Three Dimensional Modeling of Titanium-Aluminum Alloys with Application to Attachment Fatigue

A Thesis
Presented to the Academic Faculty
By
Jason R. Mayeur

In Partial Fulfillment
of the Requirements for the Degree
Master of Science in Mechanical Engineering

Georgia Institute of Technology
November, 2004
Three Dimensional Modeling of Titanium-Aluminum Alloys with Application to Attachment Fatigue

Dr. David L. McDowell

Dr. Richard. W. Neu

Dr. Min Zhou

Date Approved: 22 November 2004
ACKNOWLEDGEMENTS

First I would like to give a special thanks to my advisor Dr. David L. McDowell for his patience, guidance, and encouragement throughout the completion of this work. I have greatly benefited from his helpful comments and insight throughout the completion of this work. I would also like to thank the other committee members, Dr. Richard W. Neu and Dr. Min Zhou, for their patience and thoughtful suggestions. And lastly, I would like to thank all of my friends and colleagues for both the technical and social discourse I’ve enjoyed since I’ve been at Georgia Tech.
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SUMMARY

The increasing use of $\alpha/\beta$ Ti-Al alloys in critical aircraft gas turbine engine and airframe applications necessitates the further development of physically-based constitutive models that account for their complex microdeformation mechanisms. Alpha/beta Ti-Al alloys are dual-phase in nature consisting of a mixture of hcp ($\alpha$) and bcc ($\beta$) crystal structures, which through variation in alloying elements and/or processing techniques can be produced in a wide range of microstructural compositions and morphologies. A constitutive model for these materials should address the various sources of material anisotropy and heterogeneity at both the micro and macroscales. The main sources of anisotropy in these materials are the low symmetry of the hcp phase, the texture, the relative strengths of different slip systems, non-planar dislocation core structures, phase distributions, and dislocation substructure evolution.

The focus of this work is the development of a 3-D crystal plasticity model for duplex Ti-6Al-4V (Ti-64), an ($\alpha + \beta$) alloy. The model is used to study the process of attachment fatigue. Attachment fatigue is a boundary layer phenomenon in which most of the plastic deformation and damage accumulation occurs at depths on the order of tens of microns and encompasses regions of only a few grains into the depth of the material. The use of computational micromechanics-based crystal plasticity models to study attachment fatigue is a relatively new approach. This approach has the potential to offer
additional insight to classical homogeneous plasticity models, since the length scales over which relative slip and crack initiation occur during this process is on the order of microstructural dimensions. Emphasis is placed on understanding the effects that texture, slip strength anisotropy, and phase distribution have on the surface and subsurface deformation fields during attachment fatigue. The deformation fields are quantified in terms of cumulative effective plastic strain distributions and plastic strain maps.

The results clearly demonstrate the importance of considering the various sources of microstructural heterogeneity during the process of fretting fatigue. The main sources of microstructural heterogeneity in these materials are the distribution of phases, slip system strength anisotropy, and crystallographic texture. The necessity of including realistic 3-D textures is especially underscored in this work as the distribution and cyclic behavior of the plastic strain can be fundamentally different for different types of textured materials. If is shown that basal textured materials, in which a large number of grains in the polycrystal are able to deform by soft slip modes, that the plastic strain distributions are more evenly distributed in the subsurface regions and as a result have less intense regions of significant plastic strain accumulation. However, the sharper transverse and basal / transverse textured materials feature subsurface plastic zones in which the plastic strain accumulates in narrow vein-like structures leading to more intense regions of cumulative effective plastic strain.

Similarly, the texture of the material is observed to influence the cyclic plastic strain behavior. Due to the homogeneous distribution of plastic strain for the basal textured material, the majority of the plastic zone has already reached a state of elastic shakedown by the start of the 3\textsuperscript{rd} tangential loading cycle, which is indicative of the more
uniform distribution of residual stresses that develop for this type of textured material. However, the transverse and basal / transverse textured materials still show that a large portion of the plastic zone is still deforming via cyclic plastic ratcheting over the 3rd tangential loading cycle. Again, this is a result of the sharper nature of these type of textures in which a relatively small number of banded regions in the plastic zone are accommodating a majority of the plastic deformation. This heterogeneous distribution of deformation leads to the more pronounced plastic ratcheting for these types textures. These fundamental differences in cyclic plastic strain behavior due to the influence of microstructural heterogeneity emphasize the importance of this work, and the need for continued study of the process of fretting fatigue with physically-based micromechanical models.
CHAPTER I

INTRODUCTION

Material microstructure correlates strongly with corresponding macroscopic properties. Within the past century, significant effort has been invested in the understanding and modeling of materials at the microstructural level in hope of gaining a fundamental understanding of the physics of important deformation processes that originate at this scale, such as plasticity, fatigue, fracture, creep, phase transformation, etc. In the case of polycrystalline metals, which are composed of aggregates of single crystals (grains), anisotropy of material behavior derives from microstructure ranging from the subgrain scale to the macroscale. The key contributors to this anisotropy in metals on the macroscopic scale are the orientation distribution function (texture), the crystal structure, and the dislocation substructure of the constituent single crystals or grains. Equally influential on material response is the dependence of single grain behavior on constraints of neighboring grains in the polycrystalline aggregate.

Plastic deformation in metals is the manifestation of microstructure evolution due to dislocation motion, and can occur in various ways from dislocation glide and twinning to phase transformation. For a given material the plastic deformation mechanisms may be dominated by one of the aforementioned processes, but more realistically may involve an intricate coupling of multiple competing mechanisms over various microstructural
length scales. Regardless of which mechanisms are active for a given material, each one depends on the underlying crystallographic structure.

Traditional macroscopic models of metal plasticity are unable to capture the local details of the deformation mechanisms occurring at the microstructural level. However, the use of physically-based macro-models is still adequate for many engineering applications in which the variation of the local deformation fields in the presence of heterogeneous microstructural features is not integral to the problem at hand. For other applications, such as attachment fatigue, when the scale of the plastic deformation is on the same order as the microstructural features, more detailed plasticity models are required to capture the local changes in the deformation fields due to the heterogeneous nature of the material when observed at these length scales.

In the early work of Taylor (1934) on aluminum it was observed that at low homologous temperatures the glide of dislocations through the crystal lattice was the main source of plastic deformation in metals. In an attempt to describe the macroscopic response of a polycrystalline aggregate in terms of the deformation mechanisms occurring at the level of a single crystal, crystal plasticity theory was developed. Developing a polycrystalline model for metal plasticity, based on experimental observations of single crystal deformation, requires specification of the active deformation processes for a given material as well as some type of constraint for intergranular interactions.

The basis of crystal plasticity theory comes from the observations noted in these early works that dealt with single phase fcc metals, for which the dislocation core is split into Shockley partial dislocations in the (111) planes. The planar nature of the dislocation
core results in these materials obeying Schmid’s law. In the years since these initial observations, a wider variety of materials have been studied and our understanding of the deformation mechanisms has grown. It has become obvious that further development of the theory is necessary to model the more advanced materials currently being used in a wide variety of engineering applications.

An important class of materials that is the focus of this research is Ti-Al alloys. Industrial applications for these alloys range from aircraft gas turbine engine components to biomedical components. There are two main types of Ti-Al alloys being studied today, $\gamma$-Ti-Al and $\alpha/\beta$-Ti-Al (either $\alpha+\beta$ or $\beta$ processed). Both classes of alloys are capable of being produced in a variety of microstructural compositions through different processing techniques. The key difference between the two types of alloys is their crystallographic structure: $\gamma$-Ti-Al alloys are of mixed hcp and fcc structure, whereas the $\alpha/\beta$ alloys are of mixed hcp and bcc structure.

These multi-phase alloys have very complex microstructures with equally complex deformation mechanisms that can be difficult to quantify with current experimental techniques. One of the major difficulties of dealing with these materials is determining the elastoplastic properties of the individual phases. It is difficult, if not impossible, to isolate a single crystal of each phase of the considered alloy with its exact composition in the bulk material. Unlike fcc metals, the dislocation cores in these alloys are non-planar and therefore do not obey Schmid’s law. This is evidenced by the experimental observation of tension/compression asymmetry and anomalous temperature dependence of yield behavior. Another key issue is how the slip geometry is modified in the secondary particles and at the interfaces between the primary and secondary phases.
In the particular alloys that have a lamellar secondary phase, consisting of alternating plates of hcp and bcc (or fcc) structure, there is a need to determine how these grains affect the dislocation substructure evolution and strain hardening at the macroscale, as well as which lamellae length scale(s) govern this process.

The last two decades have seen an exponential increase in computing power, and not coincidentally, a shift in the engineering design paradigm. With product design cycles rapidly decreasing, researchers cannot afford to perform exhaustive experimental tests or rely on macroscopic models to quantify a wide range of material properties that inherently depend on the microstructure. Employing an exorbitant factor of safety for design purposes is no longer an acceptable approach in many applications. Instead, efforts have been shifted to further developing computational micromechanical models, such as crystal plasticity, that incorporate the physics of the deformation processes. These models, used in conjunction with a reduced number of experiments that are carefully designed to highlight the relevant microstructural deformation mechanisms, will lead to a more fundamental understanding of the origins of material failure at the microscopic level. Our specific application to fretting fatigue in this study is an ideal application in that it demands application of micromechanical crystal plasticity to model deformation of surface and near-surface grains in the contact boundary layer.

The main objective of this work is to develop a 3-D physically-based crystal plasticity constitutive model for multi-phase Ti-Al alloys for use in fretting fatigue analyses. While much of the recent effort has been dedicated to developing models for γ-Ti-Al alloys, this work will focus on Ti-6Al-4V, a dual phase α/β alloy. The modeling effort will address the 3-D slip geometry and the interaction of the various types of slip
systems and their relative strengths in the low symmetry hcp structure, dislocation core spreading, and the resultant tension/compression asymmetry, appropriate hardening laws that incorporate dislocation substructure evolution, and twinning.

Fretting fatigue is especially of interest since the length scale over which relative slip and crack initiation occurs during this process is on the order of microstructural dimensions. Emphasis in the fretting simulations will be placed on understanding the effects that texture, low symmetry of the hcp structure (misorientation of grains), and phase distributions have on the plastic strain distributions. This work is an extension of the 2-D crystal plasticity fretting simulations performed by Goh (2002), and will be compared to these results to highlight additional insight that is gained from the use of a 3-D constitutive model.

The thesis is organized as follows. Chapter II begins by giving a microstructural characterization of several Ti-Al alloys and discusses the various deformation mechanisms observed in these materials. This is followed by discussion of dislocation core spreading and phase distributions in these alloys. The Chapter concludes by reviewing crystal plasticity as it pertains to low symmetry crystals and multi-phase materials. Chapter III presents the 3-D crystal plasticity model formulation in two parts: a model for an hcp material (α-phase) and an implicit model for the secondary (α + β)-phase which is composed of alternating plates of hcp and bcc structure. The dual-phase material can then be represented by incorporating both descriptions of the primary α-phase as well as the implicit representation of the (α + β) lamellar structures. Chapter III concludes with a parametric study on the sensitivity of material response to changes in various model parameters. In Chapter IV, the cyclic deformation behavior (mean stress
uniaxial as well as fretting simulations) of Ti-6Al-4V is investigated using the 3D dual-phase crystal plasticity. The results of the simulations are presented and compared to the previous computational studies of Morrissey (2001) and Goh (2002) in addition to the experimental work by Swalla (2003) on Ti-6Al-4V.
CHAPTER II
BACKGROUND

Titanium, known for its high strength to weight ratio and good resistance to corrosion, can be alloyed with other metals and heat treated to achieve a wide range of attractive properties at both high and low temperatures. In particular various Ti-Al alloys offer a range of properties such as high strength and fracture toughness at low temperatures to high strength and creep resistance at elevated temperatures. This wide range of properties have led to extensive use of Ti-Al alloys in engineering applications from airframe components, to compressor blades, as well as biomedical applications. The broad spectrum of properties that can be achieved from Ti-Al alloys is made possible by the numerous microstructures that can be obtained by varying the alloying elements and their respective composition percentages, the processing methodology, and the heat treatment.

Unalloyed titanium is of hcp crystal structure at room temperature, but undergoes a phase transformation from the hcp (\(\alpha\)) phase to a bcc (\(\beta\)) phase at a temperature around 882° C. By varying the alloying elements it is possible to create materials that consist solely of all \(\alpha\) -phase, all \(\beta\) -phase, a mixture of \(\alpha\) and \(\beta\) -phases, and in the case of certain Ti-Al alloys a mixture of \(\gamma\) (fcc) and \(\alpha_2\) (hcp Ti\(_3\)Al) phases. Recently, the two most commonly studied types of Ti-Al alloys are the dual phase (\(\alpha + \beta\)) and
($\gamma + \alpha_2$) materials. The favorable properties of ($\alpha + \beta$) alloys tend to be good strength at low temperatures, high ductility, and easy workability (Picu and Majorell, 2002), whereas ($\gamma + \alpha_2$) alloys offer excellent high temperature properties such as creep resistance, microstructural stability, oxidation resistance, as well as good ductility and fracture toughness (Grujicic and Batchu, 2001). As was mentioned earlier, there are a variety of microstructures that can be realized for the same alloy depending on the processing parameters and heat treatment, each with its own unique set of material properties. In order to be able to optimize an alloy and its microstructure for a particular application, it is necessary to quantify the arrangement of phases and the active deformation mechanisms in them. In general, components made from bulk material of these alloys can exhibit highly anisotropic and texture dependent macro material response due to the inherent anisotropy and low symmetry of the hcp crystal structure. Further complicating the micro deformation processes is the fact that these are dual phase materials. Issues that arise in dealing with such materials are the variations in the properties of the individual phases due to different amounts of alloying elements, the dependence on phase distributions, microstructural length scales, and the deformation and compatibility requirements at phase interfaces. The focus of the following discussion will be on $\alpha$-titanium and the $\alpha/\beta$ class of Ti-Al alloys.
2.1 Microstructural Description

2.1.1 Crystallographic Aspects of the hcp Crystal Structure

Understanding the deformation mechanisms in titanium and Ti-Al based alloys first requires knowledge of crystallographic planes and directions of the hexagonal structure. Unlike fcc materials, in which slip predominantly occurs on the \{111\} family of planes, the hcp structure has several families of planes on which slip or twinning might occur. In most hcp materials, the primary slip planes are either basal (0001) or prismatic \{10\overline{1}0\} with the slip vector being in the closed packed \{11\overline{2}0\} direction. For a long time it was thought (Duesbery, 1989) that the deviation of the material from the ideal c/a ratio, 1.633, determined the dominant slip plane. This simple rule is based on the observation that slip occurs more easily on the family of planes with the largest inter-planar spacing, which obviously depends on the c/a ratio. A material with c/a ratio greater than ideal was thought to deform primarily on basal planes, whereas one with a c/a ratio less than ideal was thought to deform primarily on prismatic planes. There are exceptions to this rule such as Be, and we now know that the preferred slip plane depends on the dissociated dislocation core structure and stacking fault energy associated with the different families of slip planes. The works of (Duesbery, 1989; Vitek, 1992) show that the splitting of partial dislocations into any particular crystallographic plane is usually the reason why such a plane is preferred (i.e. splitting of \{111\}\{110\} dislocations into Shockley partials in fcc materials). However, titanium is known to exhibit a flow stress vs. temperature anomaly as well as orientation dependent yielding (Naka et al., 1988) which seems to indicate a non-planar core structure of primary dislocations (Bassani et al., 2001). The
core structure of dislocations in titanium and its effect on the plastic deformation of these materials will be discussed in detail in Section 2.3.

In order to accommodate an arbitrary plastic strain in three dimensions, the von Mises criterion states that a crystal must possess at least five independent slip systems (Kelly et al., 2000). This results from the fact that there are six independent components (in the non-polar case) of the general strain tensor, but since it is assumed that there is no dilatational strain \( \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = 0 \) in plastic deformation, there are only five independent components of the plastic strain tensor. The basal and prismatic planes with \( \{a\} \)-type \( \{11\overline{2}0\} \) burgers vector only comprise four independent systems, and therefore there must be some additional slip or twinning systems to account for the fifth independent system. This is usually either the first-order \( \{10\overline{1}1\} \) or second-order \( \{11\overline{2}2\} \) pyramidal system with the burgers vector \( \{1\overline{1}2\overline{3}\} \). These \( \{e+a\} \) type systems are necessary to accommodate for an arbitrary strain parallel to the c-axis. The crystallographic planes and burgers vectors discussed above are illustrated in Figure 2.1 with the slip plane highlighted red and the possible burgers vectors highlighted blue. Observations of the particular systems active in titanium and \( \alpha/\beta \) Ti-Al alloys will be discussed in Section 2.2.1.
Twinning can play an important role in the deformation and compatibility of hcp metals and alloys. Generally speaking, the activity of multiple twinning modes within an hcp structured material is the reason why certain metals, such as titanium and zirconium, exhibit good ductility. On the other hand, the brittleness of other hcp metals is the result of very few available twin systems during deformation (Yoo, 1981). As one might expect the twinning process in hcp materials is very complex and is highly dependent on the c/a ratio. A number of operative twinning systems have been reported in the literature for titanium including \{10\bar{1}1\}, \{10\bar{1}2\}, \{11\bar{2}2\}, \{11\bar{2}3\}, and \{11\bar{2}1\} (Tan et al., 1998a). Of these, the four most often observed and therefore most important are the systems \{10\bar{1}1\}, \{10\bar{1}2\}, \{11\bar{2}2\}, and \{11\bar{2}1\}. A schematic of these habit planes is given below in Figure 2.2.
Figure 2.2: Most frequently observed twin habit planes in titanium.

For titanium, which has a c/a ratio of 1.588, the \{1\bar{2}11\} and \{1211\} systems are tension twins and the \{10\bar{1}2\} and \{1\bar{2}12\} compression twins. Tension twins cause an extension of the crystal along the c-axis, whereas compression twins result in a distension of the crystal along the c-axis. As noted by Yoo (1981), the number of independent modes provided by a single twin system will depend on the sense of the twinning shear with respect to the internal stress state of the crystal. If both tension and compression twins are active, five independent deformation modes are guaranteed regardless of the internal stress state. A couple of other key aspects of twinning in hcp metals are the variations in magnitudes of the twinning shears associated with each type of system, as well as the ratio of atoms that are reshuffled during twinning to the number of atoms inside the unit cell of the twin. Both of these quantities serve as indicators as to which systems should be the easiest to activate. It should also be pointed out that the magnitude of the twinning shear is dependent on the c/a ratio. Some of the pertinent parameters
associated with each of the four main twinning systems in titanium are listed below in Table 2.1. The $\{10\overline{1}1\}$ system has the lowest magnitude of twinning shear and should be the most likely system to be activated.

Table 2.1 Crystallographic parameters of twinning systems in titanium. $N_t$ is the total number of atoms in the twin unit cell, $N_s$ is the number of atoms reshuffled during twinning, and $\gamma$ is the magnitude of the twinning shear.

<table>
<thead>
<tr>
<th>Habit Plane</th>
<th>Twinning Direction</th>
<th>$N_t$</th>
<th>$N_s/N_t$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>${10\overline{1}2}$</td>
<td>$\langle\overline{1}011\rangle$</td>
<td>8</td>
<td>3/4</td>
<td>0.174</td>
</tr>
<tr>
<td>${10\overline{1}1}$</td>
<td>$\langle\overline{1}012\rangle$</td>
<td>32</td>
<td>7/8</td>
<td>0.099</td>
</tr>
<tr>
<td>${1\overline{2}12}$</td>
<td>$\langle1\overline{1}23\rangle$</td>
<td>12</td>
<td>2/3</td>
<td>0.219</td>
</tr>
<tr>
<td>${1\overline{2}11}$</td>
<td>$\langle1\overline{1}26\rangle$</td>
<td>8</td>
<td>1/2</td>
<td>0.630</td>
</tr>
</tbody>
</table>

Owing to its hcp lattice, titanium unit cells are inherently transversely isotropic, which for both mono- and polycrystalline specimens can result in highly anisotropic behavior. The ratio of the elastic constants perpendicular and parallel to the basal plane is approximately 1.12. Also, as the loading direction of the crystal approaches the basal plane normal, the resolved shear stress for slip systems with $\langle a \rangle$- type burgers vector vanishes, which leads to the activation of harder deformation mechanisms (i.e., $\langle c+a \rangle$ slip or twinning). For these reasons, the orientation distribution function (ODF or texture) as well as the misorientation of the aggregate grains in a polycrystalline sample is extremely important. Depending on what type of processing technique is used in
forming the work piece, there are three more common textures found in these materials: basal, transverse, and basal + transverse (Peters et al., 1984). The sample ODF’s for these types of materials are represented quantitatively by basal plane pole figures given in Figure 2.3.

