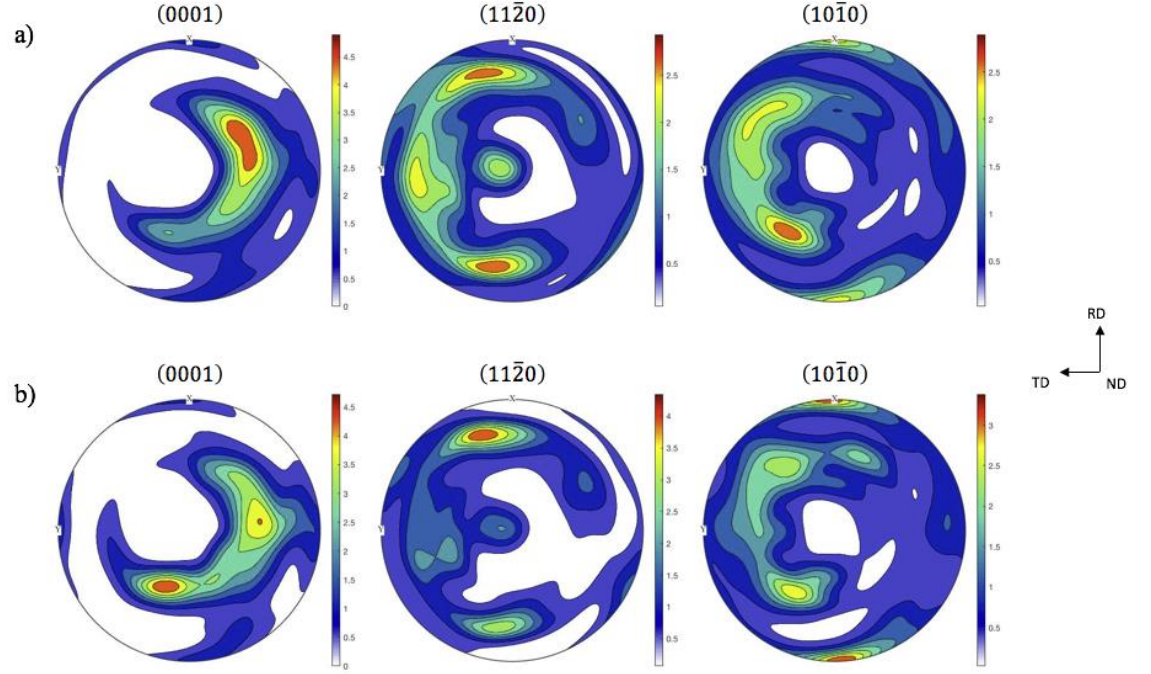


Figure 20: Pole figures for the macro-texture representation of the α -phase for the a) as-received sample and b) the post machined sample.

index notation. Texture data was analyzed, and pole figures constructed using MTEX, a free texture analysis toolbox for MATLAB [56]. The constructed pole figures for the as-received and post-machined samples are given in Figure 20. While the texture is seen to evolve due to the machining process, it should be noted that XRD captures not only the near surface machining microstructure, but also some of the lessor or unaffected microstructure beneath the near surface. Because of this, a method was devised to subtract the bulk (or base) sample texture from that of the post-machined sample texture and renormalize the texture data. In this method, the texture of the near surface microstructure for the post-machined sample is more accurately represented and usable as a comparison against VPSC simulated texture. This subtracted and renormalized texture representing the near surface texture of the post-machined sample is given in Figure 21 and the algorithm

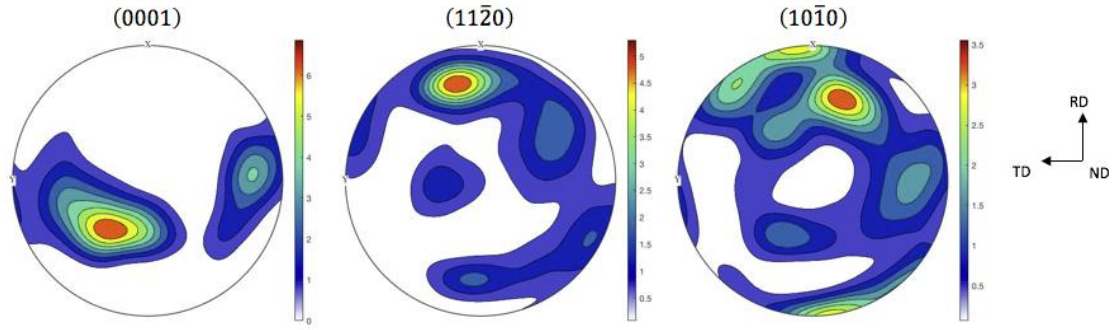


Figure 21: Pole figures representing the renormalized difference between the post-machined and as-received samples. The texture difference was subsequently renormalized and provides a more accurate representation of the true texture of the near-surface microstructure.

for the method is provided in Appendix B. Dual-phase VPSC simulations of the high-speed machining process in Chapter 6 will support this method.

5.2 EBSD Results

EBSD measurements occur using an EDAX Hikari EBSD Pro camera situated within a Tescan FERA3 scanning electron microscope. Unlike the averaged macro-texture methods of XRD, EBSD yields the micro-texture, or local texture data. Essentially, texture from XRD relies on measuring diffracted x-ray counts at specific orientations from a great number of polycrystals whereas EBSD relies on measuring a great number of locations on a materials surface to determine the orientation at each of those locations; the later could be termed a point-to-point measure of orientation data with the former being an average measure of orientation data. EBSD was conducted on the transverse section of the sample, i.e. perpendicular to the plane of XRD measurements. In this way, the texture change as a function of depth below the surface is determined along with the spatial distribution of the

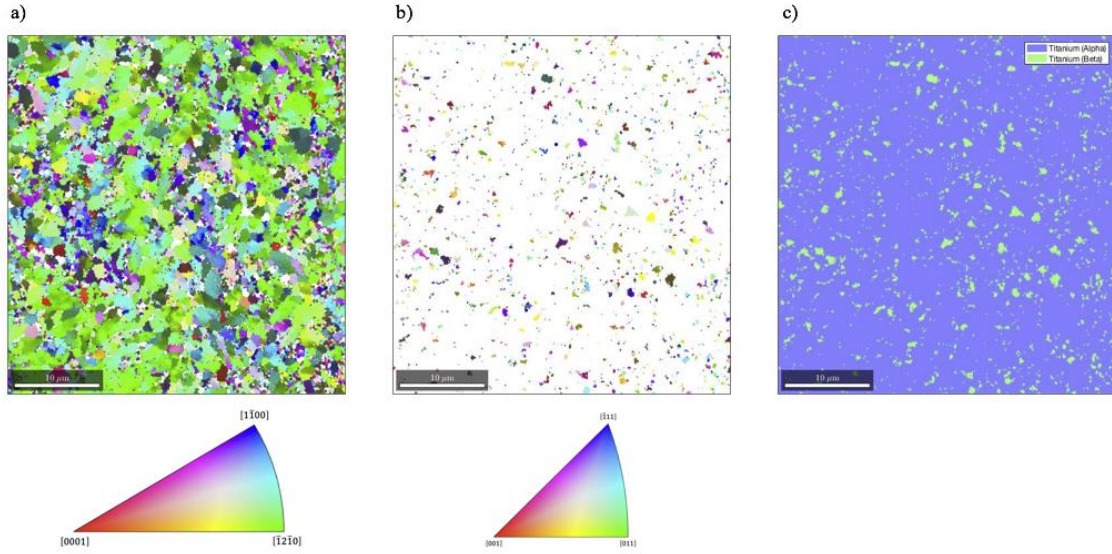


Figure 22: Spatial distribution of the a) α -phase and b) β -phase for the as-received sample color coded with respective inverse pole figure map. In, c) the α -phase is blue while the β -phase is green. From this latter figure, the β -phase is found to have a volume fraction of $\sim 6\%$.

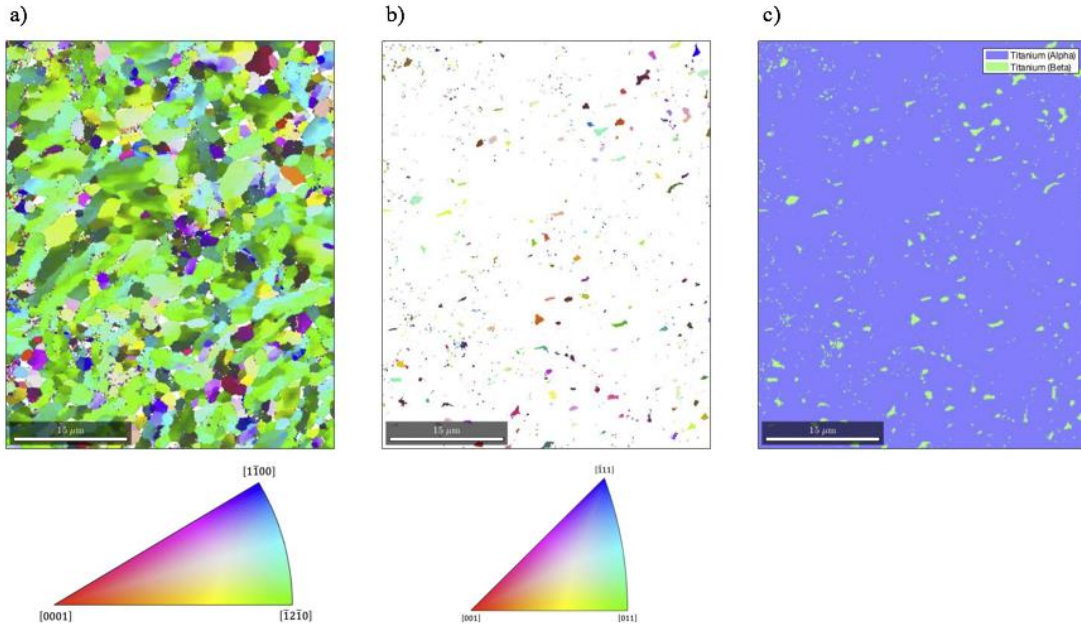


Figure 23: Spatial distribution of the a) α -phase and b) β -phase for the post-machined sample color coded with respective inverse pole figure map. In, c) the α -phase is blue while the β -phase is green. From this latter figure, the β -phase is found to have a volume fraction of $\sim 5\%$.

α - and β -phases. The spatial distribution of the α - and β -phases are given in Figures 22 and 23 for the as-received and post-machined sample, respectively. From this data, it is found that the volume fraction of the β -phase is approximately 6% for the as-received sample and 5% for the post-machined sample and the microstructure is equiaxed.

The calculated micro-texture data for each sample is given in Figures 24 and 25 and is rotated to match the sample orientation from XRD measurements. It is interesting to note that the EBSD texture for the α -phase of both samples closely resembles that of the subtracted/renormalized XRD texture, which is expected as EBSD measurements were made at and just below the surface on the order of ~ 50 micrometers. It is also pointed out that the EBSD micro-texture of each sample for the α -phase closely resemble each other and it is difficult to determine the extent to which texture evolution has occurred. The β -phase, on the other hand, shows more obvious signs of texture evolution. Although EBSD measurements are made as close as possible to the surface, a gradated texture is expected due to the decrease in temperatures and strain-rates as a function of depth below the surface that occurs during the machining process. The subtraction and renormalization method, used previously for XRD measurements, is used on the EBSD micro-texture data with the results show in Figure 26, again rotated to match the sample orientation like from XRD measurements. The subtraction and renormalization method for the EBSD micro-texture really highlights the texture changes with the greatest changes occurring at the surface, the area that we are trying to model. Subtracting out the near-surface micro-texture data also gives a closer approximation of the evolved macro-texture that was found via the XRD method.