Figure 2.3: Basal pole figures of representative textures (a) basal texture (b) basal / transverse texture and (c) transverse texture.
2.1.2 Microstructural Morphology

Alpha/beta Ti-Al alloys are two-phase in nature and, depending on processing conditions and the cooling rate to below the $\beta$ transus ($\sim 1250$ K), can be produced in a wide range of microstructural variations (Suri et al., 1999). In addition to initial processing, further heat treatments may be used on these materials to achieve even more microstructural permutations. Figure 2.4 shows some of the possible microstructures that can be engineered in $\alpha/\beta$ Ti-Al alloys.
It is obvious from Figure 2.4 that both the shape and arrangement of the phases can be altered. The processing technique most frequently used for structural applications with these alloys is obtained by forging and annealing the material within the $(\alpha + \beta)$ region of the phase diagram. The resulting microstructure will consist of equiaxed $\alpha$ grains in addition to $(\alpha + \beta)$ lamellar colonies, which are composed of alternating layers of...
secondary $\alpha$ Widmanstätten plates and an untransformed residual $\beta$-phase. This most closely resembles the micrograph shown in Figure 2.4(b). If this material is further processed above the $\beta$ transus and is cooled at a slow rate (typical of air cooling), the microstructure will consist of colonies of Widmanstätten plates surrounded by a residual $\beta$-phase similar to that shown in Fig 2.4(e). However, if the material is cooled at a fast rate, as in the case of water quenching, the resulting microstructure will be composed of an acicular martensitic $\alpha$ ($\alpha'$) phase (Manero et al., 2000). The difference in processes arises because martensite formation is not strictly thermally activated. However, in these alloys the transformation processes cannot be neatly described either as “martensitic” or “nucleation and growth” (Collings, 1984). Therefore, a clear cut transition in cooling rates and the resulting microstructure does not exist, but instead a general division (listed in order from fast to slow cooling rates) based on diffusion coefficients is suggested by Collings (1984): (i) bulk martensite, (ii) acicular martensite, and (iii) Widmanstätten. Bulk or “massive” martensite is marked by large irregular zones of fine parallel plates with significant structural coherence and without the presence of a retained $\beta$ phase. Acicular martensite due to the slower cooling rate loses some of the coherency between regions which results in a somewhat disordered array of $\alpha$ platelets. Finally, the Widmanstätten structure, as discussed earlier, is made up of acicular $\alpha$ regions separated by the residual $\beta$-phase from which they grew.

Ti-6Al-4V (Ti-64), with a microstructure made up of primary $\alpha$ grains and secondary ($\alpha + \beta$) Widmanstätten colonies, is the $\alpha/\beta$ alloy that is most commonly used in practice (Picu and Majorell, 2002) and will serve as the focus of the following
discussion. The microstructural composition of the considered alloy, as previously
discussed, consists mostly of large globular primary $\alpha$-phase grains, with a smaller
number of interspersed secondary lamellar ($\alpha + \beta$) grains. Because the secondary $\alpha$
plates form out of large $\beta$ grains as the material is being cooled down below the $\beta$
transus, they exhibit an approximate burgers orientation relation (BOR) with the
untransformed $\beta$ they are sandwiched between. The BOR has been verified by several
researchers and is given as $(101)_{\beta} \parallel (0001)_{\alpha}, [1 \bar{T} \bar{T}]_{\beta} \parallel [1 \bar{1} 2 0]_{\alpha}$ (Savage et al., 2001). The
BOR has further geometrical implications that should be pointed out here:
\{$1 \bar{T} 2\}_{\beta} \parallel \{01 \bar{T} 0\}_{\alpha}, \{111\}_{\beta} \parallel \{1 \bar{1} 2 0\}_{\alpha}$ and \{$01 \bar{T}\}_{\beta} \parallel \{01 \bar{T} 1\}_{\alpha}, \{111\}_{\beta} \parallel \{1 \bar{1} 2 0\}_{\alpha}$ (Ankem
and Margolin, 1980). There is a slight difference in the magnitude of the burgers vector
in each phase such that $|b_{\alpha}| / |b_{\beta}| \approx 1.04$ (Suri et al., 1999) which leads to a misalignment
of $\sim 10^\circ$ between one of the $\langle a \rangle$-type vectors and the other $[111]$ vector in the interface
plane ($a_1$ and $b_1$ in Figure 2.5). It has also been reported by Suri et al. (1999) that there
exists a small misalignment in the BOR such that there is an angle of $\sim 0.7^\circ$ between the
primary vectors $a_2$ and $b_2$. A view normal to the interface plane $(110)_{\beta} \parallel (0001)_{\alpha}$ of the
ideal (neglecting the $0.7^\circ$ misalignment) BOR is shown in Figure 2.5 to illustrate the
geometrical relationships. The \{110\} plane is shown in green dashed lines superimposed
over the hexagonal basal plane.
According to the ideal BOR there are 12 possible variants that can be realized during the cooling process, but it should be noted that only one such variant is observed within each individual Widmanstätten colony (Ambard et al., 2001). Ambard et al. (2001) as well as Majorell et al. (2002) have noted that primary $\alpha$ grains surrounding colony regions tend to have orientations very near those of the neighboring secondary $\alpha$ plates. In addition, the secondary $\alpha$-phase has a higher initial dislocation density than the primary $\alpha$-phase resulting from their formation out of the large $\beta$ regions (Picu and Majorell, 2002).
2.2 Deformation Mechanisms and Mechanical Behavior

2.2.1 Deformation Mechanisms

There is general agreement within the literature that the controlling mechanism of plastic deformation in titanium and Ti-Al alloys subjected to quasi-static loading at room temperature is the glide of screw dislocations on prismatic planes (Naka et al., 1988). There is less agreement on the order of operation of secondary slip modes, but most would agree that the following list is fairly typical for the ease of operation: \((\bm{a})\)-type basal, \((\bm{a})\)-type first-order pyramidal, and \((\bm{c}+\bm{a})\)-type first- or second-order pyramidal. Also, in the case of unalloyed titanium and some Ti-Al alloys twinning can play a substantial role in plastic deformation behavior. The \((\bm{c}+\bm{a})\) slip systems and twinning systems are significantly harder deformation modes than \((\bm{a})\) slip systems, but in certain orientations with respect to applied loading, these harder modes will dictate the material behavior. As was mentioned earlier, the activation of these modes in hcp metals is necessary to accommodate an arbitrary applied strain, and in particular accommodation of deformation along the c-axis. Typically, these harder modes dominate only when the mobility of \((\bm{a})\)-type screw dislocations is minimized. Low dislocation mobility can be the result of stressing the crystal along the direction of the c-axis such that the resolved shear stress on \((\bm{a})\) systems is near zero, or by deforming the material at low temperatures and/or high strain rates. Twinning and \((\bm{c}+\bm{a})\) slip are also observed, but do not dominate, near grain boundaries in polycrystalline materials where their activation is
necessary to relieve incompatibility strains that develop during deformation (Medina Perilla and Sevillano, 1995).

2.2.2 Mechanical Behavior of $\alpha$-Titanium single crystals

Several studies have focused on the deformation behavior of single crystal $\alpha$-titanium that are fundamental to our understanding of this material as well as Ti-Al alloys (cf. Naka and Lasalmonie, 1982; Naka et al., 1988, Biget and Saada, 1989). The in situ transmission electron microscopy (TEM) experiments performed by Naka et al. (1988), in which single crystals were oriented for prismatic slip, highlight several key features associated with the deformation of titanium. One of the most important observations of that study was the strong dependence of flow stress on temperature, especially at low temperatures, despite the high mobility of $\langle a \rangle$-type edge dislocations. In addition, post mortem TEM images revealed traces of elongated rectilinear $\langle a \rangle$-type screw dislocations on prismatic planes. These two observations lead to the conclusion that the low temperature plastic deformation of titanium is analogous to the behavior of bcc metals, and is controlled by the movement of $\langle a \rangle$-type screw dislocations which experience a strong frictional force.

While there is general agreement on the existence and importance of the lattice friction in titanium and its alloys, there is not a consensus view on the underlying fundamental mechanism responsible for this phenomenon. Naka et al. (1988) suggest that the friction on screw dislocations is due to an “extended Peierls mechanism” resulting from a non-planar core structure that undergoes repeated sessile-glissile transitions. Biget and Saada (1989) found that the activation area at low temperatures
was proportional to the inverse of the local stress squared, which led them to propose Friedel’s cross slip model to capture this dependence. However, in a follow-up study conducted by Farenc et al. (1993), they found inconsistencies between the effects of both proposed models and the experimental observations. They have pointed out that the Peierls model is unable to explain the dependence of activation area on stress, while Friedel’s model is unable to explain the significantly larger density of screw as compared to edge dislocations observed after deformation. A compromise, proposed by Farenc et al. (1993), containing aspects of both models, is based on a locking-unlocking (sessile-glissile) transition of \(\langle a\rangle\)-type screw dislocations. This model is able capture the dependence of activation volume on stress, the correct order of magnitude of the activation volume, as well as account for the existence of a larger density of screw dislocations after deformation. Further support for this model is the observation that the dynamic motion of screw dislocations is “jerky” which would be indicative of the wait time associated with the locking-unlocking process.

Another interesting feature of the flow stress versus temperature curve is a discontinuity that occurs between 300-500 K (Naka et al., 1988). TEM micrographs show that this is a transition from planar to wavy slip. Wavy slip lines are indicative of cross-slip, and multiple double cross-slip events between prismatic and first-order pyramidal planes have been observed. This type of behavior is expected from titanium, which is known to have a high stacking fault energy and therefore is expected to cross-slip easily (Gu et al., 1994). In the wake of these double cross-slip events, dense heterogeneously distributed dipolar arrays are created. The discontinuity is thought to be the result of the long-range stress field associated with these arrays interacting with mobile screw
dislocations. It is not obvious why cross-slip has occurred on the pyramidal plane since the prismatic system is favorably oriented and highly stressed. As they have reasoned that a non-planar core structure manifests the friction force on screw dislocations, Naka et al. (1988) have suggested that cross-slip is possible due to a core structure that can form glissile configurations in both prismatic and first-order pyramidal planes. Further evidence indicating a non-planar core structure is the dependence of flow stress on orientation of the compressive axis. Their results show a significant variation (~49-71 MPa) in the critically resolved shear stress (CRSS) for prismatic systems. The implications of the breakdown of Schmid law will be discussed in Section 2.3.

Another important study on the single crystal behavior of was conducted by Gu et al. (1994) which looked at the active deformation modes of a crystal stressed along the c-axis under various types of loading. Since the resolved shear stress for \(\{a\}\)-type systems will be minimized in these experiments, they are ideal for studying the harder modes of deformation. In these tests, the crystals were subjected to monotonic tension, tension-tension fatigue, and tension-compression fatigue at various stress amplitudes. There were very few similarities observed in the deformation microstructures after each of the tests, indicative of the complex nature of deformation in titanium. Various types of twins and \(\{1\bar{1}22\}\langle e+a\rangle\) slip were observed in nearly all specimens. However, there were no consistent patterns of dislocation and twin arrangement that could be seen throughout all tests. For example, a dense number of intersecting twins were observed in monotonic tension tests, while twins in tension-tension fatigue tests stopped at intersection points with other twins. The tension-tension test had a lower twin and dislocation density than the monotonic test, and the dislocation structure consisted largely of dipole arrays. In the
tension-compression fatigue tests, the deformation microstructure depended on the cyclic stress amplitude. At the lowest stress amplitude (~100 MPa) both twin and dislocation densities were low. In the mid-range stress amplitude (200 MPa), twin bands were observed to form early on during cycling appearing to reach a saturation value, although existing twins appeared to grow wider. Discrete cracks, which also grew with increased cycling, were observed in the middle of the twin bands. It was determined that the cracks actually formed at the intersection of $\langle 11\bar{2}2 \rangle$ and $\langle 01\bar{1}2 \rangle$ twins. These twins intersected along the direction $[2\bar{4}23]$, which lies in the prismatic plane. Since $\langle 01\bar{1}2 \rangle$ twins grow under tension and $\langle 11\bar{2}2 \rangle$ under compression, it is believed that crack formation releases the tensile stress and slows the growth of $\langle 01\bar{1}2 \rangle$ twins while the compressive stresses due to crack closure cause the $\langle 11\bar{2}2 \rangle$ twins to continue to grow. The dislocation structure was arranged in arrays perpendicular to twin boundaries, indicating the twins acted as sufficient obstacles to dislocation motion. At the highest stress amplitude (~250 MPa) the dislocation structure formed into elongated cells and loosely organized walls.

In summary, the deformation mechanisms in single crystal $\alpha$-titanium are complex and vary according to orientation, loading conditions, temperature, and strain rate. Actually, there are two types of orientation dependencies that arise in titanium. The first is related to the non-planar dislocation core structure, and the second to the multiple competing deformation mechanisms at certain intermediate orientations. The latter has been evidenced by a study on the cyclic behavior of $\alpha$-Ti single crystals by Tan et al. (1998a/b). Their study on seven differently oriented crystals found that orientation affected both the shape and position of the cyclic stress-strain curve (CSSC). The highest
stress levels were obtained in specimens with orientations that lie on the border of the 
(0001)−(10\overline{1}0) unit triangle, while the lowest stress levels had orientations near the 
(0001) pole. As in the previous study, very few definitive conclusions relating 
orientation to deformation microstructure can be drawn from the experiments. The more 
general observations are that deformation twins were observed in all specimens except 
one which was oriented predominantly for single slip. The specimens with a higher twin 
density exhibit higher hardening rates. Also, numerous dislocations have been observed 
at twin boundaries; and it is thought that their presence is necessary to accommodate the 
strain due to twinning. The various types of dislocation structures observed range from 
dipolar arrays, loops, networks, to cell structures. Low angle boundaries have also been 
observed, but they act only as minor obstacles to both twins and dislocations.

Before discussing the deformation behavior of polycrystalline titanium and $\alpha/\beta$
Ti-Al alloys, the hardening effect due to interstitial impurity atoms (O, N, and C) needs to 
be addressed. The strengthening effect can be quite pronounced, as shown in the 
previously mentioned work of Naka et al. (1988). Testing of three different impurity 
levels shows that the CRSS for prismatic slip can vary from 30-120 MPa at room 
temperature based on the impurity concentration. Most authors have used the equivalent 
oxygen content to quantify the impurity level in a given material, which is given as, 
$O^* = O + 2N + C$. The strengthening effect is more pronounced at lower temperatures 
and is barely evident at temperatures above 550 K (athermal temperature). Naka et al. 
(1988) have shown that the effect cannot be due to Fleischer type elastic interactions 
between dislocations and solute atoms because the activation energy associated with such 
interactions is inconsistent with their experimental results. Instead, they propose that the
oxygen atoms act to modify the dislocation core structure, which results in an asymmetrical configuration that is more difficult to constrict. They do note that this hardening effect is only valid for relatively high impurity contents, since the CRSS does not vary significantly below a certain critical impurity level (1500 at.p.p.m O*). It has also been shown by Doner and Conrad (1973) that impurity content has an additional contribution via dynamic strain aging in the temperature range of 600-850 K, although this effect should be minimized with decreasing impurity content.

2.2.3 Monotonic behavior of polycrystalline $\alpha$-Ti

As would be expected the deformation in polycrystalline $\alpha$-titanium is more complex than the behavior of monocrystals. The low symmetry of the hcp structure results in significant texture effects on microscopic and macroscopic behaviors, as the orientation dependence and strain compatibility of each grain must resolve with nearest neighbor grains. The role of twinning and its effect on material behavior in polycrystalline titanium is very important; it has been the subject of much recent research (cf. Chichili et al., 1998; Nemat-Nasser et al., 1999; Salem et al., 2002; Kalidindi et al, 2003), and is still not fully understood. The difficulty in quantifying these effects stems from the numerous types of interactions, including primary twin-matrix interaction, primary twin-secondary twin interaction, secondary twins growing inside a host twin, and dislocation interactions with all of these types of obstacles. There are therefore several views on how twinning affects the deformation in concert with slip. The previously mentioned single crystal studies have shed some light on the operative deformation processes, and can be used as a basis for understanding the more complex polycrystal
behavior. Some of the more important questions about twinning are how it affects initial yield strength, strain hardening behavior, and damage nucleation. It is generally thought that twinning, which results in a reorientation of parts of grains, serves to refine the microstructure by decreasing the effective grain size (counting twin boundaries as grain boundaries). Although there have been reports of dislocations penetrating twin boundaries (Gu et al., 1994), it is more often observed that they become trapped and form dense arrays. There are two different mechanisms that contribute to this: (i) dislocations that were initially in the region where the twin nucleated become trapped upon reorientation (Kalidindi et al., 2003), and (ii) moving dislocations cannot penetrate the interface (Salem et al., 2002).

Generally speaking, a material with a higher initial twin density should exhibit a higher initial yield stress and strain hardening rate that a material with a lower initial twin density, according to Hall-Petch type arguments. There is a caveat that must be discussed in light of the previous statement. Chichili et al. (1998) have chosen to investigate this by loading a sample at 77 K to induce a large twin density and then reloading the material at room temperature. This stress-strain curve is then compared to that of a similar sample (only lower twin density) to see if the smaller effective grain size resulted in a higher flow stress. They observed a decrease in the flow stress in the material with the larger initial twin density. They explained that the yield drop was due to the reorientation of the lattice which occurred in such a way as to favorably align slip systems to more easily accommodate further deformation. Therefore, upon reloading, the material should show a decrease in flow stress, reflecting a higher availability of slip systems. This phenomenon has recently been verified by Kalidindi et al. (2003) who showed using
electron back scattered diffraction (EBSD) techniques that grains initially stressed along the c-axis, developed twins whose c-axis were reoriented perpendicular to the initial loading direction. This realignment would be favorable for prismatic slip. This softening effect was also reported by Nemat-Nasser et al. (1999), but they have found that this behavior can be modified through thermal cycling of the material. This led them to propose that dynamic strain-aging could have an additional impact on the flow stress. As further proof that dislocation motion is affected by interaction with mobile point defects, they have observed that with suitable combinations of temperature and strain rate, specimens exhibit an anomalous three-stage hardening whereas samples loaded outside of these temperature and strain rate conditions exhibit only stage I hardening, which is more consistent with typical metal behavior. Three-stage hardening has also been reported in single crystal studies by Akhtar and Teghtsoonian (1975). They observed that three-stage hardening became more pronounced for an angle between the basal plane normal and loading axis less than 60º, and the deformation involved \( [10\overline{1}2] \) and \( [1\overline{1}21] \) twinning. Salem et al. (2002) do not agree with the dynamic strain aging argument, since this effect should not be significant in high purity titanium samples deformed at temperatures lower than 600 K. In their work, they have shown that the onset of stage II hardening coincides precisely with the first observation of twins. It should be noted that the samples used in these experiments had initial textures such that the basal poles were distributed 10-15º from the loading axis, which is well within the range orientations expected to exhibit three-stage hardening that has been noted by Akhtar and Teghtsoonian (1975). The samples used by Nemat-Nasser et al. (1999) had a texture where the basal poles were perpendicular to the load axis, and therefore should have been
favorably oriented for prismatic slip. Obviously, the quantitative effect of twinning on material behavior is not yet fully understood.

Some statements can be made regarding the occurrence and effect of twinning in monotonic behavior in polycrystalline titanium, several of which have been reported by Chichili et al. (1998) and verified by others. First, when deformed at quasi-static rates the twin density increases monotonically with accumulated strain. On the other hand, under dynamic loading conditions the density of twins rapidly increases at lower strains and reaches a saturation point (at unity) with increased straining. It seems that the saturation is due to significant reordering of the microstructure which enables further deformation to be accommodated via slip. Further, it is believed that the higher stresses observed in heavily twinned titanium, such as those deformed at low temperatures or high strain rates, are the result of low dislocation mobility and not the presence of twins. Twins develop because of the high stresses in the material and not vice versa.

2.2.4 Cyclic deformation behavior of \(\alpha\)-Ti

The cyclic behavior of titanium is also very complex and depends significantly on the activity of twinning and the interaction of dislocations with twins. The deformation microstructure at room temperature depends on the applied strain amplitude. For lower strain amplitudes (\(~0.5\%)\), twinning is not thought to be significant and an approximately saturate peak stress is reached at the beginning of cycling (Sun and Gu, 2001; Swalla, 2003). At slightly higher strain amplitudes, initial hardening is observed, which is then followed by a saturate staged after about 10 cycles. At strain amplitudes higher than 1.5\%, the initial hardening rate is significantly higher and is followed by a region of
either saturation or slight softening followed by saturation. The higher the strain amplitude, the more pronounced the softening effect (Sun and Gu, 2001). Data published by Zhang et al. (1998) shows an additional hardening stage following the seemingly saturated stage at higher strain amplitudes. This secondary hardening stage occurs around 30 cycles and continues throughout cycling, never reaching a true saturated level. These data appear to be in contradiction with work of Sun and Gu (2001) and Swalla (2003). Several explanations have been proposed to account for the observed regions of cyclic softening/hardening in these materials with no one explanation seeming more valid than the other.