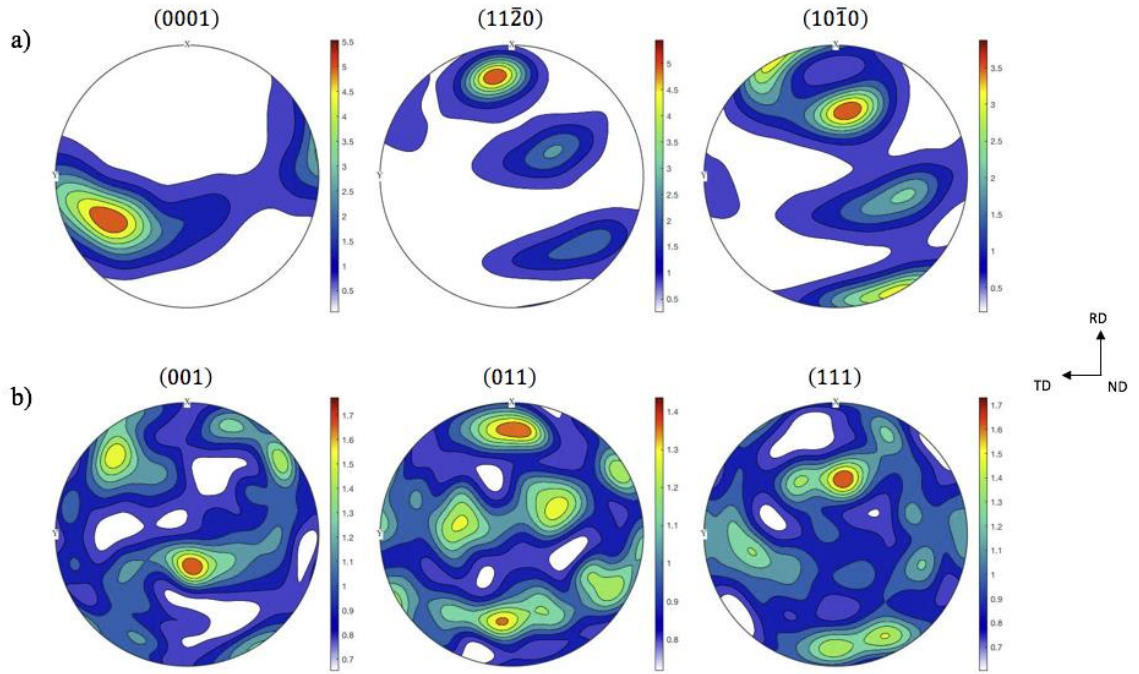


Figure 24: Pole figures for the representation of the micro texture of the a) α -phase and b) β -phase of the as-received sample.

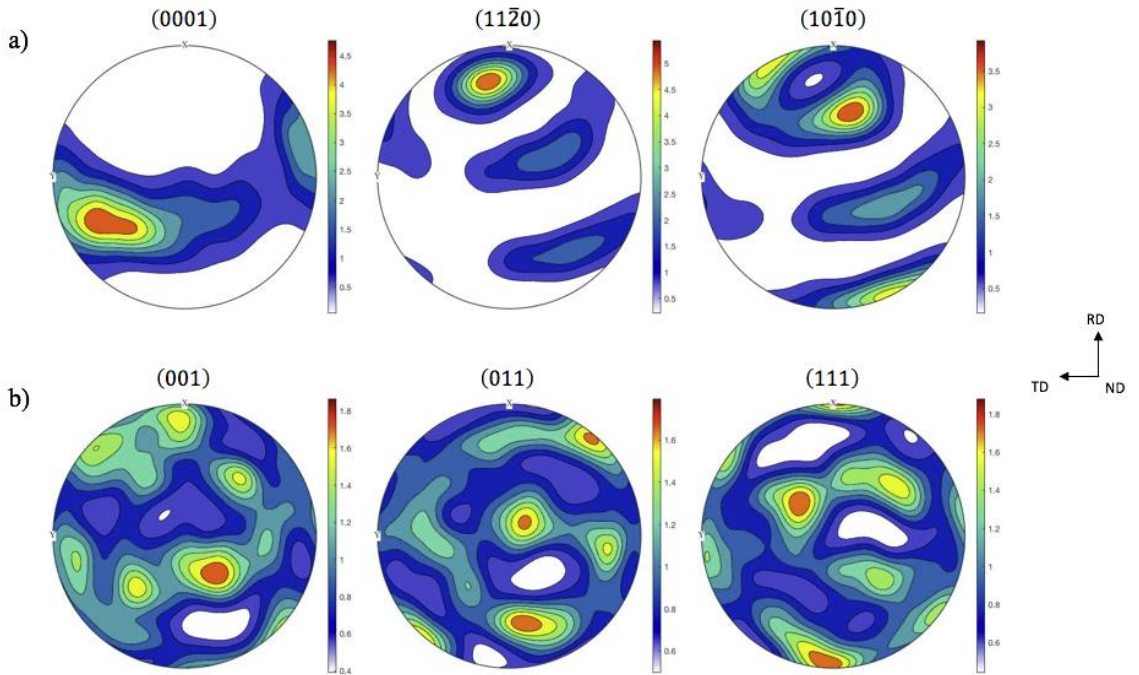


Figure 25: Pole figures for the representation of the micro texture of the a) α -phase and b) β -phase of the post-machined sample.

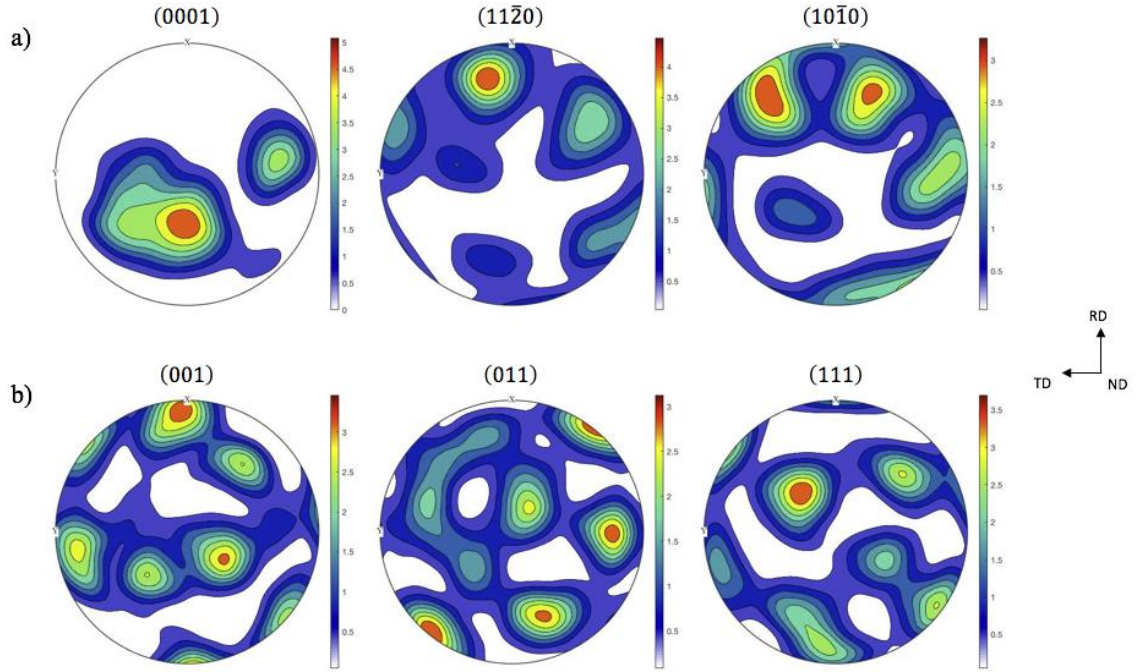


Figure 26: Pole figures representing the renormalized difference between the post-machined and as-received samples for the a) α -phase and b) β -phase.

5.3 Summary

As-received and post-machined rods of Ti-6Al-4V were investigated using XRD and EBSD techniques to find the macro- and micro-texture data. For XRD data, a subtraction and renormalization technique was devised to subtract out the bulk texture and better represent the evolved surface macro-texture of the post-machined Ti-6Al-4V rods. Because of the small amount of β -phase ($\sim 5\text{-}6\%$), inconsistency of β -peaks between samples and coincidence with α -phase peaks, the texture of the β -phase could not be determined via XRD measurements. EBSD was conducted on transverse sections of the Ti-6Al-4V rods and the micro-texture for the α - and β -phase were found. Because the texture is highly graduated with strongest texture evolution occurring at the surface, the α -phase micro-

texture was shown to be very similar pre- and post-machining, though in both samples, the data very closely resembled that from the XRD subtraction technique. To further highlight the surface texture evolution, the same subtraction and renormalization technique applied to XRD data was applied to EBSD data better approximating the texture evolution at the surface of the machined sample and providing a closer match to the texture found via XRD.

CHAPTER 6. MULTIPHASE VPSC MTS MODEL

The extension of the single-phase single-crystal MTS model to a two-phase multi-slip model presents many challenges. The previous model formulated in Chapter 4 was calibrated around the single-phase hcp α -system where each slip system was modeled using the same parameters and hardening rates. Because the critical resolved shear stress (CRSS) is expected to vary with slip system, there is no one simple scaling factor with which to re-scale the MTS model. While the model yielded an exceptional stress-strain response, it was seen that increasing deviations from the experimentally measured data occurred as temperatures increased. In this chapter, a single-crystal MTS model is introduced for the β -phase using parameters from Mandal et. al. for the near β -alloy Ti-5553 and is used in conjunction with the previously developed α -phase model to all work together [57]. This model is modified, as has been done throughout this work, to extend its applicability to high strain-rate behavior and improve estimation of the initial work-hardening behavior.

6.1 FEA Machining Simulations

One of the last remaining items needed to run the VPSC model for high-speed machining are the velocity gradients and temperature states for the machining operation. FEA simulations for the machining process were conducted using DEFORM to model a ceramic cutting tool piece interacting with a Ti-6Al-4V sample at a cutting speed of 100 m/min and a depth of cut of 0.2 mm; the feed rate was not included within the simulation. Velocity gradients and temperature profiles at the surface were recorded at different points across the cutting plane as a function of time. This data is used to define the dynamic mechanical

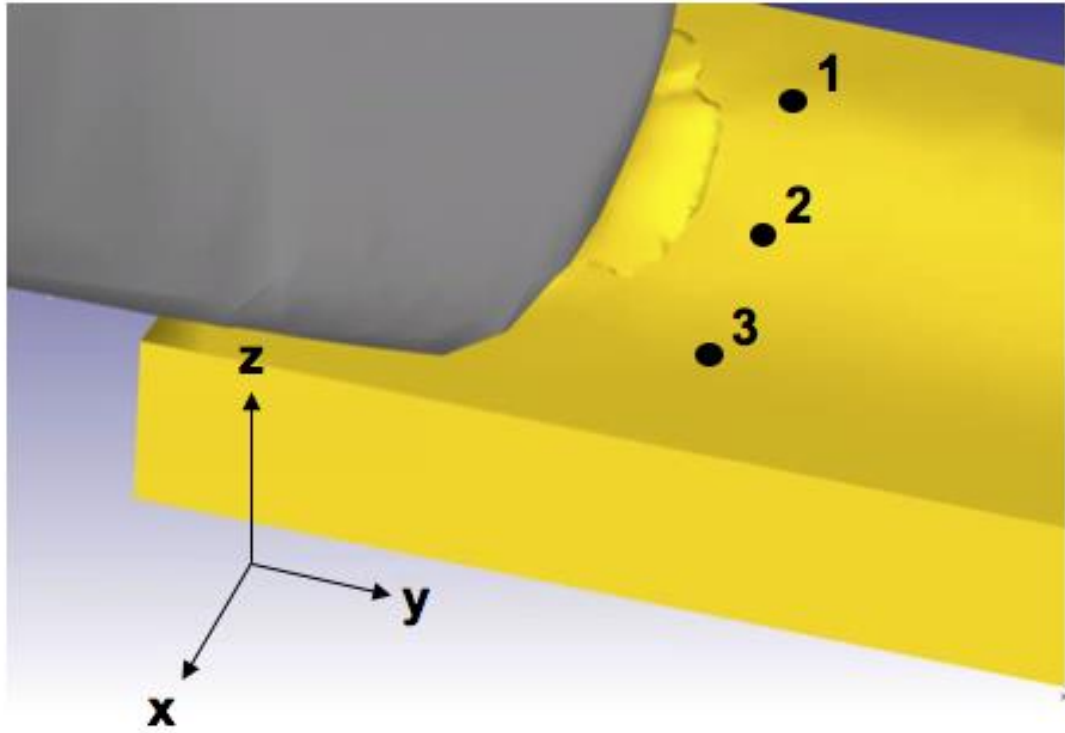


Figure 27: Representation of the FEA simulations of the cutting process. Velocity gradients and temperature profiles were recorded at the three locations indicated and used to model three passes of the cutting tool within the VPSC simulations.