Sun and Gu (2001) imply that the observed initial hardening is due to the accumulation of dislocations with increased cycling that act as obstacles for mobile dislocations. They propose that cyclic softening is caused by the formation of low energy sub-structures such as cells, and/or the interaction of dislocations resulting in annihilation. Twinning is discounted as affecting the hardening/softening response as it is claimed that it is not an important deformation mechanism at 293 K. Zhang et al. (1998) agree that initial hardening is due to mobile dislocation interaction with areas of high dislocation density, and that softening especially at low amplitudes is associated with dislocation annihilation. They mention that at higher strain amplitudes, that twinning will play a more important role and may act as a softening mechanism by reducing the internal stress concentration and promoting further deformation. They also believe that twinning is the cause of the second phase of hardening observed in their experiments at large strain amplitudes. They suggest that the continuous increase in twin fraction with increased cycling impedes further twinning and dislocation motion resulting
in the observed hardening. This view on the effect of a large density of twins differs from that observed by Kalidindi et al. (2003) for monotonic loading who argued that the number of twins saturates in response to the microstructure’s ability to accommodate further deformation via slip, resulting in a drop in flow stress. While the quantitative effect on twinning on cyclic deformation is still unsubstantiated, it is known that twin density increases with both strain amplitude and number of cycles.

2.2.5 Deformation behavior of $\alpha/\beta$ Ti-Al alloys

Since it is often impossible to isolate the individual phases of a polyphase alloy with the same composition that exists in the bulk material, single crystal studies of deformation mechanisms in such materials are difficult if not impossible. For this reason, the behavior of $\alpha/\beta$ Ti-Al alloys must be studied at the polycrystal level and is primarily interpreted within the framework of knowledge gained from the extensive single crystal studies on $\alpha$-Ti. This is appropriate considering that the onset of plastic deformation occurs and remains within the primary $\alpha$-phase at lower strain levels. Twinning is not really a factor in these materials since the process of twinning is inhibited due to alloying with aluminum. It has been shown that the occurrence of twinning decreases with increasing aluminum content (Williams et al., 2002). In alloys containing 6% or higher atomic wt. % aluminum, twinning is rarely, if ever, observed. With the role of twinning being negligible in many $\alpha/\beta$ alloys, the importance of $\langle c+a \rangle$ slip is enhanced as it is then the sole mechanism responsible for accommodating deformation along the c-axis. The most difficult and important aspect of deformation to quantify in this class of alloys is the effect of the $\beta$ and/or $(\alpha+\beta)$ regions. For this
reason, significant effort has been devoted to understanding the yield and slip transmission process in individual $\alpha/\beta$ colonies. Although most of these works do not study colonies with the same morphology as would appear in a duplex Ti-6Al-4V microstructure with lamellar ($\alpha+\beta$) regions, they offer insight into the slip transmission process that occurs across the $\alpha/\beta$ interface. This should be applicable to any such alloy.

The motion of screw dislocations on prismatic planes in the primary $\alpha$-phase is the primary mechanism of deformation in $\alpha/\beta$ Ti-Al alloys as it is in unalloyed titanium. Feaugas and Clavel (1997a) have shown in a study on Ti-6Al-2Sn-4Zr-6Mo (Ti-6246) that single prismatic slip occurred in a majority of grains, with double slip occurring in approximately 10% of $\alpha$ grains. Uniformly spaced planar slip traces that traverse the entire grain are also characteristic in these materials. The transition from planar to wavy slip occurs at a significantly higher temperature (~500 K) than it does in cp $\alpha$-titanium. The upward shift in transition temperature is due to the solid solution hardening provided by aluminum atoms, and is generally associated with the dissolution of fine Ti$_3$Al precipitates that exist in the primary $\alpha$-phase below this temperature. Neraj et al. (2000) also found that single slip was the predominate feature of the deformation microstructure. In grains where double slip was active, it was observed that prismatic dislocations were able to cross through each other with little disruption to their respective motions. Combined with the fact that single slip occurs in most grains, this seems to indicate that intragranular dislocation interactions play a secondary role in the hardening behavior of these alloys. If this is the case, then grain and $\alpha/\beta$ interface boundaries are the primary obstacles to dislocation motion. The difficulty of slip
transmission across $\alpha/\alpha$ boundaries is a result of the low symmetry of the hcp structure and is therefore highly dependent on the misorientation between grains. This is supported by the observation that, in general, persistent slip bands (PSB) are not found in these materials, in contrast to cubic materials. When PSBs have been observed, there has been a single strong component of texture that favorably aligns prismatic slip planes across many grains. As a reflection of transmission difficulty between neighboring $\alpha$ grains, slip traces intensify with continued loading and eventually enough dislocations pile-up at the boundary that a secondary slip system is activated in the neighboring grain. These secondary dislocations move at a much slower speed than primary dislocations, and usually do not travel the length of the grain. This supports the possibility that they are activated with help from pile-up stresses which decay with distance from the boundary.

Although slip transmission through $\alpha/\alpha$ boundaries can be difficult, the most effective obstacles in this alloy are the $\alpha/\beta$ interfaces. Due to their importance in enhancing the properties of Ti-Al alloys, numerous studies have been dedicated to resolving the role these interfaces play in the microdeformation process (cf. Suri et al., 1999; Ambard et al., 2001; Savage et al., 2001). With the variety of different microstructures that can be produced in these materials, it is no surprise that a wide array of mechanisms have been reported associated with $\alpha/\beta$ colonies and interfaces. Reported deformation modes range from zero slip activity at low temperature and strain (Ambard et al., 2001), $\alpha/\beta$ interfacial sliding (Ankem and Margolin, 1983), restricted basal slip (Ambard et al., 2001), and selective slip system filtration with residual dislocation by-products at the $\alpha/\beta$ interface (Suri et al., 1998). Probably the most
microstructurally significant research on the deformation processes at these interfaces has been carried out by a group at Ohio State University (Suri et al., 1999; Neeraj et al., 2000; Savage et al., 2001). They have grown single colony crystals of several $\alpha/\beta$ alloys with the intent of determining the CRSS for slip these colonies as well as investigating the slip transmission process and its effect on initial yield strength and subsequent hardening behavior. While their work is unable to investigate the constraints placed on the colony by its adjacent grains or the effect of multiple laths, it is informative to study the interface dislocation transmission process.

Recall the diagram of the BOR given in Figure 2.5 and note that the $\alpha$-phase burgers vectors are such that each is at a unique angle with respect to the corresponding slip vectors in the $\beta$-phase. The work of Suri et al. (1999) looks specifically at the transfer of $\langle a_1 \rangle$ and $\langle a_2 \rangle$ prismatic dislocations through the interface for the material Ti-5Al-2.5Sn (Ti-5-2.5). Their results show that specimens preferentially aligned for $\langle a_1 \rangle$ slip exhibit a higher yield strength and work hardening rate than specimens aligned for $\langle a_2 \rangle$ slip. They explain this behavior with the help of a slip transmission model in terms of the residual dislocations that are left behind after being transmitted through the $\beta$ region. In the case of $\langle a_2 \rangle$ dislocations, the residuals are smaller and after the passing of a small amount of primary dislocations a favorable annihilation reaction can occur. The smaller residual necessary for initial transmission and the favorable annihilation reaction seems to explain the lower yield strength and decreased work hardening rate. In a separate study, Savage et al. (2001) have measured the CRSS for the basal and prismatic systems corresponding to each unique slip vector for the material Ti-6Al-2Sn-4Zr-2Mo-
0.1Si (Ti-6242). The findings for the prismatic systems follow what would be predicted by the model discussed above with the CRSS for \(\{a_2\}\) being the smallest and with \(\{a_3\}\) having the largest value. As also would be expected from knowledge of other Ti-Al alloys, the CRSS for the three basal systems is slightly higher (\(\sim 1.2-1.5 \tau_{\text{prism}}\)) than that for prismatic systems, except for the \(\{a_3\}\) system which is approximately equal to the CRSS for the prismatic systems. This behavior cannot be explained within the context of the current slip transmission model since the transmission of the \(\{a_3\}\) system should leave the largest residual dislocation, and therefore the highest CRSS. The general tendency of higher CRSS for basal systems is explained by noting that the slip traces associated with these systems are very fine and heterogeneous, which indicates probable cross-slip and interaction among the different slip systems as opposed to the highly planar nature of prismatic slip. This type of interaction will require a larger value of macroscopic shear stress to accumulate enough dislocations to enable transmission through the interface. Chan et al. (1981) reported a similar increase in CRSS with decreasing slip line spacing regardless of the type of slip system.

A work contrary to the previous studies by Ambard et al. (2001) on polycrystalline Ti-64 contended that transmission rarely occurs and that only basal systems are active in lath colonies. This occurs even though prismatic systems are the most active within the primary \(\alpha\)-phase, and basal deformation is said to be independent of the orientation of the lath with respect to the loading axis. Their argument is that the \(\beta\) laths act as prismatic \(\alpha\) slip system blockers which would result in higher yield strength and work hardening rates upon transmission with these systems as compared to their basal counterparts. The observations reported by Ambard et al. (2001) differ
significantly from the single colony response discussed earlier. One possible explanation for the different observations could be due to the intergranular constraints placed on the lamellar colonies in the polycrystalline sample. Ankem and Margolin (1980) have shown the importance that the elastic interaction stresses can play in aiding and/or restricting slip on systems near the interface. Suri et al. (1999) found these stresses to be similar on all systems and deemed them to be a secondary effect. While they were not calculated in the work by Savage et al. (2001), they believe it is doubtful that the effect would be significant enough to explain the $\langle a_z \rangle$ basal anisotropy. Another possible explanation of the different behavior could be related to the fact that in the single colony studies, one slip system was optimally aligned for single slip; in the polycrystalline tests this cannot be done.

2.3 Dislocation Core Structure and its Effect on Plasticity

Initial studies of plastic deformation in metals by Schmid (1924) revealed that the main mechanism of plastic flow was the relative motion of close-packed crystal planes in the direction of the highest atomic density. These results led them to propose the Schmid law, which, as pointed out by Duesbery (1989), has two distinct implications. The first is that plastic flow begins when the resolved shear stress for a slip system reaches a constant critical value (CRSS), and the second is that the critical stress is not influenced by any other component of the applied stress tensor resolved onto the crystal lattice coordinate system. It is important to note that the work of Schmid (1924) was performed on hexagonal close-packed metals that primarily deform by basal slip, which will be
further addressed shortly. At around the same time, similar experiments conducted by Taylor et al. (1928) on bcc metals highlighted some intriguing aspects of slip in these materials that did not follow the Schmid law. While slip always occurred in the close-packed direction, the slip surface varied with orientation and sense of applied stress. These obvious violations were basically ignored as the main concern was determining the magnitude of the CRSS (Duesbery, 1989). The magnitudes of the CRSS determined experimentally were several orders of magnitude lower than those predicted by early theoretical models. These models considered the slip process in a perfect crystal for which it was assumed that all bonds were simultaneously broken across the slip plane. Dislocations were proposed as a possible explanation of the differences between experimental observations and the theoretical models. The introduction of dislocations into the theory of plastic deformation then led to a more thorough investigation of the CRSS. Further research revealed that the mechanisms of plastic deformation were structure dependent, with close-packed metals (fcc and hcp) obeying the Schmid law with the CRSS having very little dependence on orientation or temperature. On the other hand, for bcc metals it was observed that the CRSS and slip geometry were highly dependent on temperature and stress orientation. In addition, non-crystallographic slip was observed for certain orientations. The cause of this anomalous behavior is the dislocation core geometry which is inherently dependent on the crystal structure of the material (Duesbery, 1989). This is further supported by the fact that the continuum description of dislocations works quite well for distances of several lattice spacings from the core, which indicates that no structure dependence is expected in this region. Inside this region the continuum description of the dislocation breaks down as the discrete
nature of the lattice dominates and the strain field is non-local in nature. Although the importance of the dislocation core was recognized at an early stage in research, it was not until the emergence of computers that the massive calculations necessary to study the discrete core structure could be carried out.

To date the vast majority of core studies have been carried out on bcc metals since this class of materials has been widely noted to deviate from the Schmid law. The characteristic of the core that distinguishes bcc from fcc materials and the hcp materials that deform by basal slip (i.e. Mg, Cd, and Zn) is the non-planarity of the dissociated dislocations. In fcc metals and certain hcp materials, the dislocations dissociate into Shockley partials in the \{111\} and \{0001\} planes, respectively. Due to the planar nature of the core, the most important stress component is still the shear stress resolved in the glide plane in the direction of the total burgers vector. However, in bcc metals plastic deformation is dictated by \(a/2\{111\}\) screw dislocations. Screw dislocations having their burgers vector parallel to the dislocation line are not constrained to one particular plane and may spread onto any plane belonging to the \(\{111\}\) axis, namely the \{110\} and \{211\} families of planes. In its dissociated state, these dislocations are in a sessile configuration and must first constrict to form a glissile dislocation so that slip can occur. Depending on the geometry of the core, several types of different constriction stresses can play a role in dislocation motion. If the dissociation results in partial dislocations with a significant edge component, the resolved shear stress in the dissociated plane perpendicular to the total burgers vector will be important. However, if the reaction is of the type where one large screw dislocation dissociates into several smaller screw partials into non-parallel planes, the resolved shear stresses in the dissociated planes in the directions parallel to
the total burgers vector are the most significant components. In either case, the onset of glide depends on the constriction stress, which explains the orientation and sense dependence on the applied stress in these materials. The non-planarity of the core is also the reason that the observed CRSS for these materials increases drastically with decreasing temperature. The constriction process is very similar in nature to cross-slip, in that both involve screw dislocations and are thermally activated; in the case of cross-slip, however, the screw segments are free to glide. Constriction can be aided (or hindered for that matter) by an applied stress, but as temperature decreases the thermal component becomes minimized and the constriction stress significantly increases.

As has been noted in earlier sections, the primary mechanism of plastic deformation in $\alpha$-Ti and $\alpha/\beta$ Ti-Al alloys is the motion of screw dislocations on prismatic planes. It has also been mentioned that several of the indicators of a non-planar core structure have been experimentally observed during the study of these materials. The most notable are the significant increase in CRSS with decreasing temperature and significant variation of the CRSS with orientation (Naka et al., 1988). For these reasons and the emergence of titanium as an important alloying material for engineering applications, several studies of the screw dislocation core have been carried out. These studies, some phenomenologically motivated and others supported by atomistic simulations, have resulted in numerous proposed core structures. This can be attributed to the fact that the results of atomistic modeling of dislocation cores are highly influenced by the choice of interatomic potential. Titanium, which is a transition metal with an incomplete d-shell of electrons, exhibits directional bonding and may not be very well suited for description by classical potential functions. Presently there are no definitive
results on the core structure of screw dislocations in titanium; therefore, a summary of the results to date will be presented.

2.3.1 Core structure in hcp materials and titanium

Before the widespread use of computers to perform detailed atomistic studies of dislocation cores, the proposed dissociation reactions were based on crystallography, hard-sphere models, and/or mechanisms that could explain observed material behavior. First, the basal splitting of \( \frac{1}{3} \langle 11 \bar{2} 0 \rangle \) dislocations is relatively simple and can be reckoned on a purely crystallographic basis. The dissociation reaction is given as

\[
\frac{1}{3} \langle 11 \bar{2} 0 \rangle = \frac{1}{6} \langle 10 \bar{1} 0 \rangle + \frac{1}{6} \langle 01 \bar{1} 0 \rangle
\]  

(2.1)

This is the equivalent to the splitting into Shockley partials in fcc materials, and corresponds to the I2 intrinsic stacking fault that is present in all hcp materials. This is the most favorable core configuration for hcp materials that primarily deform by basal slip. As noted by Vitek and Igarashi (1991) this fault is ensured due to the symmetry of the hcp structure in which three mirror planes (the three prismatic planes) intersect normal to the basal plane, guaranteeing a minimum on the \( \gamma \) - surface. The \( \gamma \) - surface is a tool derived from atomistic studies to find possible metastable stacking faults and their related fault vectors (cf. Vitek, 1992). Since prismatic slip is known to be favored in titanium, core spreading of \( \frac{1}{3} \langle 11 \bar{2} 0 \rangle \) dislocations within (or out of) the prismatic planes should be more energetically favorable that basal splitting. Unfortunately the
dissociation on prism planes is not as clear and, since it cannot be predicted crystallographically, it depends on the details of interatomic bonding.

The earliest dissociation encountered in this review was deduced from the hard-sphere model and was proposed by Churchman (1954). The reaction consists of splitting within the prismatic plane, and is given by

$$\frac{1}{3}\langle 11\bar{2}0 \rangle = \frac{1}{6}\langle 11\bar{2}1 \rangle + \frac{1}{6}\langle 11\bar{2}T \rangle$$

(2.2)

The most remarkable feature of this core configuration is the significant edge component in the direction parallel to the c-axis. Several years later a similar hard-sphere based model was proposed by Tyson (1967), i.e.,

$$\frac{1}{3}\langle 11\bar{2}0 \rangle = \frac{1}{18}\langle 42\bar{6}3 \rangle + \frac{1}{6}\langle 24\bar{6}3 \rangle$$

(2.3)

The difference between this model and the previous model is the additional \( \frac{1}{18}\langle 1\bar{1}00 \rangle \) component of each partial dislocation normal to the prism plane. These components obviously lead to dissociation in a non-prismatic plane. The plane of core spreading is not a low index crystallographic plane, but is close to a first-order pyramidal plane. Both of these configurations are sessile, first requiring a constriction before slip can occur in the prismatic plane. Regnier and Dupouy (1970) proposed a dissociation which results in a thin layer of \( \{112\} \) stacking of the bcc lattice noting the hcp-bcc transition exhibited by
certain metals, including titanium. It should be pointed out that the core structure they have proposed is asymmetric since the two partials have different magnitude (Vitek and Igarashi, 1991), i.e.,

\[
\frac{1}{3}\langle 11\overline{2}0\rangle = \frac{1}{9}\langle 11\overline{2}0\rangle + \frac{2}{9}\langle 11\overline{2}0\rangle
\]  

(2.4)

In this configuration, the core is confined to the prismatic plane, and there is no edge component of the partial dislocations. Such a reaction, without any edge component that is confined in the prismatic plane, would not seem to be able to explain the existence of a Peierls stress that has been reported for titanium. Naka et al. (1988) have used components of the arguments from these earlier works as well as drawing by analogy from the splitting of \(\langle 111\rangle\) dislocations in bcc metals to propose a non-planar core model for titanium that involves first-order pyramidal planes. There are two first-order pyramidal planes which share the \(\langle 11\overline{2}0\rangle\) burgers vector with each prismatic plane, and participate in the dissociation given as

\[
\frac{1}{3}\langle 11\overline{2}0\rangle = \frac{1}{9}\langle 11\overline{2}0\rangle(10\overline{1}0) + \frac{1}{9}\langle 11\overline{2}0\rangle(10\overline{1}1) + \frac{1}{18}\langle 11\overline{2}0\rangle(10\overline{1}\overline{1}) + \frac{1}{18}\langle 11\overline{2}0\rangle(10\overline{1}\overline{1})
\]  

(2.5)

In this configuration each partial retains its initial screw character, but the partials spread in the pyramidal planes must constrict before slip can proceed in the prismatic plane. Like the model proposed by Regnier and Dupouy (1970), the stacking fault related to the
main dissociation in the prismatic plane corresponds to a local atomic stacking of the $\{112\}$ bcc lattice. Vitek and Igarashi (1991) have pointed out that this splitting is similar to that proposed by Sob et al. (1975). Naka et al. (1988) have acknowledged that the core structure differs from that found by Legrand’s (1984a) atomistic studies, but their model fits their experimental data better and has similar implications concerning the existence of a significant lattice friction.