and the thermal state of the system through every step of the VPSC simulations and provides VPSC the strain-rates and temperatures needed to calculate the evolution of the threshold stress at the slip system level. Because the FEA simulations are computationally expensive, the simulation was run as one pass of the cutting tool across the material sample. In machining, it is not uncommon for the cutting tool to pass by a material point multiple times. To account for multiple passes, velocity gradients and temperature profiles were recorded from three specific points across the cutting plane, as shown in Figure 27. Point 1 represents the leading edge of the cutting tools interaction with the material surface and

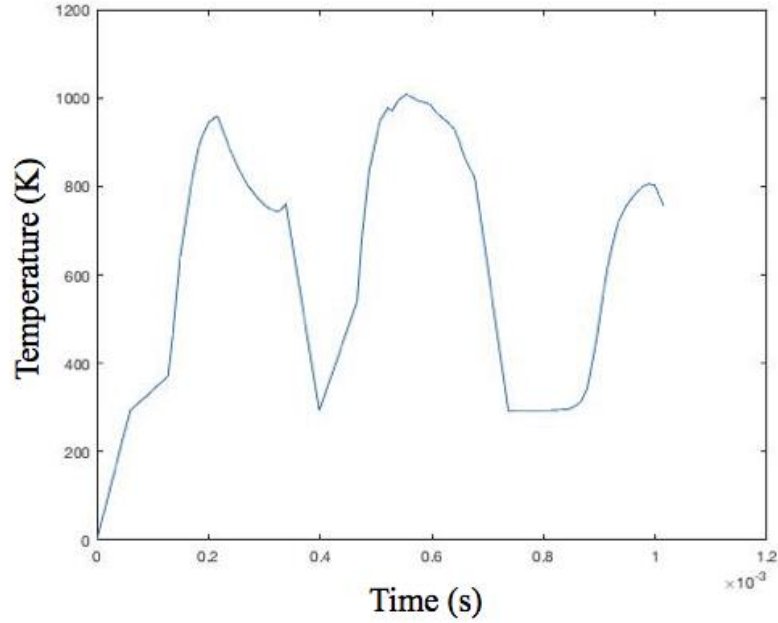


Figure 28: FEA generated temperature profile for three machining passes. The maximum temperature was found to occur during the interaction of the center of the cutting tool with the investigated materials point and reached a temperature of ~1012 K.

the first pass, while Points 2 and 3 represent the middle and trailing edge of the cutting tools interaction with the material surface and subsequent passes.

The temperature and velocity gradient profiles as a function of time are given in Figures 28 and 29, respectively, at the three specified points and again represent the thermal and mechanical state of the system during three separate interaction of different parts of the cutting tool with the same material point on the sample surface. From the simulations, the maximum surface temperature for any given pass was found to be ~1012 K with changes in temperatures occurring quite rapidly; from the data presented here, on the order of ~4100 K/ms. Simulations also indicate that strain-rates in the diagonal positions of the velocity gradients reach values as high as $\sim 24,000 \text{ s}^{-1}$ (L_{yy} , the principle cutting direction)

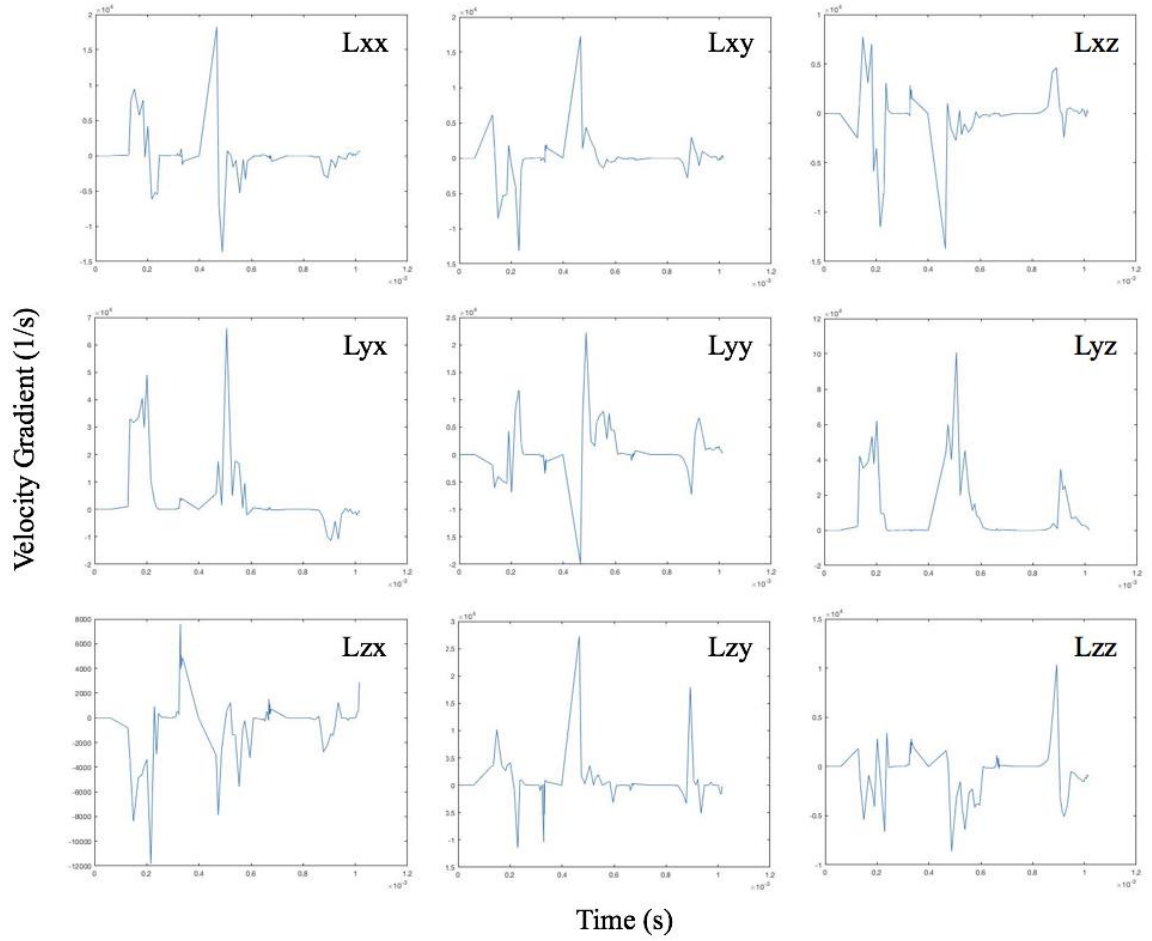


Figure 29: FEA generated velocity gradients for three machining passes. The diagonal terms are translated into strain-rates and material stretching while the off-diagonal terms are translated into shear-rates and material rotation.

while shear-rates in the off-diagonal components reach values as high as $\sim 105,000 \text{ s}^{-1}$ (L_{yz}).

All temperature and velocity gradient data is discretized with VPSC treating each discrete step as a separate simulation with constant temperature and velocity gradient; the deformation and orientation data is saved at the end of each step and fed into the next, updating at every iteration.

6.2 The Dual-Phase Model

6.2.1 Calibration Procedure

Before moving on to the full model, a discussion is presented regarding the process to calibrate the parameters. The process to calibrate the MTS model for each slip system within each phase is separated into three core steps based on the two different data sets available. In the first step, high-speed machining simulations are run using an initial set of CRSS values for each slip system. Equation (12) can be re-written in the form:

$$\tau = \tau_{crss} + \hat{\tau}_d \cdot S_d(\dot{\epsilon}, T) \frac{\mu}{\mu_0} \quad (25)$$

where:

$$\tau_{crss} = \tau_a + \hat{\tau}_i \cdot S_i(\dot{\epsilon}, T) \frac{\mu}{\mu_0} \quad (26)$$

and τ_a is the athermal shear stress and $\hat{\tau}_i$ is the mechanical threshold stress used in the form of Equation (19). In this sense, the MTS model in Equation (25) is effectively divided into two parts: 1) the CRSS term, τ_{crss} , which is analogous to the yield point in the macroscopic models and 2) a hardening term; as was done in Chapter 4, an assumption of homothetic hardening is used for each slip system, with the hardening laws differing only between the models for the α - and β -phases. Because Equation (26) is linear in τ_a and $\hat{\tau}_i$, τ_{crss} can be easily scaled and adjusted for each slip system. Once the resultant simulated texture is examined, the respective CRSS values for each slip system are adjusted after each

simulation run and the process repeated until the simulated texture yields a good qualitative fit with the experimental texture.

In the second step, high strain-rate compression simulations are run using the updated CRSS values to model the stress-strain response and results compared to experimental data. τ_a and the parameters contained within $\hat{\tau}_i$ are then adjusted and simulations re-run until the simulated stress-strain response is within ~5% of experimental data. The third step involves the repetition of the first two steps until both the simulated texture and stress-strain response are found to be acceptable. The flow chart representing the process is given in Figure 30.

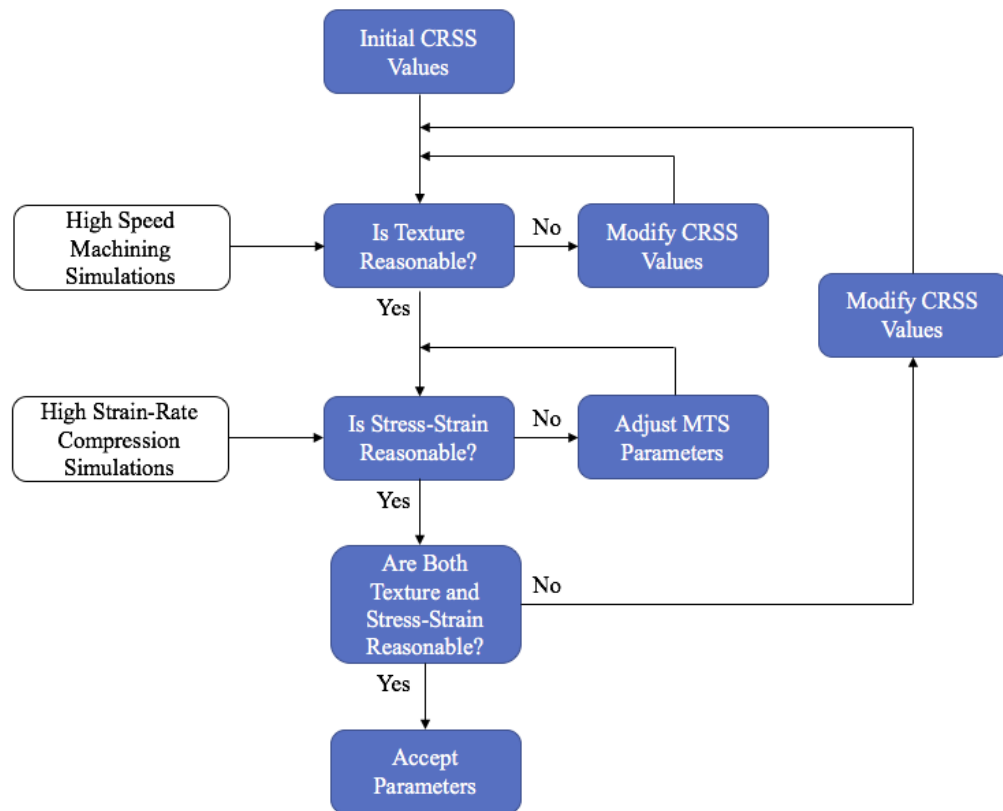


Figure 30: Flow chart describing the MTS model calibration for each slip system within each phase. The process is divided into three core processes (or loops) based on matching simulated texture and stress-strain response on the two different types of experimental data.

6.2.2 Evolution of β -Phase Fraction with Temperature

Up to this point, the Ti-6Al-4V system has been treated as a single-phase α -system without regard to the β -phase. Examination of the equilibrium binary cross-section of the ternary phase diagram at 6 wt.% Al (given in Figure 31) shows β -isomorphous behavior with alloying of Vanadium whereby the β -phase transforms into the α -phase with decreasing temperature [58, 59]. Lamellar structures of α - and β -phases typically form upon cooling from the single-phase β -phase field region whereby the α -phase nucleates at grain boundaries and grow into existing β -grains as lamellae with coarser lamellae being formed with slower cooling rates [59]. Martensitic structures may also form from β -grains at high enough cooling rates forming fine needle-like morphologies [60]. Finally, equiaxed structures of α - and β -phase form through recrystallization and growth as a consequence of deformation due to plastically working the material in the two-phase

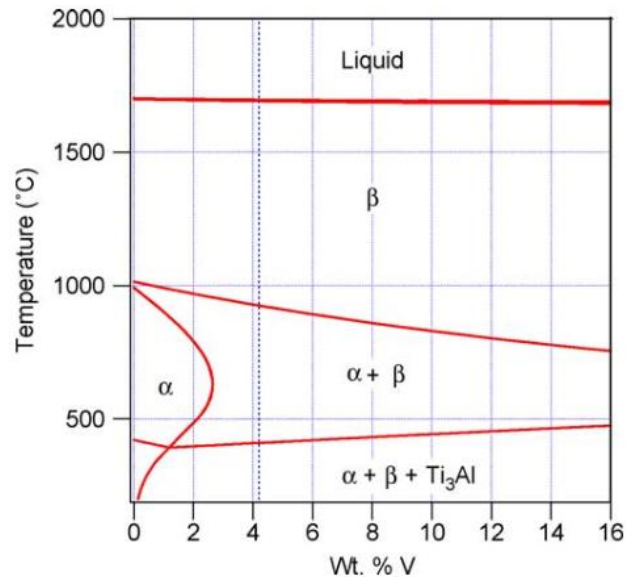


Figure 31: Calculated binary phase diagram for Ti-6Al and V. From [58].

$\alpha + \beta$ field with the volume fraction of formed α -phase depending on the temperature of the annealing process and the length of time of the annealing process dictating the coarseness of the two-phase microstructure [59].

As was shown in Figure 28, FEA machining simulations indicate that processing temperatures reach temperatures as high as ~ 1012 K while experimental data for shock compression tests reach temperatures as high as 1373 K. Analysis of the equilibrium phase diagram for Ti-6Al-4V shows that the temperatures used in this work are within those that form dual-phase α - and β -structures as well as single-phase β -structures, the β -transus occurring at ~ 1280 K. It should be noted, however, that high-speed machining is extremely dynamic and deviations from the equilibrium phase diagram do occur. Elmer et al. investigated the effects of heating rates on the volume fraction of the β -phase as a function of temperature and found that increased heating rates shift solidus and solvus lines to higher temperatures while the β -transus, though increased in temperature relative to the equilibrium phase diagram, showed very little sensitivity to the heating rate [58]. Their investigations were conducted for heating rates of 275, 283 and 303 K/s and the rate of shifts in temperatures with respect to heating rates decreased sharply as the heating rates increased. Another interesting feature found was that while the volume fraction of the β -phase stayed relatively constant up to a temperature of around 980 K, there was a loss of $\sim 2\%$ β -phase between ~ 700 -980 K at the higher heating rates. EBSD measurements on post-machined samples given in Chapter 5 appear to support this.

For this work, an assumption is made that the volume fraction of the β -phase remains constant up to 980 K and will take a value of 6%, which was the value measured

from EBSD experiments on as-received (pre-machined) samples; Elmer et al. reported constant values of $\sim 12\%$ for the samples used in their work [58]. Another assumption is made regarding the shift in transformation temperatures with respect to heating rates. While heating rates from machining approach values of ~ 4100 K/ms, the β -phase volume fraction transformation temperatures reported by Elmer et al. for heating rates of 303 K/s are assumed to be representative. This assumption is based on 1) the rate of shifts in temperatures with respect to heating rates decreased sharply as the heating rates increased and 2) a lack of any other data. Figure 32 gives the resultant hybridization of the reported β -phase volume fraction increase with temperature above 980 K and the constant β -phase volume fraction of 6% below 980 K and will be used to model the evolution of the fraction of β -phase. The interpolated fit of the reported experimental fit was made to fit the lower constant β -phase volume fraction of 6% as opposed to the $\sim 12\%$ reported by Elmer et al.

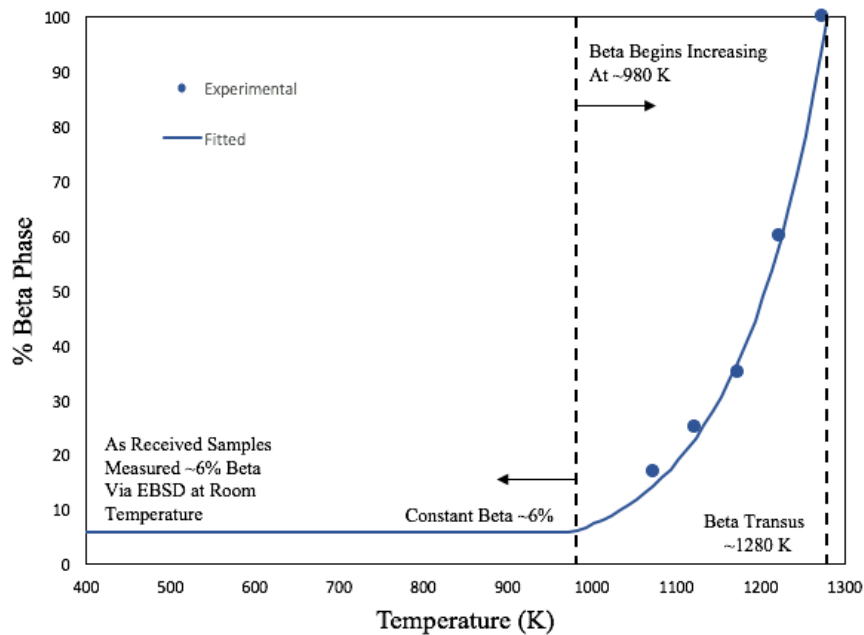


Figure 32: Hybridization of the reported β -phase volume fraction increase with temperature found by Elmer et al. and room temperature EBSD measurements of as-received samples.

6.2.3 α - and β -Phase Constitutive Relations

A single-crystal MTS model is now introduced for the β -phase using parameters from Mandal et. al. for the near β -alloy Ti-5553 [57]. Modifications to some parameters are made to best model the stress-strain response of experimental shock compression data and the experimentally measured texture of the post-machined sample. Modifications were also necessary to extend applicability to high strain-rate behavior and improve estimation of the initial work-hardening behavior. As with the α -phase model, slip systems and their respective modes must be specified within the VPSC program in order to calculate slip system activity. For the bcc system, the $\{110\}\langle 111 \rangle$ (with 12 modes), $\{112\}\langle 111 \rangle$ (with 12 modes), $\{123\}\langle 111 \rangle$ (with 24 modes) slip systems representing pencil glide are used and a schematic of the bcc slip system are given in Figure 33. As was described in subsection 6.2.1, the process to best parameterize the α - and β -phases is an iterative one and quite time consuming. Because of this, no more will be said about the calibration process other than it was followed and yielded quite good results.

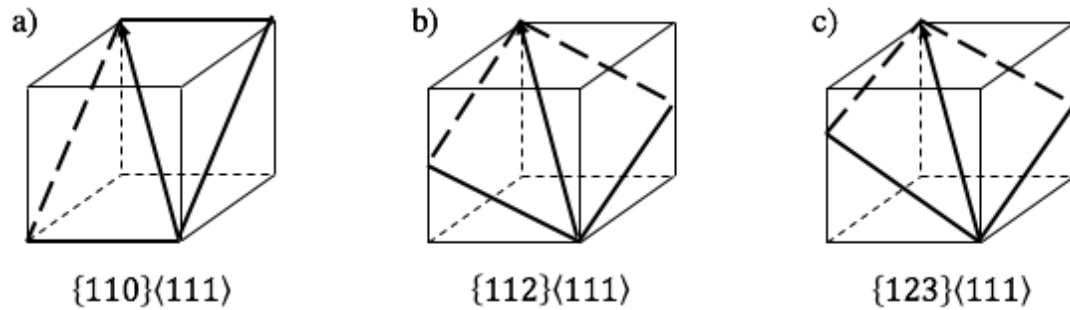


Figure 33: Representation of three slip systems representing pencil glide found in bcc materials: a) the $\{110\}\langle 111 \rangle$ (with 12 modes), b) $\{112\}\langle 111 \rangle$ (with 12 modes), c) $\{123\}\langle 111 \rangle$ (with 24 modes).

The parameters are presented in four parts. First, the common parameters used for each slip system for the α -phase is given in Table 4. In Table 5, the α -phase slip system specific parameters are given. Table 6 gives the common parameters used for each slip system used for the β -phase while Table 7 gives the slip system specific parameters.

Table 4: Common single crystal MTS model parameters used within the VPSC program for the α -phase HCP Ti-6Al-4V system

g_{oi}	1.53 J	μ_0	49020 MPa
$\dot{\epsilon}_{oi}$	$1 \times 10^{10} \text{ s}^{-1}$	a	4355 MPa
p_i	2/3	T_0	198 K
q_i	1.0	θ_0	$12000(\exp(-\epsilon))^{50} + 1300 \text{ MPa}$
g_{od}	1.6 J	τ_{ds0}	272.88 MPa
$\dot{\epsilon}_{od}$	$1 \times 10^7 \text{ s}^{-1}$	g_{ds0}	2 J
p_d	2/3	$\dot{\epsilon}_{ds0}$	$1 \times 10^7 \text{ s}^{-1}$
q_d	1.0	k_b	$1.38062 \times 10^{-23} \text{ J/K}$
κ	1	b	$2.96 \times 10^{-10} \text{ m}$

Table 5: Slip system specific single crystal MTS model parameters used within the VPSC program for the α -phase HCP Ti-6Al-4V system

Slip System	τ_a	$\hat{\tau}_i$
$\{0001\}\{11\bar{2}0\}$	46.00 MPa	$466.4 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$
$\{10\bar{1}0\}\{11\bar{2}0\}$	37.64 MPa	$396.0 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$
$\{10\bar{1}1\}\{11\bar{2}0\}$	50.18 MPa	$528.0 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$
$\{10\bar{1}1\}\{11\bar{2}3\}$	44.62 MPa	$469.5 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$
$\{11\bar{2}2\}\{11\bar{2}3\}$	41.82 MPa	$440.0 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$