In an attempt to verify these proposed models and/or find new stable core configurations, several researchers have carried out atomistic simulations on $\langle11\bar{2}0\rangle$ dislocations in hcp materials (cf. Bacon and Martin, 1981; Bacon and Liang, 1986) and specifically in $\alpha$-Ti (cf. Legrand, 1984a,b; Vitek and Igarashi, 1991; Girschick et al., 1998). Most of these studies have been performed using central force-type potentials including pair potentials, N-body potentials, and Finnis-Sinclair potentials with the notable exceptions being Legrand (1984 a,b) and Girschick et al. (1998). The latter authors have used the tight-binding method and bond-order potentials, respectively, to describe the atomic interactions. The key difference between the two groups of potentials is that the former do not take into account directional bonding while the latter do. Directional bonding is thought to play an important role in titanium; since any stable core configurations on the prismatic plane are going to be a result of the nature of atomic interactions and not crystallography, it is important to include this directional dependence of the bonding in the chosen potential. The work of Girschick et al. (1998) provides a lucid comparison of what occurs when simulating $\langle11\bar{2}0\rangle$ dislocations in titanium using both Finnis-Sinclair (F-S) and bond-order potentials (BOP). In the case of the F-S potential, the preferred core dissociation (basal or prismatic) depends on the starting
configuration of the dislocation. On the other hand, the BOP predicts that prism splitting occurs regardless of the starting configuration. This occurs because the F-S potential significantly underpredicts the stacking fault energy associated with basal splitting, resulting in it being a more favorable reaction for some cases. Another outcome of the F-S model for dislocations in prismatic planes is the prediction of a metastable stacking fault associated with the fault vector \( t = \frac{1}{6} \langle 11\overline{2}0 \rangle + 0.18 \langle 0001 \rangle \), or in other words it predicts the reaction

\[
\frac{1}{3} \langle 11\overline{2}0 \rangle = \frac{1}{6} \langle 11\overline{2}x \rangle + \frac{1}{6} \langle 11\overline{2}x \rangle, \; x = 1.08
\]  

(2.6)

It has been noted that this fault is a result of central forces and can be deduced using the hard-sphere model. No such metastable fault is predicted using the BOP. While the F-S potential as compared to the BOP leads to significantly lower values for the stacking fault energy on the basal plane as well as an artificially favorable dissociation on the prism plane, the stabilized prismatic core structure is very similar in both cases. The resultant core structure is principally spread within the prismatic plane, with some slight spreading into adjacent basal planes. The edge component of the dissociation is considered to be negligible, and these results are very similar to those found by Legragnd’s (1985) work on screw dislocations in titanium. It is possible that this type of non-planar configuration could give rise to a significant Peierls stress, as has been reported in the literature. The most interesting finding in this work is that the core configuration of \( \frac{1}{3} \langle 11\overline{2}0 \rangle \) screw dislocations in prism planes for titanium cannot be well-described by partial dislocations
separated by a metastable stacking fault. Instead the geometry of the core consists of several fractional dislocations bounding unstable planar faults (Vitek, 1992).

Experimental evidence also suggests that the core structure of $\frac{1}{3}(1\bar{1}23)$ dislocations is non-planar. However, since the primary mechanism of plastic flow in titanium at room temperature is the motion of $\frac{1}{3}(1\bar{1}20)$ screw dislocations in prismatic planes, the possible core structures of this type of dislocation will not be discussed. Further, as pointed out by Bacon and Vitek (2002), to date no such atomistic studies have been carried out for these dislocations using potentials that account for the directional nature of bonding and therefore use of conventional potentials may give misleading results.

2.4 Crystal Plasticity

Clearly, plastic deformation on the macroscopic scale in metals is a manifestation of dislocation motion and interaction on the microscopic scale. The details are intimately related to the basic crystallographic nature of the material as well as the current state of the microstructure. Macroscopic models of plasticity lack the ability to link these fundamental mechanisms to the bulk material response without rather substantial experimental characterization. Furthermore these models give relatively little physical connection between the actual deformation processes and the observed material behavior. While there have been many formulations of constitutive laws for the elastic-plastic deformation of single and polycrystals over the past 50 years (cf. Taylor, 1938a,b; Hill,
of these micromechanical models, and the focus of the following discussion, is continuum crystal plasticity based on a multiplicative decomposition of the deformation gradient. While the details of crystal plasticity can be quite intricate and are constantly changing to reflect an improved understanding of deformation at this scale, the basic premise is relatively simple: macroscopic plastic deformation is related to the cumulative process of slip (or twin) system shearing relative to the lattice. This methodology provides a sort of physical link between the processes at radically different length scales. The two basic components of a micromechanical continuum crystal plasticity model are the kinematic and kinetic relations. The kinematic relations provide the mathematical framework for describing the physical process of dislocation motion based on continuum deformation fields, whereas the kinetic relations incorporate the material and/or mechanism dependence of nonequilibrium dislocation motion and interaction. The following discussion will briefly cover some of the basic aspects of crystal plasticity, as well as some of the issues specific to Ti-Al alloys such as non-Schmid behavior, presence of multiple phases, length scale effects, cyclic deformation behavior, and twinning.

2.4.1 Kinematics of Crystalline Deformation

The basic concept of crystal plasticity is that material is convected through the lattice via dislocation motion, leaving the structure of the lattice unchanged (Asaro, 1983). Therefore, the deformation can be separated into two distinct processes: plastic slip and elastic stretching of the lattice. It is proposed that the total deformation gradient can be written as a multiplicative elastic-plastic decomposition of the form
where the dislocation motion through the lattice is captured via $F^p$, and the rigid body rotation and elastic stretching of the lattice is captured in $F^e$. A differential line segment is mapped from the reference to the current configuration according to

$$dx = FdX$$  \hspace{1cm} (2.8)$$

The velocity gradient in the current configuration is given as

$$L = \dot{F}F^{-1} = \dot{F}^eF^{e^{-1}} + F^e\dot{F}^pF^{p^{-1}}F^e^{-1}$$  \hspace{1cm} (2.9)$$

The velocity gradient in the current configuration can also be written as

$$L = D + W$$  \hspace{1cm} (2.10)$$

where $D$ is the symmetric rate of deformation tensor and $W$ is the anti-symmetric rate of spin tensor. Furthermore, the rate of deformation and rate of spin tensors can be decomposed into elastic and plastic parts as well, i.e.,

$$D = D^e + D^p, \quad W = W^e + W^p$$  \hspace{1cm} (2.11)$$

The decomposition in (2.11) invariably plays an important role in any numerical implementation based on this type of formulation. As is seen in Figure 2.6, the total
effect of dislocation motion on the $\alpha$ slip system is represented by a simple shear strain, $\dot{\gamma}^\alpha$. The shearing rate, $\dot{\gamma}^\alpha$, is related to the plastic velocity gradient through the relation (Asaro, 1983)

$$\dot{\mathbf{L}}^p = \sum_{\alpha=1}^{N_{\alpha}} \dot{\gamma}^\alpha (\mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha) = \dot{\mathbf{F}}^p \mathbf{F}^{-1}$$

(2.12)

where $\dot{\mathbf{L}}^p$ is the plastic velocity gradient in the isoclinic, lattice invariant, intermediate configuration in which $\mathbf{s}_0^\alpha$ and $\mathbf{n}_0^\alpha$ are fixed unit vectors in the slip and slip plane normal directions, respectively, and are unchanged from their values in the undeformed, reference configuration. It should be noted that in the definition of the plastic velocity gradient in the intermediate configuration given above, summation occurs over all active slip systems.

Figure 2.6 Kinematics of elastic-plastic deformation of crystalline solid deforming by crystallographic slip. (I: Undeformed, II: Intermediate, III: Deformed (or Current) Configuration)
2.4.2 Kinetics of Crystalline Deformation

Kinetic equations provide the relationship between slip system shearing rate and the driving forces (resolved shear stresses). The kinetic relations and other constitutive equations can be postulated in various forms, and can be either rate dependent or rate independent in nature. In general, all materials are rate dependent to some extent, but the rate independent approximation works reasonably well for metals subjected to deformation at low homologous temperatures. The following discussion concerns a hyperelastic rate dependent formulation.

In a rate dependent formulation, all slip systems are considered to be active for stresses above the threshold, and there is a prescribed flow rule that relates the shearing rates to the resolved shear stress and the current state of the microstructure. This relationship is often written as a function of the form

\[
\dot{\gamma}^\alpha = \hat{\psi} \left( \frac{\tau^\alpha - \chi^\alpha - \kappa^\alpha}{D^\alpha} \right) \text{sgn}(\tau^\alpha - \chi^\alpha)
\]  \hspace{1cm} (2.13)

where \( \hat{\psi} \) is some model dependent scalar function, \( \tau^\alpha \) is the driving force (CRSS) for dislocation motion, \( \chi^\alpha \) is the back stress, \( \kappa^\alpha \) is the threshold stress, and \( D^\alpha \) is the drag stress. The use of two or three internal state variables is often necessary to capture the deformation behavior of a material that cannot be suitably modeled with a single internal variable. As pointed out by Sheh and Stouffer (1990), this partitioning of hardening into kinematic (back stress) and isotropic (threshold and drag stress) parts is necessary, in general, because the sources of internal stress are fundamentally different in nature. The
back stress reflects directional dependence of prior straining on the subsequent plastic flow. These effects lead to a dependence of reverse yielding on pre-strain in the forward direction. McDowell (1994) offers several physical origins of back stress in polycrystalline metals: (i) differential yielding among grains with hard and soft orientations, (ii) pile-ups of dislocations against hard boundaries such as grain or phase boundaries, (iii) differential resistance to slip in forward or reverse directions in certain systems by virtue of irreversible pinning mechanisms in the presence of planar dislocation structures in second phases or Taylor lattices, and (iv) distribution of short-range barriers to thermally activated dislocation motion and anelastic bowing of dislocations. In light of the previously mentioned mechanisms it can be seen that back stress is an inherently a multiscale modeling concept (McDowell, 2004). It is also pointed out that the kinematic hardening variable is not the average of a self-equilibrated internal stress field, but it is instead related to the peak athermal barrier resistance to thermally-activated motion of dislocations past obstacles; it is related more to statistical mechanics arguments of distributed barriers to slip with significant activation energy. On the other hand, the threshold stress represents the elastic energy stored in the material associated with the accumulation of dislocation density and the reduction of the mean free path of dislocations, as well as lattice friction effects arising from non-planar dislocation core structures. The drag stress can evolve in a manner similar to the threshold stress, but it is usually taken as a non-evolving material specific parameter that represents an inherent friction stress that depends on the nature of atomic bonding (e.g., Peierls stress), and serves as a normalizing factor in the flow rule. It is necessary to prescribe evolution equations for the hardening variables that are based on the physics of
deformation in the microstructure. Obviously, these functions are in general material dependent, and can take on many functional forms. Specific forms of evolution equations that appear in the literature will be discussed later. Generally speaking, the drag stress and threshold stress of a particular slip system depends on the dislocation motion on all active slip systems (so-called latent hardening effects), while the back stress depends to first order only on the shearing process on that particular slip system.

At the onset of plastic deformation, the initial values of back stress and drag stress are prescribed, as is the CRSS. For a material that obeys the Schmid law, the CRSS is simply the resolved shear stress in the slip plane in the slip direction. In a hyperelastic formulation, the CRSS can be calculated in a straightforward manner. For a given increment of the total deformation gradient, the elastic part of the deformation gradient is given by

\[ \mathbf{F}^e = \mathbf{F}^F \mathbf{F}^F \]  \hspace{1cm} (2.13)

Knowing \( \mathbf{F}^e \), we can calculate the Green Strain with respect to the intermediate configuration, i.e.,

\[ \mathbf{E}^e = \frac{1}{2} (\mathbf{F}^{e^T} \mathbf{F}^e - \mathbf{I}) \]  \hspace{1cm} (2.14)

Assuming linear elasticity, the elastic response of the crystal in the intermediate configuration is then given by
\[ \sigma^{pk2} = C : E^e \] (2.15)

where \( \sigma^{pk2} \) is the symmetric 2nd Piola-Kirchoff stress tensor and \( C \) is the 4th rank elastic stiffness tensor. The Cauchy stress tensor for the crystal is obtained by pushing forward the 2nd Piola-Kirchoff stress to the current configuration through the relation

\[ \sigma = \frac{1}{\det F^e} F^e \sigma^{pk2} F^{e^T} \] (2.16)

The resolved shear stress can be calculated as

\[ \tau^\alpha = \sigma^{pk2} : (s_0^\alpha \otimes n_0^\alpha) \] (2.17)

The shearing rates on each slip system can be calculated using the flow rule. In rate dependent formulations, a typical power law flow rule has the form

\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{\tau^\alpha - \chi^\alpha - \kappa^\alpha}{D^\alpha} \right)^m \text{sgn} (\tau^\alpha - \chi^\alpha) , \quad \langle x \rangle = 0 \quad \text{if} \quad x < 0 \]
\[ \langle x \rangle = x \quad \text{if} \quad x \geq 0 \] (2.18)

Here, \( \dot{\gamma}_0 \) is a reference shearing rate. See McGinty (2001) for a review on the details of the numerical integration employed in solving the above constitutive equations. Specific forms of evolution equations for the drag stress and back stress will discussed in the
following sections, which review some the recent crystal plasticity modeling efforts relevant to multi-phase materials such as Ti-Al alloys.

2.4.3 Non-Schmid Effects

Duesbery (1989) pointed out that Schmid’s law only strictly applies to lightly deformed or virgin materials. This is due to the fact that after continued deformation, certain dislocation substructures (such as low-angle subgrain boundaries) will form and anisotropy of flow will develop as a natural consequence. This type of violation of Schmid’s law is not considered here as it is due to the evolution of state variables at the slip system level, as well as the development of back stress, such as in the formation of low angle sub-grain boundaries (cf. Butler and McDowell, 1998). The non-Schmid effect considered here is due to the fact that stress components other than the shear stress resolved in the slip plane in the slip direction influence the CRSS, as is the case for non-planar core structures. Determining the core structure of the dislocation is a necessary step for including non-Schmid effects in crystal plasticity simulations. The structure will indicate what other components of the local stress tensor could possibly affect dislocation motion. Dislocation core studies are usually carried out through atomistic simulations (cf. Duesberry, 1989; Vitek, 1992). Using atomistic simulations as input for a continuum model, Bassani et al. (2001) investigated the core structure of $1/2\{111\}$ screw dislocations in bcc metals. They showed that this type of dislocation tends to spread into three $\{110\}$ planes that contain the dislocation line, and that the critical stress for dislocation motion depends on an applied shear stress that is parallel to the burger’s...
vector but is not necessarily in the glide plane. These observations led them to propose a generalized form of Schmid’s law

$$\tau_{cr}^\alpha = \tau^\alpha + \sum_\eta a_\eta^\alpha \tau^\eta $$  \hspace{1cm} (2.19)

where $\tau^\alpha$ is the Schmid stress and $\tau^\eta$ are the non-glide stresses, and $a_\eta^\alpha$ are the weight factors that determine the relative importance of the non-glide stresses. Although Bassani et al. (2001) were able to obtain a good correlation between their atomistic and continuum simulations, they have only considered non-glide stresses in the direction of the burgers vector in planes that contain the dislocation line. They have admitted that other components of the local stress tensor, such as shear stresses perpendicular to the burgers vector, may affect dislocation motion as well. They have stated that they intend to investigate this possibility in future work. This generalized form of Schmid’s law is easily incorporated into the flow rule given by Eq. (2.18) by modifying the threshold stress to include dislocation core dependent terms. Generally speaking, the threshold stress will also depend on inherent microstructural length scales that characterize dislocation density accumulation and the reduction in the mean free path. A general form of the threshold stress is given as

$$\kappa^\alpha = \kappa_0^\alpha + \frac{C_1 Gb}{\lambda} + C_2 Gb \sqrt{\rho} + \sum_\eta a_\eta^\alpha \tau^\eta $$  \hspace{1cm} (2.20)
where the first term typically represents an inherent lattice resistance to dislocation motion, the second term and third terms are the classical Orowan and Taylor expressions, respectively, and the last term is related to non-planar core structure. Here, $\lambda$ is a characteristic mean free path of dislocation glide associated with microstructural obstacles other than forest dislocations. Specific formulations for the threshold stress are discussed in subsequent sections.

2.4.4 Multi-Phase Material Models

Extending the concepts of crystal plasticity developed for single phase materials to multi-phase materials ushers in a unique set of challenges, and is still in its relative infancy. Such models are necessary to study the deformation and failure mechanisms of these complex materials at this level in order to provide insight into how they might be microstructurally optimized for specific applications. One of the main difficulties in formulating a multi-phase model is determining the material properties and slip geometry of the multi-phase material. In many multi-phase materials, the constituent properties of each phase in the alloyed material will differ from the properties of an isolated single crystal of that same phase due to slight differences in composition (Brockman, 2003). It may also be difficult to isolate a single crystal of a respective phase for a given polycrystalline sample, as is the case for lamellar ($\alpha + \beta$) regions, so experimentally measuring the properties of each phase is not always possible. Another difficulty that arises in the implementation of a multi-phase polycrystal model is determining how the slip geometry and deformation mechanisms are modified within each individual phase, including effects of the phase interfaces. This is undoubtedly the most important
consideration when developing such a model as the possible slip systems, orientation relations between phases, and interfacial properties will ultimately control the deformation behavior of the material.

There are two general approaches to modeling multi-phase materials using crystal plasticity. In one methodology, the material is treated as a representative microstructure for which there is no crystallographic distinction between the individual phases. In this type of model, the slip geometry is the same for each individual grain, but the hardening parameters that govern the yield behavior may be assigned different values in attempt to incorporate some of the effects of anisotropy and heterogeneity of the actual material. Due to the already simplified nature of the material microstructure, the slip geometry used in this type of model is often an idealization. Recently there have been several models of this type used to study Ti-64 (Morrissey et al., 2001; Morrissey, 2001; Goh et al., 2001; Goh, 2002, Schoenfeld and Kad, 2002). The models used by Morrissey (2001), Morrissey et al. (2001), Goh et al. (2001), and Goh (2002) employ a 2-D planar triple slip idealization for the slip geometry. In this scheme, there are three active slip systems equally spaced 120° apart (see Figure 2.7) which is akin to modeling the material with basal texture deforming only by prismatic slip. The angle $\theta$ completely specifies the orientation of the grain in this 2-D model.
Schoenfeld and Kad (2002) also use a planar triple slip idealization, but in their model they have one system that accounts for prismatic slip and two systems that represent idealized pyramidal slip and/or twinning (as pseudo-slip) along the $(11\bar{2}3)$ directions. Figure 2.8 shows their idealized representation of the 2-D slip geometry. Upon examination of their model it becomes obvious that their slip geometry is essentially equivalent to that proposed by Morrissey (2001) and Goh (2002). It is noted that while the slip geometry is essentially equivalent for both planar triple slip models, that anisotropic strengths of slip systems in the Schoenfeld and Kad (2002) model will lead to different results as compared to the model of Morrissey (2001) and Goh (2002) as many of their analyses assumed isotropic slip strengths.
The other method used to model multi-phase materials distinguishes between the microstructural constituents by assigning each one with its own set of slip systems. Such models can either employ an idealized 2-D slip geometry, or specify the 3-D slip systems of the different phases based on experimental observations. This implies that each phase does not necessarily need to be represented in precise detail, but instead specific distinctions are made between the crystallographic nature of certain components of the microstructure. An excellent example of this type of model has been presented by Brockman (2003). He proposes a model for dual-phase $\gamma/(\gamma+\alpha_2)$ Ti-Al alloy, which consists of an fcc $\gamma$-phase interspersed among lamellar $(\gamma+\alpha_2)$-phase (fcc+hcp). The active slip systems for the $\gamma$-phase are the standard $\{111\}\langle110\rangle$ systems of an fcc material. However, individual lamellae of the $(\gamma+\alpha_2)$ grains are not modeled as this would prohibit the size of the polycrystal model. Instead the lamellar structures are
treated as effective grains with augmented slip geometry that accounts for both fcc and hcp systems, as well as an interlamellar system. The interlamellar systems are actually parallel to the basal systems of what would be the $\alpha_2$ phase due to the BOR, but they have a much lower CRSS and are intended to capture the soft interlamellar mode that has been observed in these types of materials. Brockman (2003) points out that the use of both fcc and hcp slip systems in the effective grains corresponds to an isostress assumption throughout the lamellae. Obviously, there are a number of models for multi-phase materials and more specifically for Ti-Al alloys, but the previous examples were selected to illustrate the difference between crystallographically equivalent and crystallographically distinct types of models.