Table 6: Common single crystal MTS model parameters used within the VPSC program for the β -phase BCC Ti-6Al-4V system

g_{oi}	0.6667 J	μ_0	47620 MPa
$\dot{\epsilon}_{oi}$	$1 \times 10^8 \text{ s}^{-1}$	a	5810 MPa
p_i	0.5	T_0	500 K
q_i	1.0	θ_0	$5533(\exp(-\epsilon))^{50} + 630 \text{ MPa}$
g_{od}	1.6 J	τ_{dso}	368 MPa
$\dot{\epsilon}_{od}$	$1 \times 10^7 \text{ s}^{-1}$	g_{dso}	0.05 J
p_d	2/3	$\dot{\epsilon}_{dso}$	$1 \times 10^7 \text{ s}^{-1}$
q_d	1.0	k_b	$1.38062 \times 10^{-23} \text{ J/K}$
κ	1	b	$3.32 \times 10^{-10} \text{ m}$

Table 7: Slip system specific single crystal MTS model parameters used within the VPSC program for the β -phase BCC Ti-6Al-4V system

Slip System	τ_a	$\hat{\tau}_i$
$\{110\}\langle 111 \rangle$	3.1 MPa	$418.5 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$
$\{112\}\langle 111 \rangle$	3.3 MPa	$445.5 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$
$\{123\}\langle 111 \rangle$	2.0 MPa	$270.0 + 0.43 \ln(\dot{\epsilon}) + 0.018 \cdot \dot{\epsilon} \text{ MPa}$

6.3 Stress-Strain Prediction

High strain-rate compression simulations were run for the various temperatures and strain-rates given in the experimental data reported by Lee and Lin as has been done throughout this work. Unlike the single-phase VPSC simulations conducted previously, where random

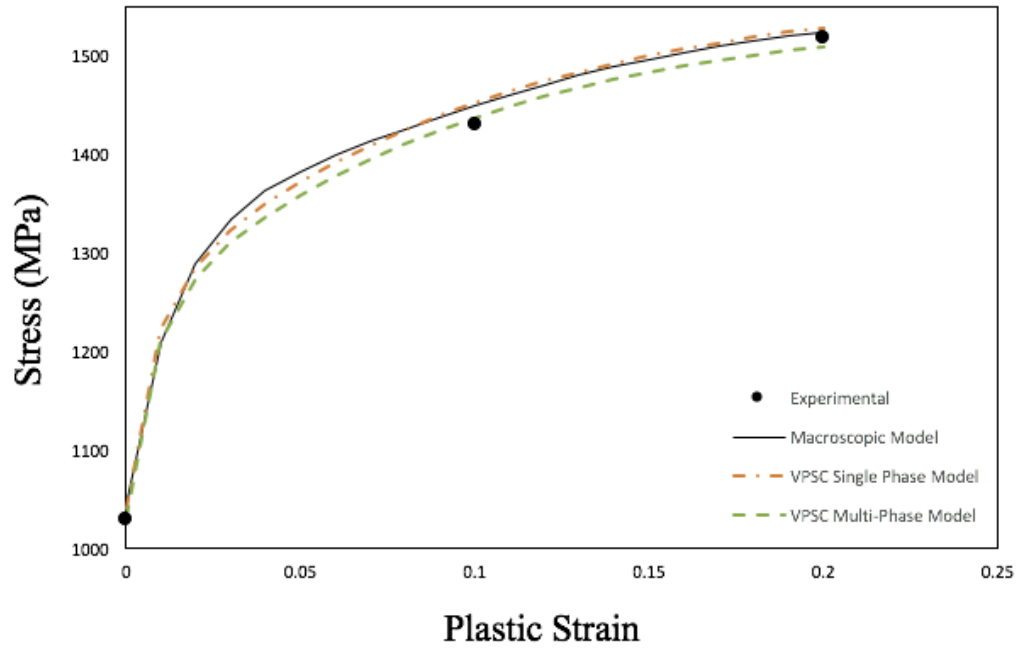


Figure 34: Results of the single-phase VPSC model using the single crystal MTS model along with the results of the macroscopic MTS model and the experimental data under compression conditions at 298 K and a strain-rate of 2000 s^{-1} .

orientation data was used as the initial state, the orientation data used here is generated from the texture measurements of the as-received sample (c.f. Figure 24). MTEX was used to generate 4632 orientations for the α -phase and 852 orientations for the β -phase; these numbers represent the unique number of orientations found from EBSD measurements and are used input into the VPSC program. Figure 34 shows the results of the dual-phase VPSC model using the single crystal MTS model for both the α - and β -phases (94% and 6% volume fractions respectively) along with the same results for the macroscopic MTS model, single-phase VPSC model and the experimental data under compression conditions at 298 K and a strain-rate of 2000 s^{-1} . The results show improvement over the macroscopic MTS model and single-phase VPSC model. The maximum percent error in relation to the

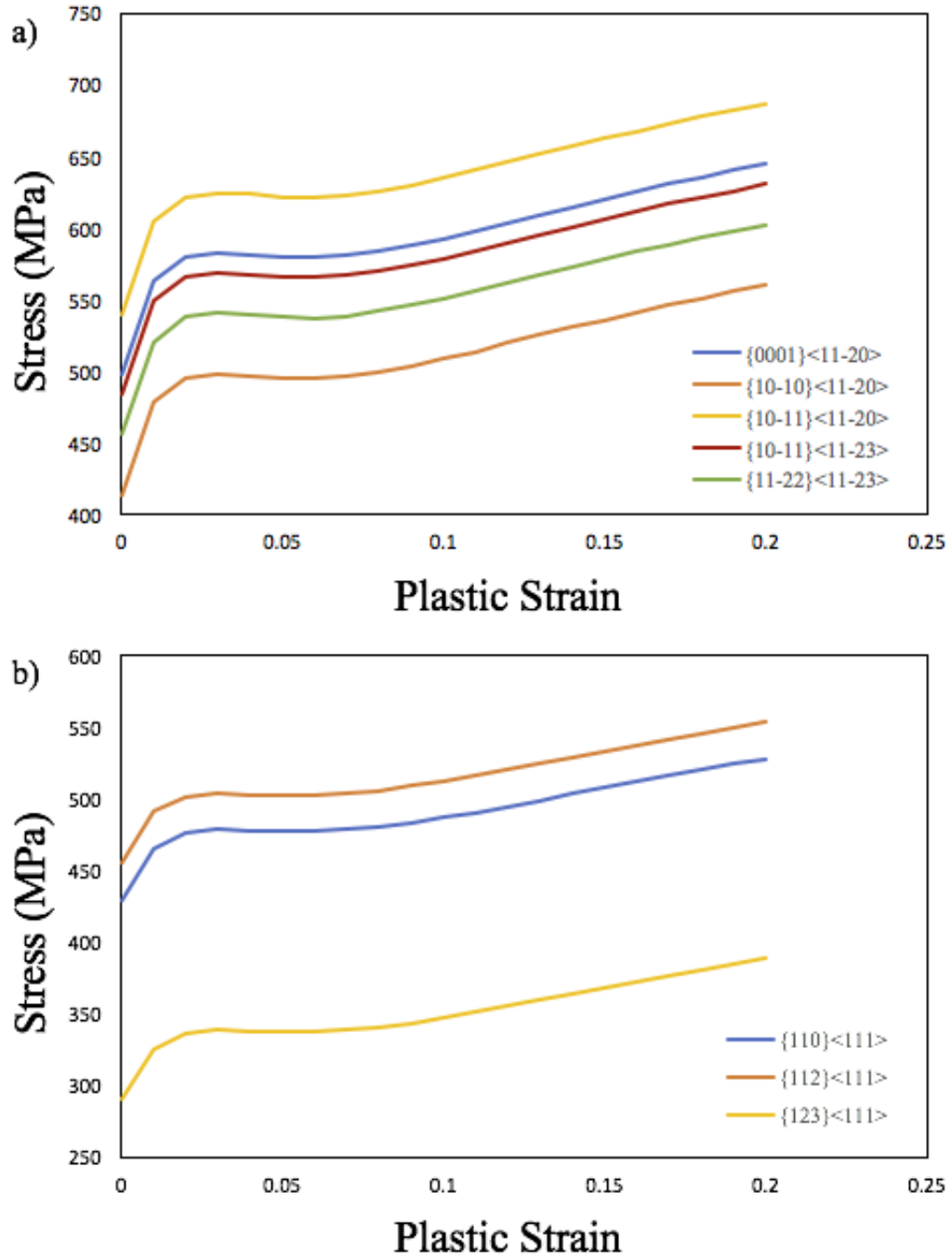


Figure 35: Stress-strain plots under compression conditions at 298 K and a strain-rate of 2000 s⁻¹ for the individual slip systems using the MTS model parameters specified in Tables 4-7 for the a) α - and b) β -phases.

experimental data is $\sim 0.60\%$. In Figure 35, the equivalent stress-strain curves for the individual slip systems are plotted for the α - and β -phases using the parameters specified in Tables 4-7.

Experimental stress-strain data and the dual-phase VPSC predictions are given in Figures 36, 37 and 38 for temperatures ranging from 298-1173 K and strain-rates from $1700\text{--}2500\text{ s}^{-1}$ with the maximum percent error being $\sim 5.02\%$ for a temperature of 1173 K and a strain-rate of 2500 s^{-1} ; tables comparing all reported experimental data points with the dual-phase VPSC results and their associated percent errors are found in Appendix A.3.

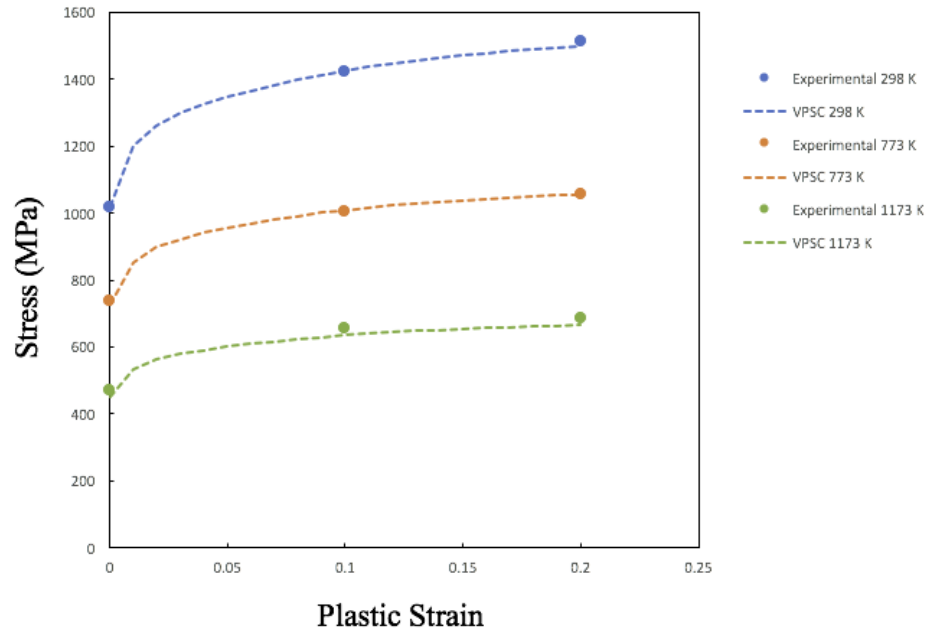


Figure 36: Comparison of the experimental flow stress behavior and dual-phase VPSC predicted behavior for a strain-rate of 1700 s^{-1} and temperatures ranging from 298–1173 K.

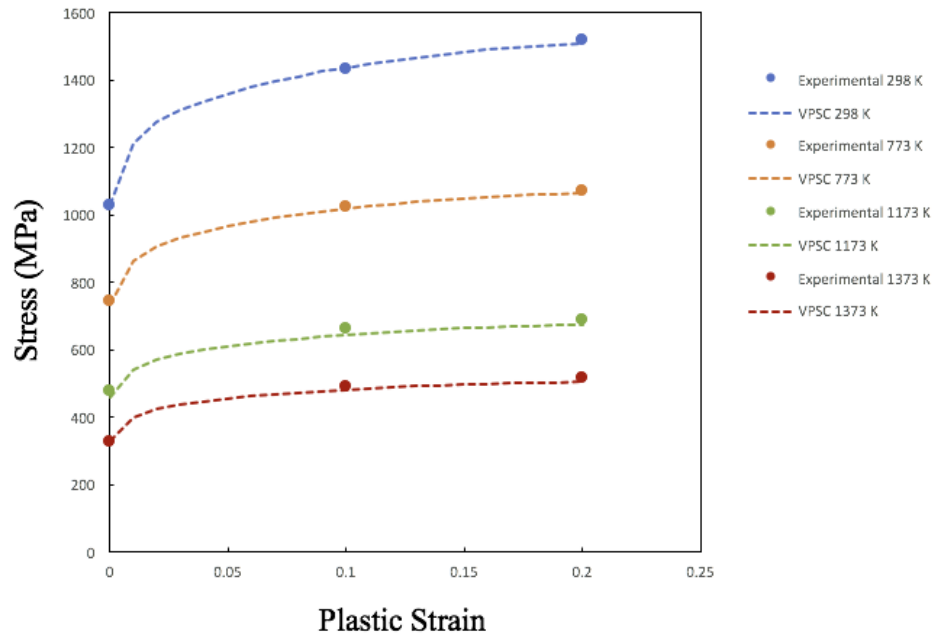


Figure 37: Comparison of the experimental flow stress behavior and dual-phase VPSC predicted behavior for a strain-rate of 2000 s^{-1} and temperatures ranging from 298–1373 K.

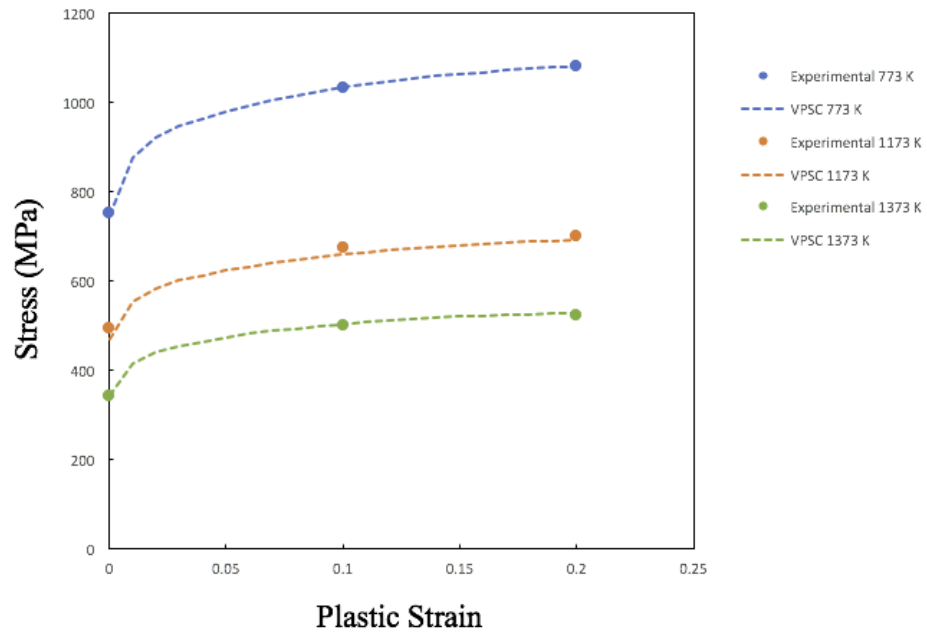


Figure 38: Comparison of the experimental flow stress behavior and dual-phase VPSC predicted behavior for a strain-rate of 2500 s^{-1} and temperatures ranging from 773–1373 K.

The volume fractions for the α - and β -phases used within the dual-phase VPSC model at temperatures 298 and 773 K are 94% and 6%, respectively, while at a temperature of 1173 K they are 65% and 35%. At a temperature of 1373 K the volume fraction is 100% β -phase. Improvements in the stress-strain response can be seen at temperatures in the single β -phase region in comparison to the previous models though the percent errors in the two-phase region at 1173 K increased. For continuity of flow, as little modifications were made to parameters in translating from the macroscopic model to the single- and dual-phase models. It may be that the parameters developed are not the most optimized for use within the dual-phase model, though the results presented are quite good. Additionally, as is shown in Figure 35, homothetic hardening is used for each slip system and changing the hardening parameters for each slip system might lead to improvements as well.

6.4 Texture Prediction

High-speed machining simulations were run using the parameters specified in Tables 4-7 and the temperature and velocity gradients given in Figures 28 and 29, respectively. As with the high strain-rate compression, 4632 orientations for the α -phase and 852 orientations for the β -phase, representing the texture of the as-received sample, were used as inputs for the initial orientation state of the system. With regards to possible phase transformations, it was seen that the maximum temperature predicted by FEA simulations was ~ 1012 K and from Figure 32, an increase in β -phase volume fraction of only ~ 2 -3% is expected. An assumption is made here that this small of an increase in volume fraction will not greatly affect the simulated results and the volume fractions for the α - and β -phases are kept constant at 94% and 6%, respectively, throughout the machining simulations. The

results of the simulation texture results are shown in Figure 39 and are compared with the experimentally measured subtracted and renormalized texture results.

Qualitatively, the simulated results are in good agreement with experimental results and lend support to the texture subtraction and renormalization method developed in Chapter 5. Although care was taken to subtract out the texture of the as-received sample from that of the post-machined sample, only approximations of the surface texture can be made as remnants of the sub-surface texture still persist in the measured data. The simulations presented here for surface texture evolution show strains up to 1400% at the surface and because of this the texture is very localized. In the machined sample, velocity gradients and temperatures decrease as a function of depth thus lessening the localization of orientations and creating a more diffuse texture as depth increases. In this sense, the measured texture intensities are expected to be much less than the more localized intensities found through simulations. Because of this, quantitative measures between the sets of texture were not used.

6.5 Summary

In this chapter, all previous work was brought together to create a set of constitutive relations for the α - and β -phases of Ti-6Al-4V for use within the VPSC model. The constitutive models were parameterized for the hcp $\{0001\}\{11\bar{2}0\}$ Basal $\langle a \rangle$, $\{10\bar{1}0\}\{11\bar{2}0\}$ Prismatic $\langle a \rangle$, $\{10\bar{1}1\}\{11\bar{2}0\}$ 1st order Pyramidal $\langle a \rangle$, $\{10\bar{1}1\}\{11\bar{2}3\}$ 1st order Pyramidal $\langle c+a \rangle$ and $\{11\bar{2}2\}\{11\bar{2}3\}$ 2nd order Pyramidal $\langle c+a \rangle$ slip systems and the bcc $\{110\}\{111\}$, $\{112\}\{111\}$ and $\{123\}\{111\}$ slip systems utilizing different model parameters and homothetic hardening for each phase. Finite element simulations were used

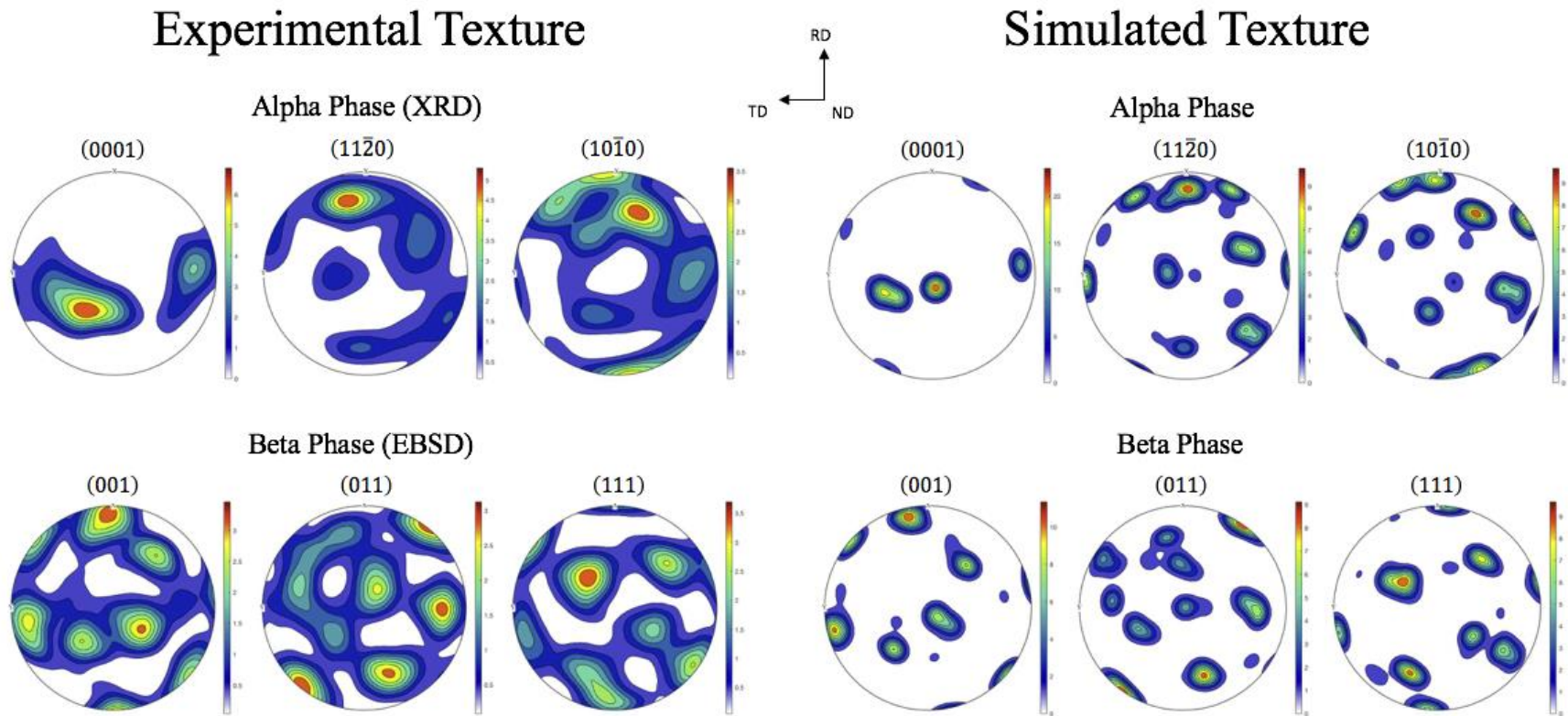


Figure 39: Experimental texture results (left) and simulated texture results (right) for the α -phase (top) and β -phase (bottom). Simulation results are in good qualitative agreement with experimentally measured results.

to model the high-speed machining process in order to generate velocity gradient and temperature profiles as inputs for the dual-phase VPSC model. A hybridized model was also put together to model the changes in β -phase volume fraction as a function of temperature utilizing room temperature β -phase volume fraction measurements and reported experimental data for dynamic heating conditions.

Following the procedure outlined in subsection 6.2.1, the complete model was calibrated using experimental data from high strain-rate compression test and experimentally measured texture from as-received and post machined samples of Ti-6Al-4V. The simulated stress-strain behavior was found to match experimental results quite well, with the maximum percent error being $\sim 5.02\%$ for a temperature of 1173 K and a strain-rate of 2500 s^{-1} . Improvements were made to the stress-strain behavior over previous results for the macroscopic MTS and single-phase VSPC model at high temperature within the single-phase β -region, though errors notably increased in the regions where the β -phase volume fraction changed as a function of temperature. This may be due to using parameters that are not the most optimized for a dual-phase system and the use of homothetic hardening for each slip system within each phase.

Simulations using the dual-phase VPSC model yielded texture results that were qualitatively in good agreement with experimentally measured results. Quantitative measures for the texture differences were not able to be achieved as experimentally measured textures tend to capture some amount of subsurface orientation data due showing some amount of diffuseness in the orientations whereas simulations only model the texture evolution at the surface and is highly localized. Overall results are quite good and should prove useful for future work.