2.4.5 Scale Effects on Flow Stress and Strain Hardening Behavior

The main advantage that crystal plasticity models have relative to traditional macroscopic models is the ability to physically link the mechanisms of dislocation motion and interaction to the deformation behavior of the material, with specific details of crystallographic orientation being directly addressed. The form of the evolution equations for the drag stress, back stress, and threshold stress can significantly affect the response of the model material. Numerous forms of evolution equations have been proposed in the literature to capture various hardening behavior. For a review of various hardening models, see McGinty (2001). For the rate-dependent internal state variable model it is important that the particular form of the evolution equations capture the different physical attributes of the state variables. Recalling that the back stress
represents directional dislocation interactions with various types of barriers on a given slip system, the evolution equation needs to allow for the sign of the back stress to change based on the loading direction in order to capture phenomena such as the Bauschinger effect. On the other hand, the threshold stress and drag stress both represent dislocation resistance due to accumulative processes (isotropic hardening), should have an evolution equation that initially increases with increased plastic strain and eventually saturates. Previous researchers (McGinty, 2001; Morrissey, 2001; Goh, 2002) have employed evolution equations that appropriately capture these features based on the direct hardening/dynamic recovery concept. Typical forms of these evolution equations for drag stress, back stress, and threshold stress are

\[
\dot{D}^{\alpha} = \sum_{\beta} \left( A h_{\alpha\beta}^{DD} - B D^{\alpha} \right) |\dot{\gamma}| 
\]

(2.21)

\[
\dot{\chi}^{\alpha} = C \dot{\gamma}^{\alpha} - D \chi^{\alpha} |\dot{\gamma}| 
\]

(2.22)

\[
\dot{\kappa}^{\alpha} = \sum_{\beta} \left( A_{\kappa} h_{\alpha\beta}^{DD} - B_{\kappa} \kappa^{\alpha} \right) |\dot{\gamma}| 
\]

(2.23)

where \( h_{\alpha\beta}^{DD} \) and \( h_{\alpha\beta}^{DC} \) are the hardening moduli for drag stress and threshold stress, respectively, and \( A, C, \) and \( A_{\kappa} \) are direct hardening coefficients and \( B, D \) and \( B_{\kappa} \) are dynamic recovery coefficients, respectively. It is important to note that the back stress evolution on a particular slip system depends only on slip history on that system, whereas the evolution of drag stress and threshold stress depend on slip on all systems.
When formulating hardening laws for a given material, it is important to consider the relevant microstructural length scales that affect dislocation mobility. For example, it has been experimentally observed in single phase polycrystalline metals that flow stress increases with decreasing grain size. This behavior is interpreted as resulting from a decrease in the mean free path a dislocation can travel before encountering an obstacle, and is often included into models via a Hall-Petch term, i.e.,

\[
\sigma = \sigma_0 + k \frac{1}{\sqrt{d}} \quad (2.24)
\]

where \( \sigma \) is the flow stress, \( \sigma_0 \) is a reference stress, \( k \) represents the strength of the barrier, and \( d \) is the limiting length scale. While the grain size serves as a simple example of a type of controlling length scale, the complex structure and behavior of multi-phase materials often merits the consideration of several microstructural length parameters. In the case of Ti-Al alloys with a duplex microstructure some possible critical length scales are the primary grain colony size, the lamellar colony size, the distance between lamellar colonies, the thickness and distribution of laths, and also possibly the distance between twins. With so many different length scales possibly affecting the stress required to move dislocations, and no clear way to experimentally isolate the effect of each, the modeling efforts to date have focused on the lamina thickness as being the dominant length scale in these types of materials as a first order approximation. It has been shown for pure metals that flow stress is inversely proportional to the mean free path, which for a Taylor lattice is directly proportional to the square root of the dislocation density (Kuhlman-Wilsdorf, 1985). This observation is
of particular significance because it enables the additional incorporation of explicit length scales into the state variable evolution equations. Instead of writing the back stress, threshold stress and drag stress as functions of shear strain, the kinetics can be written in terms of evolution of dislocation density. Typically, the evolution equations for dislocation density are written in terms of the plastic shear strain rates, and initially it may seem that expressing the internal stress variables in terms of dislocation density is an unnecessary complication since the change in dislocation density is ultimately related to the plastic shear strain rates. Yet, this distinction sets the stage for another important capability of crystal plasticity models based on a multiplicative decomposition of the deformation gradient to relate to the underlying physics of the material.

Generally speaking, dislocations can be classified as either statistically stored dislocations (SSDs) or geometrically necessary dislocations (GNDs). SSDs are defined as dislocations for which a given burgers circuit enclosing them does not produce a net burgers vector; elastic strain is stored in the lattice associated with SSD density. GNDs are generated during deformation to maintain a compatible deformation, and are usually prevalent near grain or phase boundaries. However, under large deformation GNDs can develop within individual grains as significant misorientation leads to formation of subgrains. There is no way to directly determine the density of SSDs from the kinematics of continuum crystal plasticity, but there is a way to measure the density of GNDs from compatibility and integrability requirements (Bammann, 2001). At this point it should be noted that there are numerous measures of GND density reported in the literature stemming from the multiplicative decomposition and integrability requirements. For a
review of the different measures and their inter-relationships the reader is referred to Cermelli and Gurtin (2001). Referring to the mapping in Eq. 2.7, compatibility requires

\[ \oint_{c} \mathbf{x} \cdot dl = \oint_{c} \mathbf{F} \cdot d\mathbf{X} \cdot dl = 0 \]  

(2.25)

This contour integral can be converted into an area integral using Stoke’s theorem and is given as

\[ \oint_{c} \mathbf{F} \cdot d\mathbf{X} \cdot dl = -\int_{s} (\mathbf{F} \times \nabla) \cdot \mathbf{N} \cdot dA = 0 \]  

(2.25)

In Eq. (2.7), neither \( \mathbf{F}^e \) nor \( \mathbf{F}^p \) alone produces a compatible deformation. Therefore, forcing compatibility in terms of integrability in the intermediate configuration gives a natural measure of the GND density in terms of the deformation gradients that can be incorporated directly into the constitutive formulation. This then results in the direct inclusion of a length scale based on the kinematics of the model. The mathematical details of such a formulation are involved and can be posed in several different ways. For this reason the reader is referred to several works that deal with these concepts in detail (cf. Steinmann, 1996; Bammann, 2001, Clayton and McDowell, 2003, Clayton et al., 2004; Gurtin, 2002; Acharya and Bassani, 2000; Shizawa and Zbib, 1999). Only recently has there been a significant effort put into implementing these types of models, and none to date have been applied to modeling of dual-phase Ti-Al alloys.
Most of the current models incorporate length scales phenomenologically either by introducing a Hall-Petch term into the threshold stress, or by introducing a measure of dislocation density into the flow rule without distinguishing between GNDs and SSDs. It is common in such models that the dislocation density evolution equation is of the Kocks-Mecking form or a slight variation of it. Brockman (2003) has developed a model for \( \gamma / (\gamma + \alpha_2) \) Ti-Al with lamellar colonies. In his model he is mainly interested in capturing the stress-strain variations in polycrystalline samples at the level of a grain. To account for the reduction in the mean free path of dislocations on slip systems with burgers vector components normal to the lamellar interface, the critical flow stress of these systems is modified according to a Hall-Petch type correction given as

\[
\tau_c = \tau_0 + \frac{k}{\sqrt{d_L}}
\]  

(2.26)

where \( d_L \) is the lamellar spacing. Brockman does point out that this modification should not be necessarily interpreted as physically accurate, and that it merely provides a way to account for variations in material strengths that have been measured by various researchers working in different labs with different material variants.

Dimiduk et al. (2001) have proposed an alternative model for \( (\gamma + \alpha_2) \) Ti-Al attempting to capture the experimental behavior of both single and polycrystalline samples. In this work, they initially investigate the behavior by incorporating a Hall-Petch modified flow stress similar to that of Brockman (2003). They found that this type of model can capture the heterogeneous stress-strain response of a polycrystal at the grain
level, but cannot adequately capture the heterogeneity that develops at the subgrain level. It is noted that the deformation mechanisms governing fracture and ductility originate at these subgrain length scales, and this serves as their motivation for incorporating more clearly defined length scales into the constitutive formulation. They first propose an alternative to the Hall-Petch model based on Ashby’s model that relates the yield stress to the reciprocal of the square root of the grain size. This model is motivated by the idea that GNDs are needed to produce a compatible deformation field in polycrystalline materials. Therefore, the average glide resistance imposed by the accumulation of GNDs will govern the yield stress, i.e.,

$$\tau = \tau_0 + CGb \frac{4\gamma}{\lambda_{avg} b}$$

(2.27)

where

$$\gamma = \sum \int \dot{\gamma}^a dt$$

(2.28)

where $C$ is a constant, $G$ is the shear modulus, $b$ is the magnitude of the Burger’s vector, $\gamma$ is the accumulated plastic strain, and $\lambda_{avg}$ is the average lamellar spacing. In this type of model the effective length scale is proportional to the square-root of the dislocation density. Dimiduk et al. (2001) fit the experimental stress-strain data for PST crystals with a square-root relationship, and found a poor correlation for all sets of data. Searching for a better correlation, they proposed another model that accounted for the
limiting of the dislocation source size by the lamellar thickness, the average dislocation density $\rho_{avg}$, and a distribution of lamellar thicknesses as opposed to some average quantity. The yield stress in this model is given by

$$\tau = \tau_0 + C Gb \sqrt{\rho_{avg}} = \tau_0 + \frac{C Gb}{\lambda} + C Gb \sqrt{\rho_{avg}}$$ (2.29)

where $\rho_{avg} = \frac{4\gamma}{\pi \lambda b}$ and the lamellae thickness is given by $\lambda$. Equation (2.29) is solved successively assuming uniform deformation within the lamellae for a log-normal distribution of lath thicknesses to determine an average yield stress for the PST single crystal. This model is able to fit the experimental stress-strain data very well, and indicates that consideration of the statistical aspects of the microstructure, such as actual lamellae distribution, is important in micromechanical modeling of these materials.

While the results produced by incorporating a clearly defined length scale into this model are encouraging, there still exists an opportunity to incorporate the more physical interpretation of the dislocation density and evolution by making the distinction between GNDs and SSDs and using compatibility arguments to get the measure of GNDs. One possible approach is implementing the multiscale gradient theory of crystalline elastoplasticity as outlined by Clayton and McDowell (2003a,b) and Clayton et al. (2004). In this work a three-term multiplicative decomposition of the volume averaged deformation gradient is assumed of the form
Here, $\mathbf{\bar{F}}$ is the net residual deformation gradient which is further decomposed as $\mathbf{\bar{F}} = \mathbf{\bar{F}}^p \mathbf{\bar{F}}^i$, where $\mathbf{\bar{F}}^p$ is attributed to volume averaged dislocation motion and $\mathbf{\bar{F}}^i$ is a two-point tensor that can be envisioned as an indicator of residual lattice elasticity in the elastically unloaded configuration. The deformation tensor $\mathbf{\bar{F}}^i$ contains both residual elastic and residual plastic contributions and enables the incorporation of residual stresses that might arise due to the heterogeneity of the elastic-plastic deformation fields. For example, if the homogenization volume encompasses a single crystal, it is concluded that $\mathbf{\bar{F}}^i$ represents the contribution of grain subdivision processes (Clayton et al., 2004) to the total deformation gradient. However, $\mathbf{\bar{F}}^i$ does not describe the incompatibility of the average recoverable elastic deformation from volume element to volume element. By invoking compatibility arguments for the global configuration an expression is derived for the tensorial measure of GND density. The evolution of $\mathbf{\bar{F}}^i$ and the GND density are necessarily coupled and both will play a role in determining the effective length scale(s) of the microstructure. The details of this formulation are quite involved and the interested reader is referred to the previously listed references. While this framework is in relative infancy, it provides a rigorous methodology for addressing multiscale issues in plasticity such as, for example, the behavior of lamellar regions in duplex-type microstructures.
2.4.6 Incorporation of Twinning into Models

Twinning can be an important deformation mechanism in some hcp metals and alloys, and should be included in the constitutive formulation of these materials if it contributes significantly to material behavior. The two features of twinning that need to be accounted for in crystal plasticity models are the reduction in the effective size of the microstructure (assuming twins act as grain boundaries) and the ability to accommodate deformation in orientations and loading conditions in which slip is restricted. In most of the models proposed to date, twinning is treated in a fairly idealized manner as a type of pseudo-slip system with its own unique CRSS. However, it is different from the process of dislocation glide in that it only occurs for one sense of the CRSS and it is irreversible. The main difficulty of incorporating twinning into these models is handling the reorientation of the grains in the twinned regions without making the problem computationally infeasible. In light of this difficulty, several models have been proposed in the literature, none of which can fully account for all of the important aspects related to the actual process. A review of the pertinent details and discussion of the shortcomings of several of these models is undertaken in the following discussion.

Kalidindi (1998) has incorporated twinning into a crystal plasticity model in a manner that follows the elastic-plastic decomposition given in Section 2.4.1, as shown in Figure 2.9.
Although this schematic shows only one twin system as being activated, the model allows for multiple twinning systems to be activated in the same grain. Further twinning is prohibited in the twinned region, and slip in the twinned regions is allowed to occur only if there is a slip system with burgers vector coplanar with the twin habit plane. It is argued that dislocations that are not coplanar with the twin habit plane become trapped upon reorientation of the crystal. Implicit in Fig 2.9 is that the twinned and untwinned regions undergo the same deformation gradients (Taylor assumption). In the intermediate configuration, the lattice orientations of the twinned regions are related to the lattice in the untwinned regions by a 180° rotation of the lattice about the twin habit plane normal.
This particular relationship between the lattice in the parent and the twin regions holds for twins that are of the compound type (Staroselsky, and Anand, 2003). This adheres to the classical definition of twinning which requires that the twin and parent lattices are related by either a reflection in some plane or by a 180° rotation about some axis (Christian and Mahajan, 1995). Due to the lattice orientation mismatch in the twinned and untwinned regions, there will be a mismatch in stresses due to the anisotropy of elasticity within the crystal. Kaladindi (1998) assumes that the Cauchy stress in the crystal is equal to the volume average of the Cauchy stress in each of these regions. The same hyperelastic formulation given in Section 2.4.1 can be used to calculate stress and strain within a crystal with some slight modifications to account for the volume averaging of the stresses as well as the additional terms in the plastic velocity gradient due to the occurrence of twinning. Since the twinned and untwinned regions undergo the same deformation gradient, the difference of the 2nd Piola-Kirchoff stress between the parent and the twin is due solely to the dependence of the elastic stiffness tensor to lattice orientation in each region. In the intermediate configuration, the relationship between the elastic stiffness tensors is given by

\[
C_{ijkl}^{tw} = C_{pqrs}^{mt} Q_{ip} Q_{jq} Q_{kr} Q_{ls}
\]  

(2.31)

where \( Q_{ij} \) is the transformation between the lattice orientation in the matrix region to the lattice orientation in the twinned region, given by

\[
Q_{ij} = 2n_in_j - \delta_{ij}
\]  

(2.32)
where $n_i$ is the twin plane normal. After mapping the 2nd Piola-Kirchoff stress of the twinned and untwinned regions to the current configuration using Eq. 2.16, the volume averaged Cauchy Stress is given as

$$\sigma = \left(1 - \sum_{\alpha} f^{\alpha}\right)\sigma^{mat} + \sum_{\alpha} f^{\alpha}\sigma^{tw} \quad (2.33)$$

where $f^{\alpha}$ is the volume fraction of the grain that has been twinned to the $\alpha$-twin system.

The plastic velocity gradient in the intermediate configuration then takes the form

$$\dot{\mathbf{L}} = \left(1 - \sum_{\beta} f^{\beta}\right)\sum_{\alpha=1}^{N^{\alpha}} \dot{\gamma}^{\alpha} S_{s-m}^{\alpha} + \sum_{\alpha} f^{\alpha}\dot{\gamma}^{\alpha} S_{m}^{\alpha} + \sum_{\alpha} f^{\alpha}\left(\sum_{\beta} \dot{\gamma}^{\alpha} S_{m}^{\alpha \cdot s} - \dot{\mathbf{F}}^{\alpha} \dot{\mathbf{F}}^{\beta} \right) = \dot{\mathbf{F}}^{\alpha} \dot{\mathbf{F}}^{\beta} \quad (2.34)$$

where the first term accounts for shearing due to slip in the matrix region, the second term is the shearing that results from twinning, and the third term is due to slip in the twinned region. To complete the description of the model, criterion for twin nucleation and the evolution of the twin volume fraction must be specified. Kaladindi (1998) assumes that twin nucleation and twin volume fraction evolution depend only upon the resolved shear stress and an initial twin resistance (similar to drag stress), and both are described using simple power law equations similar to Eq. 2.18. These assumptions have been made because the variables that influence the rate of increase of the twin volume fraction are not clearly understood at the present time. The restrictions placed on the form of the evolution of $f^{\beta}$ are: the twin volume fraction must be nonnegative, the sum...
of the twinned regions cannot be greater than the volume of the grain, and the twinned
volume fraction can never decrease. This type of power relation for the evolution of the
twin volume fraction may be a good first approximation, but even Kalidindi (1998)
admits that it does not seem very physical. It has been mentioned earlier that Chichili et
al. (1999) had observed that twin volume fraction evolved in an entirely different manner
at high and low strain rates. Secondly, there is not really a need for an evolution equation
for twinned volume fraction. Instead of specifying a phenomenological equation, the
volume fraction should be tracked in terms of portions of the grain that have met some
critical criteria and have undergone the twinning transformation. The work of Idesman et
al. (1999) does indeed treat twinning as a thermodynamic transformation process,
although not in a crystal plasticity context, and will be discussed shortly. This should not
be a difficult addition to the model, since the twinned regions could be monitored through
reorienting the lattice. However, it should also be noted that not all twinning modes in
titanium are compound twins, and therefore the relationship between the parent and twin
cannot always be represented as a 180° rotation about the normal to the interface plane.
Applying the particular model to titanium would also require the slight modification of
allowing further twinning in prior twinned regions as this behavior has been
experimentally observed. Such a modification would additionally complicate equation
2.33 which would have to include a term to account for this situation.

In the model proposed by Karaman et al. (2001) for deformation twinning in
Hadfield steel, a self-consistent crystal viscoplasticity formulation is employed with a
power law flow rule similar to that given in Eq. (2.18). Attention here will be focused on
the predominant twin reorientation (PTR) scheme that is used to update the orientations
of the twinned regions. In the PTR scheme the real volume fraction of twinning in the polycrystal aggregate is defined as

\[
f_R = \sum_r f^r \sum_{t_i} \frac{g^{r,t_i}}{s^i}
\]

(2.35)

where \( g^{r,t_i} \) is the accumulated twinning shear associated with each twinning system \( t_i \), \( s^i \) is the characteristic shear associated with the twin system, and \( f^r \) is the volume fraction of the grain in the aggregate. When an entire grain is reoriented as a result of twinning, the effective twin volume fraction is updated as

\[
f_E = \sum_r f^r \Delta^r
\]

\[
\Delta^r = \begin{cases} 0 & \text{when the grain is untwinned} \\ 1 & \text{when the grain is twinned} \end{cases}
\]

(2.36)

where \( r \) represents the number of grains in the simulation. After each step in the solution, the amount of shear accumulated in each twinning system is compared with a threshold volume fraction

\[
f_T = A_1 + A_2 \frac{f_E}{f_R},
\]

(2.37)

where \( A_1 \) and \( A_2 \) are empirical constants. If the accumulated shear for a particular system exceeds the threshold value, the crystal will be reoriented with respect to this dominant
twin system. This scheme is designed to allow the model to self-adjust itself such that the reorientation of crystals occurs using the twinning systems that are the most active. A consequence of this scheme is that the effective volume fraction is forced to coincide with the real volume fraction, because if \( f_E > f_R \) then the threshold volume fraction will increase and further restrict twinning reorientation in the aggregate until the real volume fraction catches up to the effective volume fraction.

Both of the models above consider twinning as a type of pseudo-slip. Each twinning system has a specified CRSS and initial twin resistance, and the increase in twins determined by an evolution equation for the volume fraction of twins. The major element that these models are lacking is consideration of the thermodynamics of the twinning process. As will be shown in the following model for twinning that is based on thermodynamics, the activated twin system should be the one that maximizes the dissipation of the free energy of the system. This suggests that a thermodynamic driving force based on free energy minimization is more appropriate than prescribing a CRSS and twin resistance governing twin formation. A secondary problem with models like the one proposed by Karaman et al. (2001) is that after the grain is reoriented as a result of twinning, it is allowed to undergo further slip and twinning without restriction. As Kalidindi (1998) has pointed out, slip in these regions should be restricted to slip systems that are co-planar with the twin habit plane.

The model for twinning proposed by Idesman et al. (1999), unlike the previously discussed two models, is not yet incorporated into a crystal plasticity framework. In their model, they consider twinning as a special case of phase transformation which occurs instantaneously in some material region based on thermodynamics, without the need of
introducing volume fraction or a related evolution equation. They employ a
decomposition of the deformation gradient of the form

\[
F = F^e F^t F^p = V^e R^e F^t F^p
\] (2.38)

where \( F^t \) corresponds to the twinning portion of the deformation gradient and \( V^e \) and
\( R^e \) are the left stretch tensor and rotation tensor, respectively, resulting from the left
polar decomposition of the elastic deformation gradient. An order parameter
\( \xi \) \((0 \leq \xi \leq 1)\) associated with \( F^t \) is introduced such that twinning begins when \( \xi = 0 \) and
finishes at \( \xi = 1 \). During this time, the transformation deformation gradient evolves
from the identity tensor to a final value of \( \bar{F}^t \), which is determined completely by the
crystallography of the reorientation due to twinning. It should be noted that the system is
in equilibrium only when \( \xi = 0 \) or \( \xi = 1 \). The kinematical equations of the model are
listed below. All quantities are expressed in the current configuration.