CHAPTER 7. CONCLUSIONS AND FUTURE WORK

7.1 Conclusions

The main focus of this work is the development of development of dual-phase constitutive relations for Ti-6Al-4V based on the Mechanical Threshold Stress (MTS) model. In the process, modifications and deviations from normal methodologies were made that yielded better fits to experimental data and made the parameterization of the MTS model much easier. In Chapter 3, an alternative approach to fitting the mechanical threshold stress within the MTS model was examined to model the transition region where the deformation controlling mechanism transitions from thermal activation to drag mechanisms. It was found that fitting the mechanical threshold stress as a function of strain-rate lead to the “hockey-stick” behavior (linear behavior at low strain-rates and exponentially increasing behavior at high strain-rates) of the yield stress as a function of strain-rate typically found in many high strain-rate experiments. Additionally, it was found that modifications to the work-hardening rate provided a more realistic fit to the experimental data in the early stages of hardening post yield.

In Chapter 4, the calibrated macroscopic MTS model was adapted to a single crystal system and incorporated within the VPSC program to simulate the stress-strain response of a hypothetical single-phase hcp Ti-6Al-4V system undergoing high strain-rate compression. The MTS model was modified using a simple scalar factor (or Taylor factor) of ~ 2.17 to rescale the macroscopic model to the slip system level. The work-hardening rate parameter, unable to be scaled in the same manner, was fitted until the desired stress-strain response was achieved. The hcp $\{0001\}\langle 11\bar{2}0 \rangle$ Basal $\langle a \rangle$, $\{10\bar{1}0\}\langle 11\bar{2}0 \rangle$ Prismatic

$\langle a \rangle$, $\{10\bar{1}1\}\{11\bar{2}0\}$ 1st order Pyramidal $\langle a \rangle$, $\{10\bar{1}1\}\{11\bar{2}3\}$ 1st order Pyramidal $\langle c+a \rangle$ and $\{11\bar{2}2\}\{11\bar{2}3\}$ 2nd order Pyramidal $\langle c+a \rangle$ slip systems were used with each slip system utilizing the same constitutive model and model parameters along with homothetic hardening. Simulations were carried out in compression using an equivalent Von Mises strain measure with the initial material state having 10,000 random orientations (individual grains). While the stress-strain results for the macroscopic MTS and the single-phase VPSC models are in excellent agreement with each other, there two items limited the applicability of the model the evolution of texture. Firstly, using the same MTS parameters for each slip system prohibit a realistic texture evolution of the α -phase as it is well established that the critical resolved shear stress (CRSS) varies with the different slip systems. Secondly, the lack of a model for the β -phase prohibits the modeling of the full evolution of texture for the dual-phase Ti-6Al-4V system.

In Chapter 5, as-received and post-machined rods of Ti-6Al-4V were investigated using XRD and EBSD techniques to find the macro- and micro-texture data. For XRD data, a subtraction and renormalization technique was devised to subtract out the bulk texture and better represent the evolved surface macro-texture of the post-machined Ti-6Al-4V rods. EBSD was conducted on transverse sections of the Ti-6Al-4V rods and the micro-texture for the α - and β -phase were found. Because the texture is highly graduated with strongest texture evolution occurring at the surface, the α -phase micro-texture was shown to be very similar pre- and post-machining, though in both samples, the data very closely resembled that from the XRD subtraction technique. To further highlight the surface texture evolution, the same subtraction and renormalization technique applied to XRD data

was applied to EBSD data better approximating the texture evolution at the surface of the machined sample and providing a closer match to the texture found via XRD.

Finally, In Chapter 6 all previous work was brought together to create a set of constitutive relations for the α - and β -phases of Ti-6Al-4V for use within the VPSC model. The constitutive models were parameterized for the hcp $\{0001\}\langle 11\bar{2}0 \rangle$ Basal $\langle a \rangle$, $\{10\bar{1}0\}\langle 11\bar{2}0 \rangle$ Prismatic $\langle a \rangle$, $\{10\bar{1}1\}\langle 11\bar{2}0 \rangle$ 1st order Pyramidal $\langle a \rangle$, $\{10\bar{1}1\}\langle 11\bar{2}3 \rangle$ 1st order Pyramidal $\langle c+a \rangle$ and $\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$ 2nd order Pyramidal $\langle c+a \rangle$ slip systems and the bcc $\{110\}\langle 111 \rangle$, $\{112\}\langle 111 \rangle$ and $\{123\}\langle 111 \rangle$ slip systems utilizing different model parameters and homothetic hardening for each phase. Velocity gradient and temperature profiles generated from finite element simulations of the machining process were as inputs for the dual-phase VPSC model and volume fraction changes of the β -phase were modeled using a hybridization of data utilizing room temperature β -phase volume fraction measurements and reported experimental data for dynamic heating conditions.

The simulated stress-strain behavior was found to match experimental results quite well and improvements were made to the stress-strain behavior over previous results for the macroscopic MTS and single-phase VSPC model at high temperature within the single-phase β -region. Errors notably increased in the regions where the β -phase volume fraction changed as a function of temperature, though this may be due to using parameters that are not the most optimized for a dual-phase system and the use of homothetic hardening for each slip system within each phase. Simulated texture results were in good qualitative agreement with experimentally measured results. Quantitative measures for the texture differences were not able to be achieved as experimentally measured textures tend to capture some amount of subsurface orientation data due showing some amount of

diffuseness in the orientations whereas simulations only model the texture evolution at the surface and is highly localized. Overall results are quite good and should prove useful for future work.

7.2 Future Work

The work presented here was intended to accomplish several tasks related to the formation of dual-phase constitutive models for Ti-6Al-4V. Starting with an existing MTS model, modifications were made that extended applicability into the high-strain rate regime as well as modifications made to more accurately describe initial work-hardening behavior post yielding. The MTS model and modifications were then successfully implemented within the VPSC program to describe the stress-strain behavior under high strain-rate compression and dual-phase texture evolution under high-speed machining conditions. With the completion of this current study, there are several areas of research where this work can be further extended or applied.

The texture evolution in this work was modeled for one sample that was machined with a cutting speed of 100 m/min, a depth of cut of 0.2 mm and a feed rate of 0.0508 mm/revolution. Other samples were machined with various cutting speeds, depth of cuts and feed rates, but FEA simulations have not been implemented to generate velocity gradient and temperature profiles for those specific conditions. The first suggestion for future work entails the completion of FEA simulations to further validate texture evolution simulations from this model with machined samples under differing process conditions.

The second suggestion for future work relates to running VPSC simulations with the dual-phase MTS constitutive relations at various points below the surface to model the

stress-strain response as a function of depth. XRD glancing angle methods have been used to analyze residual stress in the machined surface of all samples related to this project, though not part of this work. Because residual stress development is in part due to the competition of decreasing plastic strength with decreasing strain-rates and increasing plastic strength with decreasing temperatures as a function of depth below the machined surface, VPSC simulations are capable of describing the constitutive response of a material, again as a function of depth, undergoing high-speed machining. FEA simulations can provide the necessary velocity gradients and temperature profiles as a function of depth for each of the various machining conditions.

The third suggestion for future work relates to more modern approaches to the micromechanical modeling of material properties. The VPSC model is a mean-field approach to micromechanical modeling and is reliant on one-point statistics, or volume fractions of phases or heterogeneities to calculate homogenization relations; this is well outside the scope of this thesis and the reason it was not addressed in the background material. Another useful program to model the anisotropic properties of viscoplastic polycrystals, also developed at Los Alamos, is the FFT code. This program, based off of the work of Moulinec and Suquet, uses the method of fast-Fourier transforms over periodic heterogeneous microstructures (representative volume elements) to provide exact solutions mechanical equilibrium equations [61, 62]. Unlike the VPSC model, the FFT model uses two-point statistics, or spatial distributions of heterogeneities, to better estimate the local response of polycrystalline materials. EBSD images taken as part of this work already provide the necessary microstructure information for construction of representative volume elements for two-phase materials. Currently, the FFT code only uses a modified Voce

hardening law to model the evolution of threshold stress and it is recommended that work be undertaken to incorporate the MTS model within the FFT code to expand its capability for use under dynamic processing conditions and further test the MTS model developed in this work.

The final recommendation for future work involves further investigation of the modifications made to the work-hardening rate coefficient (Equation (21)) in the MTS model. Certain combinations of parameters within this equation lead to a stress-strain response that mimic the yield-point phenomenon (i.e. upper and lower yield-point behavior) due to alloying effects. Chen and Gray examined the compression behavior of tantalum with 2.4, 5.2 and 9.6 wt% tungsten additions over temperatures ranging from 298-873 K and strain-rates ranging from 0.001-2500 s⁻¹ [63]. In addition, the authors fitted the MTS model for each system. The data for tantalum with 9.6 wt% tungsten is particularly attractive as it displays the yield-point phenomenon quite nicely. The authors were contacted and provided the raw experimental data for these data sets. To that effect, it would be an interesting exercise to examine the modification made to the work-hardening rate coefficient within this work and see if there is any consistency to which it could potentially model the yield-point phenomenon experimentally measured.

APPENDIX A. MODEL COMPARISONS TO EXPERIMENTAL DATA

In this appendix, the simulated stress-strain data is compared with all reported experimental data points for each model. Appendix A.1 gives the comparison for the macroscopic MTS model, A.2 gives the comparison for the single-phase VPSC model and A.3 gives the comparison for the dual-phase VPSC model. The percentage error is calculated using:

$$\% \text{ Error} = \left(\frac{\sigma_{sim}}{\sigma_{meas}} - 1 \right) \times 100\% \quad (27)$$

where σ_{sim} are the simulated stress values and σ_{meas} are the measured stress values.

A.1 Comparison of Macroscopic MTS Model to Full Experimental Results

Table 8: Experimentally measured and calculated yield stress values for various temperature and strain rates. Calculated values were made using the macroscopic MTS model.

Temperature (K)	Strain Rate (s ⁻¹)	$\sigma_{ys\ meas}$ (MPa)	$\sigma_{ys\ MTS}$ (MPa)	% Error
298	400	970	980.9	1.12
	450	982	983.1	0.11
	800	998	997.3	-0.07
	1400	1010	1020.2	1.01
	1700	1017	1031.3	1.40
	2000	1030	1042.2	1.19
573	800	861	821.7	-4.57
	1400	876	842.0	-3.88
	1700	884	851.7	-3.66
	2000	891	861.1	-3.35
	2500	909	876.6	-3.57
	2700	923	882.7	-4.37
773	800	717.9	693.9	-3.34
	1400	729	712.4	-2.27
	1700	736.9	721.0	-2.16
	2000	746	729.3	-2.23
	2500	754	742.8	-1.48
973	800	580	567.4	-2.17
	1700	595	591.5	-0.59
	2000	615	598.6	-2.66
	2500	630	610.2	-3.15
	3300	644	627.9	-2.50
1173	1700	470	464.0	-1.28
	2000	480	470.0	-2.09
	2500	495	480.0	-3.14
1373	2000	330	345.0	4.53
	2500	343	352.4	2.74

Table 9: Experimentally measured and calculated stress values at a strain of 0.1 for various temperature and strain rates. Calculated values were made using the macroscopic MTS model.

Temperature (K)	Strain Rate (s ⁻¹)	σ_{meas} (MPa)	σ_{MTS} (MPa)	% Error
298	800	1404.8	1403.8	-0.07
	1400	1413.7	1427.7	0.98
	1700	1421.3	1439.1	1.25
	2000	1431.5	1450.3	1.31
573	800	1149.2	1155.8	0.58
	1400	1162.1	1178.1	1.38
	1700	1167.4	1188.4	1.80
	2000	1178.9	1198.4	1.66
	2500	1189.3	1214.7	2.13
	2700	1197.2	1221.0	1.99
773	1400	1004.1	996.5	-0.75
	1700	1006.4	1006.0	-0.04
	2000	1025.7	1015.0	-1.04
	2500	1033.8	1029.5	-0.41
973	800	832.5	796.8	-4.28
	1700	835.2	825.0	-1.23
	2000	838.16	833.0	-0.61
	2500	849.3	845.8	-0.42
	3300	864.2	865.0	0.09
1173	1700	654.6	646.6	-1.22
	2000	661.9	653.6	-1.25
	2500	674.8	664.7	-1.52
1373	2000	491.3	478.9	-2.52
	2500	501.6	487.9	-2.73

Table 10: Experimentally measured and calculated stress values at a strain of 0.2 for various temperature and strain rates. Calculated values were made using the macroscopic MTS model.

Temperature (K)	Strain Rate (s^{-1})	σ_{meas} (MPa)	σ_{MTS} (MPa)	% Error
298	1700	1513.8	1513.4	-0.03
	2000	1519.6	1524.7	0.34
573	1700	1228.1	1248.0	1.62
	2000	1237	1258.2	1.71
	2500	1244.6	1274.6	2.41
	2700	1251.4	1281.1	2.37
773	1700	1058.5	1055.0	-0.33
	2000	1074.2	1064.3	-0.92
	2500	1080.6	1079.1	-0.14
973	1700	878.2	863.7	-1.65
	2000	876.7	872.0	-0.54
	2500	883.6	885.1	0.17
	3300	895.2	904.7	1.06
1173	1700	686.5	675.4	-1.62
	2000	691.2	682.7	-1.23
	2500	700.1	694.0	-0.88
1373	2000	515.3	498.6	-3.24
	2500	524	507.9	-3.06

A.2 Comparison of Single-Phase VPSC Model to Full Experimental Results

Table 11: Experimentally measured and calculated yield stress values for various temperature and strain rates. Calculated values were made using the single-phase MTS model within VPSC.

Temperature (K)	Strain Rate (s ⁻¹)	$\sigma_{ys\ meas}$ (MPa)	$\sigma_{ys\ VPSC}$ (MPa)	% Error
298	400	970	980.3	1.06
	450	982	982.4	0.04
	800	998	996.7	-0.13
	1400	1010	1019.5	0.94
	1700	1017	1030.6	1.34
	2000	1030	1041.5	1.12
573	800	861	821.2	-4.63
	1400	876	841.5	-3.94
	1700	884	851.1	-3.72
	2000	891	860.6	-3.41
	2500	909	876.0	-3.63
	2700	923	882.1	-4.43
773	800	717.9	693.5	-3.39
	1400	729	712.0	-2.33
	1700	736.9	720.7	-2.20
	2000	746	728.9	-2.29
	2500	754	742.4	-1.54
973	800	580	567.2	-2.22
	1700	595	591.2	-0.65
	2000	615	598.3	-2.71
	2500	630	609.8	-3.20
	3300	644	627.5	-2.56
1173	1700	470	463.8	-1.33
	2000	480	469.8	-2.13
	2500	495	479.3	-3.18
1373	2000	330	344.8	4.50
	2500	343	352.3	2.71

Table 12: Experimentally measured and calculated stress values at a strain of 0.1 for various temperature and strain rates. Calculated values were made using the single-phase MTS model within VPSC.

Temperature (K)	Strain Rate (s^{-1})	σ_{meas} (MPa)	σ_{VPSC} (MPa)	% Error
298	800	1404.8	1406.0	0.09
	1400	1413.7	1429.9	1.15
	1700	1421.3	1441.4	1.41
	2000	1431.5	1452.7	1.48
573	800	1149.2	1157.8	0.75
	1400	1162.1	1180.1	1.55
	1700	1167.4	1190.5	1.98
	2000	1178.9	1200.5	1.83
	2500	1189.3	1216.8	2.31
	2700	1197.2	1223.2	2.17
773	1400	1004.1	998.3	-0.58
	1700	1006.4	1007.8	0.14
	2000	1025.7	1016.9	-0.86
	2500	1033.8	1031.4	-0.23
973	800	832.5	798.4	-4.10
	1700	835.2	826.5	-1.04
	2000	838.16	834.6	-0.42
	2500	849.3	847.4	-0.22
	3300	864.2	866.7	0.29
1173	1700	654.6	648.0	-1.01
	2000	661.9	655.0	-1.04
	2500	674.8	666.0	-1.31
1373	2000	491.3	480.0	-2.29
	2500	501.6	489.1	-2.50

Table 13: Experimentally measured and calculated stress values at a strain of 0.2 for various temperature and strain rates. Calculated values were made using the single-phase MTS model within VPSC.

Temperature (K)	Strain Rate (s^{-1})	σ_{meas} (MPa)	σ_{VPSC} (MPa)	% Error
298	1700	1513.8	1517.7	0.26
	2000	1519.6	1529.1	0.63
573	1700	1228.1	1251.9	1.94
	2000	1237	1262.2	2.04
	2500	1244.6	1278.7	2.74
	2700	1251.4	1285.2	2.70
773	1700	1058.5	1058.6	0.01
	2000	1074.2	1067.9	-0.59
	2500	1080.6	1082.7	0.19
973	1700	878.2	866.8	-1.29
	2000	876.7	875.2	-0.17
	2500	883.6	888.3	0.53
	3300	895.2	908.1	1.44
1173	1700	686.5	678.1	-1.22
	2000	691.2	685.4	-0.83
	2500	700.1	696.8	-0.48
1373	2000	515.3	500.9	-2.80
	2500	524	510.3	-2.62

A.3 Comparison of Dual-Phase VPSC Model to Full Experimental Results

Table 14: Experimentally measured and calculated yield stress values for various temperature and strain rates. Calculated values were made using the dual-phase MTS model within VPSC.

Temperature (K)	Strain Rate (s ⁻¹)	$\sigma_{ys\ meas}$ (MPa)	$\sigma_{ys\ VPSC}$ (MPa)	% Error
298	400	970	968.7	-0.13
	450	982	970.9	-1.13
	800	998	985.6	-1.24
	1400	1010	1009.1	-0.09
	1700	1017	1020.6	0.35
	2000	1030	1031.9	0.18
573	800	861	818.7	-4.91
	1400	876	839.7	-4.14
	1700	884	849.7	-3.88
	2000	891	859.5	-3.53
	2500	909	875.6	-3.67
	2700	923	882.0	-4.45
773	800	717.9	697.1	-2.89
	1400	729	716.3	-1.75
	1700	736.9	725.2	-1.59
	2000	746	733.9	-1.63
	2500	754	748.0	-0.80
973	800	580	576.5	-0.61
	1700	595	601.4	1.08
	2000	615	608.9	-0.99
	2500	630	621.1	-1.42
	3300	644	639.8	-0.65
1173	1700	470	450.9	-4.06
	2000	480	458.3	-4.51
	2500	495	470.2	-5.02
1373	2000	330	329.9	-0.04
	2500	343	344.1	0.32

Table 15: Experimentally measured and calculated stress values at a strain of 0.1 for various temperature and strain rates. Calculated values were made using the dual-phase MTS model within VPSC.

Temperature (K)	Strain Rate (s^{-1})	σ_{meas} (MPa)	σ_{VPSC} (MPa)	% Error
298	800	1404.8	1389.6	-1.08
	1400	1413.7	1414.2	0.04
	1700	1421.3	1425.9	0.32
	2000	1431.5	1437.6	0.43
573	800	1149.2	1151.1	0.17
	1400	1162.1	1174.2	1.04
	1700	1167.4	1185.0	1.51
	2000	1178.9	1195.4	1.40
	2500	1189.3	1212.3	1.93
	2700	1197.2	1218.9	1.81
773	1400	1004.1	999.3	-0.48
	1700	1006.4	1009.2	0.28
	2000	1025.7	1018.7	-0.68
	2500	1033.8	1033.9	0.01
973	800	832.5	804.6	-3.35
	1700	835.2	834.5	-0.09
	2000	838.16	843.0	0.58
	2500	849.3	856.6	0.86
	3300	864.2	877.1	1.49
1173	1700	654.6	635.3	-2.94
	2000	661.9	645.0	-2.55
	2500	674.8	659.9	-2.22
1373	2000	491.3	482.6	-1.77
	2500	501.6	504.0	0.47

Table 16: Experimentally measured and calculated stress values at a strain of 0.2 for various temperature and strain rates. Calculated values were made using the dual-phase MTS model within VPSC.

Temperature (K)	Strain Rate (s^{-1})	σ_{meas} (MPa)	σ_{VPSC} (MPa)	% Error
298	1700	1513.8	1498.7	-1.00
	2000	1519.6	1510.5	-0.60
573	1700	1228.1	1242.5	1.17
	2000	1237	1253.2	1.31
	2500	1244.6	1270.1	2.04
	2700	1251.4	1277.3	2.07
773	1700	1058.5	1055.9	-0.25
	2000	1074.2	1065.8	-0.78
	2500	1080.6	1081.5	0.08
973	1700	878.2	870.8	-0.84
	2000	876.7	879.8	0.35
	2500	883.6	893.9	1.16
	3300	895.2	915.1	2.22
1173	1700	686.5	665.1	-3.11
	2000	691.2	676.0	-2.20
	2500	700.1	692.5	-1.09
1373	2000	515.3	504.5	-2.09
	2500	524	529.5	1.04

APPENDIX B. METHOD OF TEXTURE SUBTRACTION

B.1 MATLAB Code for Method of Texture Subtraction

```
%% Import Script for ODF Data - MUST RUN IN MTEX 5.03
%
% This script was automatically created by the import wizard. You should
% run the whole script or parts of it in order to import your data. There
% is no problem in making any changes to this script.

%% Specify Crystal and Specimen Symmetries

% crystal symmetry
CS = crystalSymmetry('6/mmm', [2.95 2.95 4.686], 'X||a*', 'Y||b', 'Z||c', 'mineral',...
'Titanium', 'color', 'light blue');

% specimen symmetry
SS = specimenSymmetry('1');

% plotting convention
setMTExpref('xAxisDirection','north');
setMTExpref('zAxisDirection','outOfPlane');

%% Specify File Names

% path to files
pname = '... /Ti64_XRD_Data';

% which files to be imported
fname = [pname '/as_received_sample_orientations.txt'];

%% Specify File Names

% path to files
pname1 = '... /Ti64_XRD_Data';

% which files to be imported
fname1 = [pname1 '/post_machined_sample_orientations.txt'];

%% Import the Data
```

```

% specify kernel
psi = deLaValeePoussinKernel('halfwidth',10*degree);

% create an EBSD variable containing the data for as-received sample
odf1 = loadODF(fname,CS,SS,'density','kernel',psi,...
    'interface','generic',...
    'ColumnNames', { 'phi1' 'Phi' 'phi2' 'Weights'}, 'Bunge');

% create an EBSD variable containing the data for post-machined sample
odf2 = loadODF(fname1,CS,SS,'density','kernel',psi,...
    'interface','generic',...
    'ColumnNames', { 'phi1' 'Phi' 'phi2' 'Weights'}, 'Bunge');

% subtract as-received texture from post-machined texture
odf3 = minus(odf2, odf1);

% creates a new equispaced grid on the surface of a sphere
ori = equispacedSO3Grid(CS,SS,'resolution',2.5*degree);

% evaluates the odf difference above (odf3) at each grid point over the spherical
% surface and takes the maximum between the point to point texture values or zero,
% whichever is greater
v = max(0,odf3.eval(ori));

% creates a new odf based on the previously calculated texture difference or zero
% values that are now applied at the grid points on the surface of a sphere and
% interpolates the rest of the data between each grid point
ODF4 = ODF.interp(ori,v);

% export new odf orientation values into a list of Euler Angles for VPSC inputs or further
% plotting
export_VPSC(ODF4,'9-13alphadiff.txt','points',20000);

```

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