**Kinematics**

\[
F = F^e F^t F^p = V^e R^e F^t F^p
\] (2.39)

\[
F^t = I + \xi (\bar{F}^t - I) \quad \xi \in [0,1]
\] (2.40)

\[
D = \left( \hat{F}^e F^e^{-1} \right)_{sym} + D^t + D^p
\] (2.41)

\[
D^p = \left( F^e F^t F^p F^p^{-1} F^e^{-1} F^t^{-1} \right)_{sym}
\] (2.42)

\[
D^t = \left( F^e F^t F^e^{-1} \right)_{sym} = \left( F^e F^t F^e^{-1} \right)_{sym} \xi
\] (2.43)
Twinning occurs within a material volume $V_n$ when the average dissipation associated with transformation reaches some critical value, $k_c$, and the dissipation for that variant of $\mathbf{F}^i$ is maximized. The dissipation is given as

$$\overline{X} = \frac{1}{m_n} \int_{V_n} \int_{0}^{1} \sigma : \mathbf{D}^i \frac{dt}{d\xi} dV_n = k_c$$  \hspace{1cm} \text{(2.44)}$$

where $m_n$ is the mass of the transforming volume and $t$ is time. This dissipation equation was derived from considering the thermodynamics of a free energy function of the following form

$$\psi = \hat{\psi}(\mathbf{B}^e, T, \xi)$$  \hspace{1cm} \text{(2.45)}$$

$$\mathbf{B}^e = \frac{1}{2} \left( \mathbf{F}^e \mathbf{F}^{e^t} - \mathbf{I} \right)$$  \hspace{1cm} \text{(2.46)}$$

where $\mathbf{B}^e$ is the elastic strain tensor in the current configuration, $T$ is the temperature, and $\xi$ is the dimensionless order parameter. An extremum principle is used to determine whether or not a particular variant of $\mathbf{F}^i$ maximizes the dissipation compared to all other admissible variants of $\mathbf{F}^i$ in $V_n^o$ and is expressed as

$$\overline{X}(V_n^o, \mathbf{F}^{i^t}) - k_c < \overline{X}(V_n, \mathbf{F}^i) - k_c$$  \hspace{1cm} \text{(2.47)}$$
While there is perhaps a more satisfying basis for this model as compared to the previous two, the present numerical implementation of Idesman et al. (1999) is computationally expensive and would not be feasible for large polycrystal simulations. In a global iteration of a finite element formulation of this model, each element is individually assigned an increment of the transformation strain until the final value is reached while all of the other elements are treated as elasto-plastic only. For each increment of transformation strain, the elasto-plastic boundary value problem is solved to update the stress fields and the amount of energy dissipation. This process is then repeated for every element. The element that meets the twinning criteria and dissipates the largest amount of energy is allowed to twin, and the global iteration process is repeated until the complete boundary value problem is solved. Therefore, it is not feasible to incorporate this type of twinning methodology into a crystal plasticity model in its current form.
CHAPTER III
MATERIAL MODELING

The material model discussed herein is a hyperelastic crystal viscoplasticity formulation as has been outlined in Section 2.4. The model has been developed and implemented in an ABAQUS (2003) User Material (UMAT) subroutine (McGinty, 2001). The UMAT uses a fully implicit integration scheme that is based on an extension of the work of Cuitino and Ortiz (1992), and is able to accommodate general 3-D deformation. It has been previously discussed in Chapter 2, that hcp titanium and its alloys have various sources of anisotropy and complex deformation mechanisms. The modeling effort is an extension of the work of Morrissey (2001), Morrissey et al. (2003), Goh et al. (2001), and Goh (2002) and incorporates more of the material complexities including three-dimensional anisotropic slip systems, realistic textures, as well as non-Schmid effects for prismatic glide to further investigate their influence on the deformation behavior of \( \alpha \)-titanium and \( \alpha / \beta \) Ti-Al alloys. Section 3.1 will outline the model for bimodal Ti-64 which consists of two distinct phases; the primary \( \alpha \)-phase and the secondary \( \alpha + \beta \) lamellar phase. Section 3.2 outlines the basics of texture quantification. Section 3.3 will investigate how variation of model parameters (texture, relative strengths of slip systems, non-Schmid behavior, phase distributions) affects deformation behavior.
3.1 Crystal Plasticity Model for Duplex Ti-6Al-4V

3.1.1 Primary α-phase

The primary mechanism of plastic deformation in α-titanium is the prismatic glide of screw dislocations. For this reason, the planar triple slip (PTS) approximation used by Morrissey et al. (2003) and Goh et al. (2001) is well-suited to capture this mode of deformation. However, such models are limited in their ability to model realistic microstructures due to the restrictions placed on the orientation of the grains in a polycrystalline model. Recalling the PTS model described in Section 2.4, only one angle is needed to specify the orientation of an individual grain. This model assumes a strong c-axis texture for which all of the grains have c-axes perpendicular to the plane of deformation and therefore is unable to capture the anisotropy that results from the multiple competing deformation modes. By incorporating more of the active slip systems of the hexagonal crystal structure and allowing specification of three-dimensional orientation distributions of grains, it is possible to study the heterogeneity of a greater range of crystallographic textures, including more realistic textures.

There are 24 active slip systems included in the model for the α-phase: 3 basal \(\langle 1\bar{1}2\bar{0}\rangle\{0001\}\), 3 prismatic \(\langle 1\bar{1}2\bar{0}\rangle\{10\bar{1}0\}\), 6 \(\langle a \rangle\) first-order pyramidal \(\langle 1\bar{1}2\bar{0}\rangle\{10\bar{1}1\}\), and 12 \(\langle c + a \rangle\) first-order pyramidal \(\{10\bar{1}1\}\{11\bar{2}3\}\), as illustrated below.
It should be noted that twinning can play a significant role in the deformation of $\alpha$-Ti, but has not been included in the current model for two reasons. To date it can be argued that there is a lack of physically and/or computationally tractable crystal plasticity formulations that incorporate twinning. Second, the main focus of this work is to study Ti-64 and twinning does not contribute significantly to its deformation due to high content of aluminum atoms in solid solution. It has been observed experimentally that the likelihood of twinning decreases with increasing aluminum content and is very rare in alloys containing 6% or greater atomic wt. aluminum (Williams et al., 2002).

The rate of shearing on each slip system is calculated via the isothermal flow rule given in Eq. (2.18), i.e.,

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{|\tau^\alpha - \chi^\alpha| - \kappa^\alpha}{D^\alpha} \right)^m \text{sgn}(\tau^\alpha - \chi^\alpha)$$  

(3.1)
where \( \dot{\gamma}_0 \) is the reference shearing rate, \( \tau^\alpha \) is the resolved shear stress, \( \chi^\alpha \) is the back stress, \( \kappa^\alpha \) is the threshold stress that defines initial yielding, \( D^\alpha \) is the drag stress representing the slip system resistance, and \( m \) is the rate sensitivity exponent. The anisotropy of the CRSS is mostly accounted for through the drag and threshold stresses with a small contribution coming from the back stress. While there are no “exact” values for the CRSS in these materials per se, consistent trends do emerge from the literature. A summary of various authors’ findings is presented in Table 3.1. All values have been normalized by the reported value of the CRSS for prismatic slip, i.e., \( \tau_{\text{CRSS}}^\text{basal} / \tau_{\text{CRSS}}^\text{prism} \).

Table 3.1 Relative CRSS of slip systems reported in the literature for \( \alpha \)-titanium and \( \alpha / \beta \) Ti-Al alloys, normalized to CRSS for prismatic slip.

<table>
<thead>
<tr>
<th>( \tau_{\text{CRSS}}^\text{basal} / \tau_{\text{CRSS}}^\text{prism} )</th>
<th>( \tau_{\text{CRSS}}^{\text{pyra prism}} / \tau_{\text{CRSS}}^\text{prism} )</th>
<th>( \tau_{\text{CRSS}}^{\text{pyra prism}} / \tau_{\text{CRSS}}^\text{prism} )</th>
<th>( \tau_{\text{CRSS}}^\text{prism} / \tau_{\text{CRSS}}^\text{prism} )</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.93 - 1.3</td>
<td>1</td>
<td>1.1 - 1.6</td>
<td>Medina Perilla and Sevillano, 1995</td>
<td></td>
</tr>
<tr>
<td>1.25</td>
<td>-</td>
<td>2.625</td>
<td>Paton et al., 1973</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>8.0 - 15.0</td>
<td>Fundenberger et al., 1997</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>1</td>
<td>3</td>
<td>Dunst and Mecking, 1996</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-</td>
<td>8</td>
<td>Lebensohn and Canova, 1997</td>
<td></td>
</tr>
<tr>
<td>1.43</td>
<td>-</td>
<td>4.23</td>
<td>Bieler and Semiatin, 2001</td>
<td></td>
</tr>
</tbody>
</table>

The drag stress is taken as a non-evolving constant, i.e., \( D^\alpha = 0 \). The saturated level of slip system back stress will be kept to a relatively small value compared to the drag and threshold stresses, \( \chi_{\text{sat}}^\alpha = 5 \text{ MPa} \), because very little hardening is observed in these materials at the slip system level due to the extremely planar nature of slip at room temperature. It is assumed that most of the apparent back stress in the stress-strain response arises from interactions of grains/phases with different elastic properties and
resistance to flow. Similar assumptions have been made by both Morrissey (2001) and Goh (2002). Therefore, the slip system back stress it is kept to a minimum so that the focus will be on the initial yielding behavior due to the anisotropy associated with differing CRSS and the ODF. The back stress evolves according to an Armstrong-Fredrick direct hardening/dynamic recovery type of equation (cf. Goh, 2002) and is given by

\[ \dot{\chi}^\alpha = h_d \left( b \dot{\gamma}^\alpha - \chi^\alpha \| \dot{\gamma}^\alpha \| \right) = h_d \dot{\gamma}^\alpha - h_d \chi^\alpha \| \dot{\gamma}^\alpha \| \]  

(3.2)

The threshold stress is also assumed constant, i.e., \( \kappa^\alpha = 0 \), for all but prismatic systems. In this formulation the threshold stress defines the initial slip system strength based on the free slip length of each slip system via a Hall-Petch type relation. The threshold stress is also used to incorporate the non-Schmid behavior for prismatic systems that arises from the non-planar dislocation core structure (Bassani, et al., 2001). The core structure asserted in the model is that outlined by Naka et al. (1988) as described in Section 2.4.3. The dissociation is given by the reaction

\[
\frac{1}{3} \langle 1 \overline{1} 2 0 \rangle = \\
\frac{1}{9} \langle 1 \overline{1} 2 0 \rangle (10 \overline{1} 0) + \frac{1}{9} \langle 1 \overline{1} 2 0 \rangle (10 \overline{1} 0) + \frac{1}{18} \langle 1 \overline{1} 2 0 \rangle (10 \overline{1} 1) + \frac{1}{18} \langle 1 \overline{1} 2 0 \rangle (10 \overline{1} 1)
\]

(3.3)

and is illustrated in Figure 3.2.
The dissociated core structure of prismatic screw dislocations assumed here first requires a recombination of the partial dislocations from the first-order pyramidal planes in the prismatic plane before slip can occur. Therefore, the CRSS for the three prismatic systems is a function of the resolved shear stress in the prismatic plane as well as the two associated first-order pyramidal planes. To incorporate this dependence into the model, the threshold stress is given as

\[ \kappa^\alpha = \kappa_0 + k_y \left( \frac{d^\alpha}{d} \right)^{0.5} + A \left( \tau_1^\alpha - \tau_2^\alpha \right) \]  

(3.4)
where \( \kappa_0 \) is a constant amount of frictional stress that is taken to be equal for all slip system families, \( k_y \) is the Hall-Petch slope and \( d^\alpha \) is the microstructural dimension relating to the free slip length of the slip system. In the case of the primary \( \alpha \)-phase, \( d^\alpha \) simply corresponds to the mean \( \alpha \) grain size. The third term in the Eq. (3.4) relates to the driving force for recombination of the partial dislocations in prismatic planes and will either increase or decrease the threshold stress, depending on the sense of the applied load with respect to the crystal orientation. The non-Schmid term is included only for prismatic systems (\( A = 0 \) for non-prismatic systems) and leads to tension/compression yield asymmetry for these systems. The constant \( A \) determines the strength of the sessile core configuration, where \( \tau_1^\alpha \) and \( \tau_2^\alpha \) are the non-Schmid resolved shear stresses required for recombination of the dissociated partial dislocations in the prismatic plane. For example, in Figure 3.2 \( \tau_1^\alpha \) is the resolved shear stress in the \((10\overline{1}1)\) plane in the \(\{11\overline{2}0\}\) direction and \( \tau_2^\alpha \) is the resolved shear stress in the \((10\overline{1}1)\) plane and in the \(\{11\overline{2}0\}\) direction. The sign of \( A \) determines whether yielding will occur at higher or lower stress level in tension versus compression. In a single crystal optimally oriented for prismatic slip (c-axis perpendicular to the loading direction), yield in tension will be higher than in compression if \( A \) is positive and vice versa. Care must be taken in specifying the magnitude of \( A \) such that \( \kappa_0 + k_y (d^\alpha)^{-0.5} \geq -A(\tau_1^\alpha - \tau_2^\alpha) \) to avoid an aphysical yielding condition because \( \kappa^\alpha \) must always be greater than or equal to zero. For this particular form of evolution equations and constants, the resulting material exhibits nearly perfectly plastic yield behavior at the slip system level. However, the variation of the drag stress among different slip systems and the inclusion of dependence on non-Schmid stresses for
prismatic slip will result in heterogeneous macro yield behavior due to the differential yielding of primary $\alpha$ grains for a polycrystal or for an $\alpha$/$\beta$ phase morphology. In fact, as will be discussed later, cyclic hysteresis loops are modeled fairly well with this framework.

3.1.2 Secondary $\alpha+\beta$ lamellar phase

Presently the deformation behavior of the secondary $\alpha+\beta$ lamellar regions is not well understood. It is impossible to create an isolated lamellar single crystal in the same phase arrangement and composition that it appears in the Ti-64 bimodal microstructure. This prohibits experimental determination of basic deformation mechanisms at the single crystal level for this particular phase morphology. While nanoindentation is potentially useful, there are many issues concerning its interpretation for such layered microstructures that must yet be addressed. As it was mentioned in Section 3.1.1 the lamellar $\alpha+\beta$ regions are significantly harder than the primary $\alpha$-phase. It is believed that these lamellar regions influence deformation by providing a considerable obstacle to slip transmission from neighboring primary $\alpha$-grains, resulting in a strengthening effect (cf. Suri et al., 1999; Savage et al., 2001, Ambard et al., 2000). While it is generally accepted that the lamellar grains are appreciably harder than the primary $\alpha$-grains, in several computational studies the CRSS for the $\{111\}\overline{1}\{110\}$ bcc slip systems of the $\beta$-phase is assumed to be less than or equal to the CRSS for prismatic systems in the primary $\alpha$-phase (cf. Dunst and Mecking, 1996; Lebensohn and Canova, 1997; Barton and Dawson, 2001). This is based on the observation that $\beta$-Ti alloys are mechanically softer than $\alpha$-Ti alloys. This approach seems to be counter-intuitive to the notion that
the presence of lamellar colonies increases the strength of these materials. If all possible slip systems in the $\beta$-phase were easier to activate than prismatic glide in the primary $\alpha$-phase, then the presence of $\alpha + \beta$ regions could conceivably result in weaker mechanical response. It is more likely that only a limited number of the bcc slip systems exist in the lamellar regions which, for certain orientations, are more easily activated than slip systems in the primary $\alpha$-phase. In this approach, the lamellar phase will be harder than the primary $\alpha$-phase for arbitrary orientations, but will still offer an easy deformation mode for favorable orientations. The extremely small thicknesses of the secondary $\alpha$ (1-3 $\mu$m) and $\beta$ (200-1000 nm) laths compared to the size of the primary $\alpha$ grains make it computationally infeasible to explicitly model the individual lamellae in a polycrystalline model. Instead an approach similar to that used by Brockman (2003) for modeling lamellar $\gamma$-TiAl is used to incorporate features of slip in both hcp and bcc phases into the equivalent model of $(\alpha + \beta)$ grains.

There are 24 possible slip systems in these lamellar regions: 3 basal $\langle 11\bar{2}0 \rangle (0001)$, 3 prismatic $\langle 11\bar{2}0 \rangle \{10\bar{1}0 \}$, 6 $\langle a \rangle$ first-order pyramidal $\langle 11\bar{2}0 \rangle \{10\bar{1}1 \}$, and 12 $\langle 111 \rangle \{110 \}$ bcc systems, as illustrated in Figure 3.3. Prior to assigning grain orientation, the bcc slip systems are transformed into the hexagonal coordinate system according to the burgers orientation relation (BOR) $\langle 0001 \rangle_a \| \{110 \}_\beta$, $\langle 11\bar{2}0 \rangle_a \| \{111 \}_\beta$. The crystallographic relationships between the secondary $\alpha$ and $\beta$ laths maintained by the BOR are shown in Figure 3.4. Since there are 12 $\langle 111 \rangle \{110 \}$ slip systems in bcc a material and there are 3 $\langle 11\bar{2}0 \rangle (0001)$ slip systems in an hcp material, there are 36
possible permutations for the BOR at the hcp/bcc interface. However, using the UMAT to investigate the difference in mechanical response for each of the variants for an arbitrarily oriented lamellar grain, it was determined that there are only six unique responses among the 36 permutations. As a first approximation of the material behavior, only one of the six variants will be used in the model. This is consistent with experimental observations that only a limited number of variants are present in the final as-processed material.

Figure 3.3 Slip geometry for equivalent representation of $\alpha + \beta$ grains.
First-order pyramidal $\langle c+a \rangle$ systems are not included in the model of the lamellar grains because this hard mode of deformation is unlikely to be active in the secondary $\alpha$ laths. Additionally, the accommodation of plastic deformation along the c-axis in these lamellar regions can be accounted for by the bcc systems. The lamellar slip systems are governed by the same flow rule as the primary $\alpha$-phase given in Eq. (3.1). The drag stress values for the hcp slip systems are taken to be the same as their counterparts in the primary $\alpha$-phase (i.e., $D^{\text{prism}}_\alpha = D^{\text{prism}}_{\alpha+\beta}$, $D^{\text{basal}}_\alpha = D^{\text{basal}}_{\alpha+\beta}$, etc.) whereas the drag stress for the bcc systems is taken to be slightly lower than the drag stress for prismatic systems ($D^{\text{[111]}[110]}_{\alpha+\beta} = 0.9D^{\text{prism}}_\alpha$) to represent the mechanically softer nature of $\beta$-Ti alloys.

It has been argued (Suri, et al., 1999; Savage, et al., 2001; Savage et al., 2003) that the CRSS for the lamellar prismatic and basal systems depends on the magnitude of the residual dislocation that is left behind at the $\alpha/\beta$ interface after dislocation transmission. The magnitude of the residual dislocation is related to the misalignment of...
burgers vectors in the $\alpha$ and $\beta$ phases and can be calculated using the BOR. The argument is that leaving behind a larger net residual dislocation should result in a higher CRSS for that system. This hypothesis has been tested (Savage et al., 2001; Savage et al., 2003) on a single colony crystal of the $\alpha/\beta$ alloy Ti-6246. The $\alpha/\beta$ morphology in these experiments was a honeycomb type of arrangement, and while it is not a true lamellar structure, the BOR is maintained with respect to the $\alpha/\beta$ interface plane. Their results agree with the residual dislocation argument reasonably well for prismatic slip; however, the basal slip system that is expected to leave behind the largest net residual dislocation has the lowest value of CRSS. This seems to suggest that there may be other aspects that may influence the interfacial dislocation transmission process.

The approach taken in this work is that the relative ease of activation for the different slip systems in the lamellar regions will be incorporated in the threshold stress via the Hall-Petch type term; three different microstructural length scales, $d$, corresponding to the secondary $\alpha$ lath thickness, the $\beta$ lath thickness, and the lamellar colony size are used to distinguish between hard and soft deformation modes. The hard deformation modes are the slip systems in which slip transmission is impeded by the $\alpha/\beta$ interface due to the lack of corresponding parallel slip planes in both hcp and bcc phases. The specific slip systems that comprise the set of hard deformation modes depends on the particular BOR variant, but in general includes 2 prismatic systems, 6 first-order pyramidal systems, and 10 $\{111\}\{110\}$ bcc slip systems. Amongst the set of hard deformation modes, the hcp slip systems are governed by the secondary $\alpha$ lath thickness while the bcc slip systems are governed by the $\beta$ lath thickness. The soft deformation modes are the slip systems which either glide parallel to the $\alpha/\beta$ interface
or have parallel slip planes in both the $\alpha$ and $\beta$ phases. This set of soft deformation modes consists of 3 basal, 1 prismatic, and 2 \{111\}{110} bcc slip systems. Within the set of soft deformation modes assumed in this study, the prismatic system glides parallel to the $\alpha$/$\beta$ interface, whereas the basal and bcc planes are parallel and dislocations gliding in these planes are able to traverse the length of the lamellar colony. Figure 3.5 illustrates the relevant microstructural length parameters as well the soft lamellar deformation modes. It is noted that our definition of soft modes associated with slip transmission differ somewhat from those identified by Savage et al. (2004) based on residual dislocations. In this work Savage et al. (2004) look at the transmission of the unique individual basal and prismatic dislocations identified in Figure 2.5 and measure the anisotropy of CRSS for each type of dislocation transmission and correlate their findings with respect to the misorientation angle between the burgers vectors in the $\alpha$ and $\beta$ phases. This level of detail has not been included in the current model. Essentially, we assume that all three basal slip systems are soft by virtue of the slip planes being aligned in the $\alpha$ and $\beta$ phases. The veracity of either assignment of easy slip requires further research for clarification.
3.2 Grain Orientation

Having defined the constitutive equations and slip geometry, specification of grain orientation is necessary. Prior to specifying grain orientation, the slip directions and plane normals for the hexagonal structure given in Miller-Bravais indices are converted into a standard orthogonal coordinate system. This system is defined such that \( x_1 = [100] = [2\overline{1}00] \), \( x_2 = [010] = [01\overline{1}0] \), and \( x_3 = [001] = [000\overline{1}] \) and is shown in Figure 3.4. For the sake of overall clarity, the negative \( x_2 \)-axis, \([0\overline{1}0]\), is shown in Figure 3.6. It should be noted that all Euler angles and crystallographic transformations related to the BOR are done with respect to the right-handed coordinate system\([100]−[010]−[001]\), and that Figure 3.6 displays a left-handed coordinate system.
merely to present the clearest picture of the relationship between the Miller-Bravais
directions and the associated orthogonal system.

![Diagram](image)

Figure 3.6 Coordinate relationship between the orthogonal system used in the model and
the Miller-Bravais system.

Individual grain orientation is specified via three Euler angles which give the
relationship between the local crystal coordinate system (the orthogonal system
\([\text{100}]−[\text{010}]−[\text{001}]\)) of each grain with respect to a fixed specimen coordinate system
(e.g. finite element model global coordinate system). The set of Euler angles for each
grain in the polycrystal comprises the ODF and can be quantitatively represented by basal
plane pole figures, i.e., \((0001)\) pole figures. For a given grain, the Euler angles are
defined as shown in Figure 3.7.
Figure 3.7 Schematic illustrating the Bunge convention for Euler angle specification (Randle and Engler, 2000).

Figure 3.7 illustrates the Bunge convention for describing Euler angles. The angle definition as given by Randle and Engler (2000) is listed below; in this convention, the specimen coordinate system is transformed to the local crystal coordinate system, i.e.,
1. $\varphi_1$ about the normal direction ND (Z-axis), transforming the transverse direction TD (Y-axis) into TD’ (Y’) and the rolling direction RD (X-axis) into RD’ (X’).

2. $\Phi$ about the axis RD’ (in its new orientation).

3. $\varphi_2$ about ND’ (in its new orientation).

The rotation through $\varphi_1$ about the ND brings the RD into the crystal XY-plane. Then by rotating through $\Phi$ about RD’ the ND becomes coincident with the crystal Z-axis. To complete the transformation, the final rotation through $\varphi_2$ about ND’ is necessary to align RD’ with the crystal X-axis. These three successive rotations can then be easily combined to give total transformation matrix relating the specimen coordinate system to the crystal coordinate system. The relationship can be written in the form (Randle and Engler, 2000)

$$C_c = g \cdot C_s$$  \hspace{1cm} (3.5)

where $C_c$ is the matrix of base vectors representing the crystal coordinate system, $C_s$ is the matrix of base vectors representing the specimen coordinate system, and $g$ is the transformation matrix relating the two coordinate systems. The transformation matrix $g$ is then given as the product of the three successive rotations as

$$g = g_{\varphi_2} \cdot g_{\Phi} \cdot g_{\varphi_1}$$  \hspace{1cm} (3.6)
where

\[
\begin{bmatrix}
c_{\varphi_1} & s_{\varphi_1} & 0 \\
-s_{\varphi_1} & c_{\varphi_1} & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
c_{\varphi_2} & s_{\varphi_2} & 0 \\
-s_{\varphi_2} & c_{\varphi_2} & 0 \\
0 & 0 & 1
\end{bmatrix}
= \begin{bmatrix} 1 & 0 & 0 \\
0 & \cos \Phi & \sin \Phi \\
0 & -\sin \Phi & \cos \Phi \end{bmatrix}
\]

Therefore,

\[
\begin{bmatrix} g_{11} & g_{12} & g_{13} \\
g_{21} & g_{22} & g_{23} \\
g_{31} & g_{32} & g_{33} \end{bmatrix}
= \begin{bmatrix} c_{\varphi_2} c_{\varphi_1} - s_{\varphi_2} c_{\Phi} s_{\varphi_1} \\
-c_{\varphi_2} s_{\varphi_1} + s_{\varphi_2} c_{\Phi} c_{\varphi_1} \\
s_{\varphi_2} s_{\Phi} \end{bmatrix}

(3.7)
\]

\[
g_{21} = -s_{\varphi_2} c_{\varphi_1} - c_{\varphi_2} c_{\Phi} s_{\varphi_1} \\
g_{22} = -s_{\varphi_2} s_{\varphi_1} + c_{\varphi_2} c_{\Phi} c_{\varphi_1} \\
g_{23} = c_{\varphi_2} s_{\Phi} \\
g_{31} = s_{\varphi_2} s_{\varphi_1} \\
g_{32} = -s_{\Phi} c_{\varphi_1} \\
g_{33} = \cos \Phi
\]

(3.8)

To obtain the transformation matrix for an individual grain used in the UMAT to initialize the grains from the local to global coordinate system Eq. 3.5 can be inverted, i.e.,
since \( g^T = g^{-1} \) for proper orthogonal transformations. To generate a set of Euler angles representative of an initially random uniform orientation distribution the angles can be determined from the relation

\[
\phi_i = 2\pi \xi_i, \quad \Phi = \arccos\left(2\pi \xi_{i+1} - 1\right), \quad \varphi_2 = \pi \xi_{i+2}
\]  

(3.7)

where \( \xi_i \) is a series of uniformly distributed random deviates, \( 0 \leq \xi_i \leq 1 \) (McGinty, 2001). It should also be noted that by restricting the range of certain combinations of the Euler angles, it is possible to create the specialized textures (basal, transverse, and basal/transverse) that have been discussed in Chapter II. Texture can significantly affect the deformation behavior of these materials due to both anisotropic elasticity and anisotropy of the CRSS, and its influence on material response will be investigated in the parametric studies.

Section 3.3 Parametric Studies of Model Parameters

Prior to calibrating the model for use in a specific application it is useful to investigate the sensitivity of the predicted material response to changes in the model parameters. A series of simulations is conducted to study the effects of the variation in the relative slip system strength according to slip family (i.e., prismatic, basal,
pyramidal ($a$), pyramidal ($c + a$)) for a fixed level of threshold stress (grain size), any tension/compression asymmetry resulting from non-Schmid behavior, texture, and phase distribution. In an attempt to better understand the contributions of each of these items, the simulations are divided into three different material representations. To study the effect of varying relative slip system strengths, a microstructure with random texture consisting entirely of primary $\alpha$-phase is used in order to isolate this behavior from the interplay between CRSS, texture and phase distribution. A second set of three primary $\alpha$ microstructures are then created: one each with basal, transverse, and basal/transverse textures with fixed values of threshold and drag stress to determine the effect of texture on material response without the influence of multiple phases. A third and final set of microstructures are constructed incorporating the dual-phase nature of the bimodal microstructure to determine the influence of phase distribution on material response. For each type of texture (i.e., basal, transverse, and basal/transverse) three different phase distributions are investigated. Simulations are performed under quasi-static (0.005 s$^{-1}$) monotonic (tension and/or compression) strain-controlled loading conditions.

**Section 3.3.1 Influence of CRSS**

In Section 3.1 it was noted that a significant range of variation exists in the reported measurements for strengths of the various slip system families. It has also been pointed out in Chapter II that plastic deformation in bimodal Ti-64 occurs predominantly within the primary $\alpha$-phase, and the lamellar $\alpha + \beta$ regions are appreciably harder in terms of slip activity. The lamellar colonies act as a strengthening phase in $\alpha/\beta$ Ti alloys with this type of duplex microstructure. Therefore, the first set of parametric
studies will focus on the effect of variation of the relative CRSS amongst the primary \( \alpha \) slip system families and the resultant deformation behavior. The deformation behavior will be quantified in terms of axial yield stress \( \sigma_{22}^\alpha \), the saturated axial stress \( \sigma_{22}^s \), the difference between the saturated and yield stress \( (\Delta \sigma = \sigma_{22}^s - \sigma_{22}^\alpha) \), and the maximum effective plastic strain \( \tilde{\varepsilon}_{\text{max}}^\rho \). The axial yield stress is defined as the 0.2\% offset stress of the statistical volume element consisting entirely of primary \( \alpha \) grains, the saturated flow stress is defined as the true axial stress at 5\% true axial engineering strain of the same statistical volume element, and the effective plastic strain is defined as

\[
\tilde{\varepsilon}_{\text{max}}^\rho = \sqrt{2 \overline{\varepsilon} : \varepsilon^p}
\]

where

\[
\varepsilon^p = \sum_\alpha \gamma^\alpha \left(s_0^\alpha \otimes m_0^\alpha \right)_{\text{sym}}
\]

The choice of variables chosen to quantify the deformation behavior offers insight into both the average \( (\sigma_{22}^\alpha, \sigma_{22}^s, \text{ and } \Delta \sigma) \) and local \( (\tilde{\varepsilon}_{\text{max}}^\rho) \) material response. The following set of simulations are carried out for fixed primary \( \alpha \) grain size of 30 \( \mu \)m (i.e., constant value of threshold stress) such that any changes in the CRSS enter via the drag stress since the initial slip system yield strength is approximately equal to the sum of the drag and threshold stresses, i.e., \( \tau_{\text{CRSS}} \approx \kappa + D \), by virtue of the high value of the exponent on stress in the flow rule for Ti-64.
There is wide consensus in the literature that the primary mechanism of plastic deformation in \( \alpha \)-titanium at room temperature is prismatic glide of \( \langle \mathbf{a} \rangle \) dislocations. Therefore, the drag stress for prismatic systems is held constant throughout the simulations, as the prismatic systems serve as the reference point for the relative variation in CRSS of the other slip system families. The other active slip systems in the primary \( \alpha \)-phase include basal \( \langle \mathbf{a} \rangle \), first-order pyramidal \( \langle \mathbf{a} \rangle \), and first-order pyramidal \( \langle \mathbf{c} + \mathbf{a} \rangle \). The drag stresses for these families of systems are varied such that their normalized CRSS \( \tau_{\text{CRSS}}^{\text{basal}} / \tau_{\text{CRSS}}^{\text{prism}} \) ranges fall within the reported ranges in the literature summarized in Table 3.1. The elastic behavior of each grain is given by the room temperature single crystal elastic constants for \( \alpha \)-titanium as reported by Simmons and Wang (1971). Recall that \( \alpha \)-titanium is of hcp crystal structure at room temperature, and is therefore transversely isotropic and is completely defined by five elastic constants. The model parameters are listed in Table 3.2.
Table 3.2 Model parameters used in parametric study.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Low</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>162,400 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>92,000 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$C_{13}$</td>
<td>69,000 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$C_{33}$</td>
<td>180,700 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td>46,700 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$\dot{\gamma}_0$</td>
<td>0.001</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$\kappa_0$</td>
<td>0 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$k_y$</td>
<td>17.3 MPa-mm^{-0.5}</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$d_{ap}$</td>
<td>30 µm</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$A$</td>
<td>0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$D_{prism}$</td>
<td>250 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$h$</td>
<td>500 MPa</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$h_D$</td>
<td>100</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$m$</td>
<td>63</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$\tau_{basal}^{CRSS}/\tau_{prism}^{CRSS}$</td>
<td>-</td>
<td>1</td>
<td>1.5</td>
</tr>
<tr>
<td>$\tau_{pyr(a)}^{CRSS}/\tau_{prism}^{CRSS}$</td>
<td>-</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>$\tau_{pyr(c+a)}^{CRSS}/\tau_{prism}^{CRSS}$</td>
<td>-</td>
<td>3</td>
<td>5</td>
</tr>
</tbody>
</table>

All of the simulations in this first study have an initially random orientation distribution of grains in order to evaluate the influence of the CRSS without the effect of texture. It should be emphasized that the material constants used in these simulations have not been determined by fitting the model response to any specific set of experimental data since the purpose is to merely understand the sensitivity of material response to variation in the relative CRSS ratios. The reference shear rate, $\dot{\gamma}_0$, the flow exponent, $m$, and the back stress hardening coefficients, $h$ and $h_D$, listed in Table 3.2 are taken from the work of Goh (2002), and the Hall-Petch constant, $k_y$, is taken as an average of values reported in
the literature (Picu and Majorell, 2000; Kalidindi et al. 2003). The frictional portion of
the threshold stress, $\kappa_0$, is neglected because its contribution to the threshold stress is
expected to be small (~5-10 MPa) compared to the contribution from the grain size
effects (Picu and Majorell, 2002). The value of the prismatic drag stress (250 MPa) is
chosen such that the CRSS for these systems is in the neighborhood of CRSS values
reported in the literature, ~300-500 MPa (Medina Perilla and Gil Sevillano, 1995). The
values used for the Hall-Petch, $k_y$, constant and the primary $\alpha$ grain size, $d_{\alpha}$, lead to a
threshold stress value of approximately 100 MPa resulting in an initial prismatic CRSS
equal to 350 MPa. The non-Schmid coefficient, $A$, is set to zero in this first set of
simulations as no tension/compression asymmetry is expected for the case of random
texture. The activation of the non-Schmid terms in the threshold stress for prismatic
systems may also lead to plastic strain localization, and the goal of this first series of
simulations is to determine the patterns and magnitudes of the effective plastic strain
distribution due to the relative differences in CRSS while minimizing the influence of the
other model features.

Before the parametric study can be conducted, it must be determined how many
grains need to be included in the statistical volume element (SVE) of material to obtain a
converged solution in terms of the macroscopic stress-strain response for the ensemble of
grains. To determine this, four simulations with 52 grains, 137 grains, 188 grains, and
247 grains, respectively were carried out for a 30 $\mu$m grain size. The use of this grain
size is justified by noting that by using a different grain size would simply alter the level
of initial threshold stress based on the free slip length argument, and that by appropriately
modifying the drag stress to reflect the same initial CRSS ($\tau_{\text{CRSS}} \approx \kappa + D$) for the high
value of flow exponent used here) would leave the results essentially unaffected. Additionally, the value of the Hall-Petch constant used to define the threshold stress does not result in significant changes in the initial value of threshold stress in the range of 15-30 μm grains, i.e., 138 MPa versus 100 MPa. Hexagonal shaped grains are used to capture the importance of triple point junctions. All simulations employ doubly periodic boundary conditions as described by van der Sluis et al. (2000). The boundary conditions are illustrated in Figure 3.11. The displacement is applied in the $x_2$-direction, and model parameters used in these simulations were arbitrarily chosen to be the “high” values listed in Table 3.2. The generalized plane strain boundary conditions allow for the material to expand and/or contract in the out-of-plane direction, but restrict the plane strain surfaces from relative rotations. The axial stress-strain results of these simulations are given in Figure 3.8. The results do not show a significant difference in the stress-strain response for the ensembles of grains considered here outside of some slight variation that is expected from any type of averaged material response. In balancing the number of grains included in the statistical volume element and the computational requirements, an ensemble of 137 grains is chosen for the following simulations.
The mesh was created using a Fortran code that ensures a regular pattern of equally sized elements per grain. There are a total of 48 generalized plane strain elements per grain; 36 4-noded quadrilateral elements for the grain interior and 12 3-noded triangular elements around the perimeter of the grain. The grains have an aspect ratio \( \frac{L}{h} \) of 1.67 with the length dimension being 30 µm. The aspect ratio of a grain and the resulting mesh are shown in Figure 3.9 and Figure 3.10, respectively.
Figure 3.9 Aspect ratio of hexagonal grains.

Figure 3.10 Mesh used in parametric studies.
To provide structure to the set of parametric simulations, a $2^k$ factorial design of experiments methodology (DeVor et al., 1992) was employed. The simulation test matrix is given in Table 3.3, where T/C indicates tension and compression, respectively, and the rest of the fixed model constants are as defined in Table 3.2. The (+ / -) indicates the corresponding (high / low) value for the parameters listed in Table 3.2. In the test matrix, tension corresponds to (+) and compression to (-). Since three different variables are being principally investigated in this study (the CRSS for basal, pyramidal $\langle a \rangle$, and pyramidal $\langle c + a \rangle$ slip systems) there are a total of eight combinations of CRSS values investigated (i.e. +++ , +-+, etc.). Each CRSS combination is repeated every eighth test. Therefore, the test matrix can be subdivided into two main subsections; Cases 1-8 are compression tests and Cases 9-16 are tension tests.
Table 3.3 Simulation test matrix.

<table>
<thead>
<tr>
<th>Case</th>
<th>( \tau_{\text{basal}}^{\text{CRSS}} / \tau_{\text{prism}}^{\text{CRSS}} )</th>
<th>( \tau_{\text{pyr}(a)}^{\text{CRSS}} / \tau_{\text{prism}}^{\text{CRSS}} )</th>
<th>( \tau_{\text{pyr} (+a)}^{\text{CRSS}} / \tau_{\text{prism}}^{\text{CRSS}} )</th>
<th>T/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>8</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>9</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>10</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>11</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>12</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>13</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>14</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>15</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>16</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
</tbody>
</table>

The previously defined quantities of interest (i.e., \( \sigma_{22}^y \), \( \sigma_{22}^x \), \( \Delta \sigma \), and \( \bar{e}_{\max}^{p} \)) are listed for each simulation in Table 3.4. The results can be interpreted in a relatively straight-forward manner. Cases 1 and 9 are the baseline simulations which to compare the other simulations to, noting that Cases 1-8 are compression tests and Cases 9-16 are tension tests. For example, by comparing Cases 1 and 2 as well as Cases 9 and 10, the effect of increasing \( \tau_{\text{basal}}^{\text{CRSS}} \) while leaving \( \tau_{\text{pyr}(a)}^{\text{CRSS}} \) and \( \tau_{\text{pyr}(+a)}^{\text{CRSS}} \) fixed on the output variables is determined. Similar comparisons are made for all of the different permutations of increases in relative CRSS and the results are listed in Tables 3.5 and 3.6. The change in output variables due to the increase of the relative CRSS values (i.e., \( \Delta \sigma_{22}^y \), \( \Delta \sigma_{22}^x \), and \( \Delta(\Delta \sigma) \)) are given as the average of the absolute value of the change in the output variable from both tension and compression simulations. For example, increasing \( \tau_{\text{basal}}^{\text{CRSS}} \)
while leaving $\tau_{\text{CRSS}}^{\text{prv}(a)}$ and $\tau_{\text{CRSS}}^{\text{prv}(c+a)}$ fixed leads to an change of $\sigma_{22}^{y}$ of -80 MPa in compression and an increase of 100 MPa in tension; therefore, $\Delta \sigma_{22}^{y}$ is given as 90 MPa for an increase of $\tau_{\text{CRSS}}^{\text{basal}}$. This provides an illustrative example of how to interpret the results in Tables 3.5 and 3.6. Table 3.5 shows the effect of increasing the relative CRSS for only one of the slip system families (basal, pyramidal $\langle a \rangle$, and pyramidal $\langle c+a \rangle$) whereas Table 3.6 shows the effect of increasing the relative CRSS for multiple slip system families (i.e., basal and pyramidal $\langle a \rangle$, basal and pyramidal $\langle c+a \rangle$, etc.)

Table 3.4 Simulation results. Stress quantities are expressed in MPa.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\sigma_{22}^{y}$</th>
<th>$\sigma_{22}^{s}$</th>
<th>$\Delta \sigma$</th>
<th>$\varepsilon_{\text{max}}^{p}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-880</td>
<td>-1203</td>
<td>-323</td>
<td>0.3018</td>
</tr>
<tr>
<td>2</td>
<td>-960</td>
<td>-1320</td>
<td>-360</td>
<td>0.3391</td>
</tr>
<tr>
<td>3</td>
<td>-955</td>
<td>-1292</td>
<td>-337</td>
<td>0.3165</td>
</tr>
<tr>
<td>4</td>
<td>-1130</td>
<td>-1489</td>
<td>-359</td>
<td>0.2744</td>
</tr>
<tr>
<td>5</td>
<td>-880</td>
<td>-1299</td>
<td>-419</td>
<td>0.3002</td>
</tr>
<tr>
<td>6</td>
<td>-960</td>
<td>-1439</td>
<td>-479</td>
<td>0.3280</td>
</tr>
<tr>
<td>7</td>
<td>-955</td>
<td>-1395</td>
<td>-440</td>
<td>0.3017</td>
</tr>
<tr>
<td>8</td>
<td>-1130</td>
<td>-1659</td>
<td>-529</td>
<td>0.3127</td>
</tr>
<tr>
<td>9</td>
<td>920</td>
<td>1234</td>
<td>314</td>
<td>0.3526</td>
</tr>
<tr>
<td>10</td>
<td>1020</td>
<td>1364</td>
<td>344</td>
<td>0.3617</td>
</tr>
<tr>
<td>11</td>
<td>1010</td>
<td>1331</td>
<td>321</td>
<td>0.3162</td>
</tr>
<tr>
<td>12</td>
<td>1220</td>
<td>1547</td>
<td>327</td>
<td>0.2902</td>
</tr>
<tr>
<td>13</td>
<td>920</td>
<td>1334</td>
<td>414</td>
<td>0.3058</td>
</tr>
<tr>
<td>14</td>
<td>1020</td>
<td>1500</td>
<td>480</td>
<td>0.3244</td>
</tr>
<tr>
<td>15</td>
<td>1010</td>
<td>1444</td>
<td>434</td>
<td>0.3018</td>
</tr>
<tr>
<td>16</td>
<td>1220</td>
<td>1723</td>
<td>503</td>
<td>0.3178</td>
</tr>
</tbody>
</table>
Table 3.5 Effect of increasing CRSS for one slip family (MPa).

<table>
<thead>
<tr>
<th></th>
<th>$\Delta \sigma_{22}$</th>
<th>$\Delta \sigma_{22}^r$</th>
<th>$\Delta (\Delta \sigma)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Increase Basal</td>
<td>90</td>
<td>123.5</td>
<td>33.5</td>
</tr>
<tr>
<td>Increase Pyr $\langle a \rangle$</td>
<td>82.5</td>
<td>93</td>
<td>10.5</td>
</tr>
<tr>
<td>Increase Pyr $\langle c+a \rangle$</td>
<td>0</td>
<td>98</td>
<td>98</td>
</tr>
</tbody>
</table>

Table 3.6 Effect of increasing CRSS for multiple slip families (MPa).

<table>
<thead>
<tr>
<th></th>
<th>$\Delta \sigma_{22}^r$</th>
<th>$\Delta \sigma_{22}$</th>
<th>$\Delta (\Delta \sigma)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Increase Basal and Pyr $\langle a \rangle$</td>
<td>275</td>
<td>299.5</td>
<td>24.5</td>
</tr>
<tr>
<td>Increase Basal and Pyr $\langle c+a \rangle$</td>
<td>90</td>
<td>251</td>
<td>161</td>
</tr>
<tr>
<td>Increase Pyr $\langle a \rangle$ and Pyr $\langle c+a \rangle$</td>
<td>82.5</td>
<td>201</td>
<td>118.5</td>
</tr>
<tr>
<td>Increase All</td>
<td>275</td>
<td>472.5</td>
<td>197.5</td>
</tr>
</tbody>
</table>

Upon examination of the results a few things are readily apparent. For each combination of CRSS, the yield strength in tension is between 4-8% higher than the yield strength in compression. Since non-Schmid behavior has not been included in the simulations, it is clear that this slight yield asymmetry is due to the low symmetry of the hcp crystal structure and the differences in intergranular compatibility requirements that result in tension versus compression. Similar behavior has been experimentally observed by Medina Perilla and Gil Sevillano (1995) although they report that the yield strength is higher in compression than in tension. They have argued that the tension/compression (t/c) asymmetry is a result of the non-centrosymmetry of the first-order pyramidal $\langle c+a \rangle$ slip systems by which they have reasoned that the CRSS for $-\langle c+a \rangle$ slip is appreciably higher than the CRSS for $\langle c+a \rangle$ slip. Directionally dependent CRSS have not been
included in the current model for first-order pyramidal \( (c+a) \) slip systems due to the non-universality of these findings, and may explain the discrepancy between the current simulation results and these experimental observations. It should be noted the experiments of Perilla and Gil Sevillano (1995) were performed on specimen cut from a highly textured (transverse texture) sheet which could lead to alternate explanations of the discrepancy in material behavior.

The results listed in Table 3.5 that the yield strength is more sensitive to an increase in the basal CRSS as opposed to an increase in the pyramidal \( (a) \) CRSS, and is not affected at all by increase in the pyramidal \( (c+a) \) CRSS. This is to be expected for the case of a randomly textured polycrystal in which the pyramidal \( (c+a) \) slip systems should only contribute to the deformation process at higher strain levels for compatibility purposes due to the availability of prismatic, basal, and pyramidal \( (a) \) systems which posses a markedly lower CRSS. It is also interesting that the relative change in the t/c asymmetry increases with increases in the CRSS for basal and pyramidal \( (a) \) systems. The t/c asymmetry for the baseline case (Cases 1 and 9) is approximately 4.5%. Increasing \( \tau_{basal}^{CRSS} \) results in a 6.25% t/c asymmetry while increasing \( \tau_{pyr(a)}^{CRSS} \) results in a 5.76% t/c asymmetry. Since an increase of \( \tau_{pyr(c+a)}^{CRSS} \) does not effect the yield strength of the material, obviously it does not effect the magnitude of the t/c asymmetry. The higher t/c asymmetry observed for an increase of \( \tau_{basal}^{CRSS} \) as compared to an increase of \( \tau_{pyr(a)}^{CRSS} \) is a result of the yield strength being more sensitive to an increase of \( \tau_{basal}^{CRSS} \). An increase of both \( \tau_{basal}^{CRSS} \) and \( \tau_{pyr(a)}^{CRSS} \) leads to the highest relative T/C asymmetry of 7.96%.
results indicate that the observed T/C asymmetry in the absence of non-Schmid behavior is inherently linked to the low symmetry of the hcp crystal structure and the availability of lower strength deformation modes. As the relative CRSS values for each slip system increase, competition between the available deformation modes, the grain orientation, and the intergranular compatibility requirements leads to larger magnitudes of the t/c asymmetry.

The sensitivity of the saturated stress level, $\sigma_{22}'$, to changes of the relative CRSS ratios does not depend greatly on which particular slip system that the CRSS is increased. Increasing $\tau_{\text{basal}}^{\text{CRSS}}$ leads to the maximum increase of the saturated stress level ($\Delta \sigma_{22}'$) of 123.5 MPa whereas increasing $\tau_{\text{pyr(a)}}^{\text{CRSS}}$ leads the minimum value of 93 MPa, while the increase of $\tau_{\text{pyr(c+a)}}^{\text{CRSS}}$ results in an intermediate increase of 98 MPa. A more significant result is the effect that increases of the various CRSS has on the difference between the yield stress and the saturated stress level ($\Delta (\Delta \sigma)$). While increasing $\tau_{\text{basal}}^{\text{CRSS}}$ or $\tau_{\text{pyr(a)}}^{\text{CRSS}}$ only leads to moderate changes of $\Delta \sigma$ of 33.5 and 10.5 MPa, respectively, an increase of $\tau_{\text{pyr(c+a)}}^{\text{CRSS}}$ leads to a significantly higher change of 98 MPa. This verifies the earlier proposition that pyramidal $\langle c+a \rangle$ slip dominates deformation behavior at higher strains as deformation by the easier slip modes stagnates and the material must find alternative modes to accommodate the imposed deformation.

The localized nature of the effective plastic strain distributions does not permit a straight-forward interpretation of the effect that changes in the relative CRSS values and sense of loading have on the location and magnitude of the maximum effective plastic strain. These results are best presented in the form of contour plots which are given
below in Figures 3.12-3.18. When viewing the effective plastic strain distributions it is important to remember that the results are plotted for a 5% applied axial strain.

Figure 3.12 $\bar{\varepsilon}^p$ Distributions for a) Compression b) Tension

$\tau_{\text{CRSS}} = \tau_{\text{basal}} + \tau_{\text{prism}}$ and $\tau_{\text{prism}}^{\text{pyr}+a} = 3\tau_{\text{prism}}^{\text{pyr}}$

Figure 3.13 $\bar{\varepsilon}^p$ Distributions for a) Compression b) Tension

$\tau_{\text{CRSS}}^{\text{basal}} = 1.5\tau_{\text{prism}}^{\text{pyr}}$, $\tau_{\text{CRSS}}^{\text{prism}} = \tau_{\text{prism}}^{\text{pyr}}$, and $\tau_{\text{CRSS}}^{\text{pyr}+a} = 3\tau_{\text{prism}}^{\text{pyr}}$
Figure 3.14 $\tau^p$ Distributions for a) Compression b) Tension

\[ \tau_{basal}^{CRSS} = \tau_{prism}^{CRSS}, \tau_{pyr(a)}^{CRSS} = 2\tau_{prism}^{CRSS}, \text{ and } \tau_{pyr(c+a)}^{CRSS} = 3\tau_{prism}^{CRSS} \]

Figure 3.15 $\tau^p$ Distributions for a) Compression b) Tension

\[ \tau_{basal}^{CRSS} = 1.5\tau_{prism}^{CRSS}, \tau_{pyr(a)}^{CRSS} = 2\tau_{prism}^{CRSS}, \text{ and } \tau_{pyr(c+a)}^{CRSS} = 3\tau_{prism}^{CRSS} \]
Figure 3.16  $\bar{\varepsilon}^p$ Distributions for a) Compression b) Tension.

$r_{\text{basal}} = r_{\text{CRSS}}$, $r_{\text{prism}}^{p(c+a)} = r_{\text{prism}}^{p(c+a)}$, and $r_{\text{prism}}^{p(c+a)} = 5r_{\text{CRSS}}$

Figure 3.17  $\bar{\varepsilon}_{\text{p}}$ distributions for a) Compression b) Tension.

$r_{\text{basal}} = 1.5r_{\text{prism}}$, $r_{\text{prism}}^{p(c+a)} = r_{\text{prism}}^{p(c+a)}$, and $r_{\text{prism}}^{p(c+a)} = 5r_{\text{prism}}^{p(c+a)}$
Figure 3.18  $\varepsilon^p$ distributions for a) Compression b) Tension.

$\tau_{\text{basal}}^{\text{CRSS}} = \tau_{\text{prism}}^{\text{CRSS}}$, $\tau_{\text{prism}}^{\text{pyr(a)}} = 2\tau_{\text{prism}}^{\text{CRSS}}$, and $\tau_{\text{prism}}^{\text{pyr(c+a)}} = 5\tau_{\text{prism}}^{\text{CRSS}}$

Figure 3.19  $\varepsilon^p$ Distributions for a) Compression b) Tension

$\tau_{\text{basal}}^{\text{CRSS}} = 1.5\tau_{\text{prism}}^{\text{CRSS}}$, $\tau_{\text{prism}}^{\text{pyr(a)}} = 2\tau_{\text{prism}}^{\text{CRSS}}$, and $\tau_{\text{prism}}^{\text{pyr(c+a)}} = 5\tau_{\text{prism}}^{\text{CRSS}}$
Examination of the contour plots in Figures 3.12-3.19 reveals that the effective plastic strain distributions, in general, are not quite as sensitive to changes in the relative CRSS ratios as compared to the macroscopic stress-strain response of the material. While the magnitude of the maximum effective plastic strain ranges from approximately 28-34% in compression and from 29-36% in tension due to changes in the CRSS ratios, the locations of the maximum effective plastic strain do not change and the effective plastic strain distributions remain qualitatively similar. All simulations show a heterogeneous distribution of plastic strain in which bands of intense plastic strain ($\varepsilon^p \approx 9-20\%$) are separated by regions of relatively low plastic strain ($\varepsilon^p \approx 0.1-4\%$). Since the simulated microstructure consists entirely of primary $\alpha$ grains and the same random texture is used in for all cases, the location and spacing of the bands of intense strain localization are linked to the grain size as well as the local variations in texture, which result in “soft” areas of the microstructure that are favorably aligned to accommodate deformation with lower strength slip systems. It is interesting to note that the effective plastic strain distributions are qualitatively different in tension versus compression with the bands of plastic strain localization being more homogeneously distributed in compression as compared to tension. These observations support the earlier conclusion that the low symmetry of the hcp crystal structure is responsible for the observed t/c asymmetry of material behavior. The one noteworthy outcome of varying the relative values of CRSS is an increase of $\tau_{CRSS}^{basal}$ which leads to a reduction in the number of bands of plastic strain localization while increasing the intensity of the plastic strain in the remaining bands. The effective plastic strain distributions are relatively insensitive to changes of $\tau_{CRSS}^{mr(e)}$ and $\tau_{CRSS}^{mr(e+u)}$ for a microstructure with random texture.
Section 3.3.2 Influence of Texture

The low symmetry of the hcp crystal structure and the anisotropy of slip system strengths results in material behavior for $\alpha$-Ti and $\alpha/\beta$ Ti-Al alloys that is highly dependent on the orientation of grains within the polycrystal with respect to imposed deformation, and strong effects of misorientation at grain/phase boundaries. Section 3.3.1 focused on the effects of CRSS anisotropy and the sense of the applied load for an initially random orientation of grains. In this Section, the effect of texture on material response is investigated. Additionally, a small subset of the relative drag stress ratios (as in Section 3.3.1) will be included in the simulations to determine any interrelated effects that might arise between texture and slip system anisotropy.

The simulations in this study use the same mesh as shown in Figure 3.10 and the same material parameters as listed in Table 3.2 with a couple of restrictions being made on the basis of experimental observations. In addition, the non-Schmid behavior for prismatic systems is activated and the strength of the dissociated core configuration, $A$, is taken to be -0.1. Medina Perilla and Gil Sevillano (1995) have shown that the yield locus for a polycrystalline sheet of Ti-64 shows macroscopic yielding at a higher stress level in compression as compared to tension. Although they do not show a measured difference in the CRSS for prismatic glide in tension versus compression, the sign of the non-Schmid coefficient in these simulations is taken to be negative to reflect the appropriate sense of the macroscopic tension/compression asymmetry. It is also noted that while the measured ranges of respective CRSS ratios for the different slip families vary from source to source, the following order of operation is consistent throughout the literature and will be adhered to in the simulations.
\[ \tau_{\text{CRSS}}^{\text{prism}} \leq \tau_{\text{CRSS}}^{\text{basal}} \leq \tau_{\text{CRSS}}^{\text{pyr}(a)} < \tau_{\text{CRSS}}^{\text{pyr}(c+a)} \] (3.10)

In other words, the CRSS for first-order pyramidal \( \langle c + a \rangle \) slip will always be greater than the CRSS for first-order pyramidal \( \langle a \rangle \) slip.

The simulations will investigate the material response of the three distinct textures that are common in \( \alpha / \beta \) Ti-Al alloys and have been illustrated in the form of basal pole figures in Figure 2.3: Basal, Transverse, and Basal/Transverse. The basal texture is characterized by a distribution of grains with the basal plane normals within a 30-50° donut about the normal (out of plane) direction. Therefore the texture is symmetric within the TD-RD plane and material response is not expected to vary with loading direction in the TD-RD plane. The transverse texture, which results from unidirectional rolling, is characterized by a concentration of grains with basal plane normals roughly parallel to the transverse direction. Hence, the material behavior is expected to differ significantly depending on the loading direction as loading in the transverse direction essentially represents a hard deformation mode as the resolved shear stress for slip systems with \( \langle a \rangle \)-type burgers vector will be minimized. The basal/transverse texture is a combination of transverse and basal textures and the material response should differ with loading direction, but not nearly as much as it does in the case of transverse texture as the grains with basal orientation will offer an easier deformation mode as compared to pyramidal \( \langle c + a \rangle \) slip which should result in a slighter mechanically softer material response.
For each distinct texture, eight simulations are performed. Half of which will be subjected to an applied tensile displacement in the transverse \((x_1)\) direction and the other half will be subjected to an applied tensile displacement in the rolling \((x_2)\) direction. For each combination of texture and loading direction four simulations are carried out each with a different combination of slip system CRSS as summarized in Table 3.7. The basal CRSS, \(\tau_{\text{CRSS}}^{\text{basal}}\), is held fixed in the simulations because the focus is interpreting the effects of grain orientation on material response by minimizing the availability of the softer (prismatic and basal) deformation modes. This gives a total of 24 unique simulations that are carried out in this portion of the parametric study.

<table>
<thead>
<tr>
<th>Property</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\tau_{\text{CRSS}}^{\text{basal}} / \tau_{\text{CRSS}}^{\text{prism}})</td>
</tr>
<tr>
<td>Value</td>
</tr>
<tr>
<td>Low</td>
</tr>
<tr>
<td>High</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>-</td>
</tr>
<tr>
<td>-</td>
</tr>
<tr>
<td>(\tau_{\text{CRSS}}^{\text{pyr}(a)} / \tau_{\text{CRSS}}^{\text{prism}})</td>
</tr>
<tr>
<td>-</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>(\tau_{\text{CRSS}}^{\text{pyr}(c+a)} / \tau_{\text{CRSS}}^{\text{prism}})</td>
</tr>
<tr>
<td>-</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>5</td>
</tr>
</tbody>
</table>

For a given texture and loading direction, the four cases are summarized below:

- **Case 1 (5):** \(\tau_{\text{CRSS}}^{\text{pyr}(a)} = \tau_{\text{CRSS}}^{\text{prism}}\), \(\tau_{\text{CRSS}}^{\text{pyr}(c+a)} = 3\tau_{\text{CRSS}}^{\text{prism}}\)
- **Case 2 (6):** \(\tau_{\text{CRSS}}^{\text{pyr}(a)} = 2\tau_{\text{CRSS}}^{\text{prism}}\), \(\tau_{\text{CRSS}}^{\text{pyr}(c+a)} = 3\tau_{\text{CRSS}}^{\text{prism}}\)
- **Case 3 (7):** \(\tau_{\text{CRSS}}^{\text{pyr}(a)} = \tau_{\text{CRSS}}^{\text{prism}}\), \(\tau_{\text{CRSS}}^{\text{pyr}(c+a)} = 5\tau_{\text{CRSS}}^{\text{prism}}\)
- **Case 4 (8):** \(\tau_{\text{CRSS}}^{\text{pyr}(a)} = 2\tau_{\text{CRSS}}^{\text{prism}}\), \(\tau_{\text{CRSS}}^{\text{pyr}(c+a)} = 5\tau_{\text{CRSS}}^{\text{prism}}\)

In the simulations, Cases 1, 2, 3 and 4 will correspond to loading in the rolling direction and Cases 5, 6, 7, and 8 will correspond to loading in the transverse direction. The
results are presented in Tables 3.8-3.10 in the same manner as they have been presented in the previous Section. The simulations are performed with the same loading and boundary conditions as the simulations in the previous Section for an imposed axial strain of 5%.

Table 3.8 Results: – Basal Texture. Stress quantities expressed in MPa.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\sigma_{22}^y$</th>
<th>$\sigma_{22}^x$</th>
<th>$\Delta \sigma$</th>
<th>$\bar{\varepsilon}_\text{max}^p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RD</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>865</td>
<td>1076</td>
<td>211</td>
<td>0.1446</td>
</tr>
<tr>
<td>2</td>
<td>954</td>
<td>1186</td>
<td>232</td>
<td>0.1214</td>
</tr>
<tr>
<td>3</td>
<td>865</td>
<td>1186</td>
<td>321</td>
<td>0.1792</td>
</tr>
<tr>
<td>4</td>
<td>954</td>
<td>1331</td>
<td>377</td>
<td>0.1811</td>
</tr>
<tr>
<td>TD</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>871</td>
<td>1092</td>
<td>221</td>
<td>0.1401</td>
</tr>
<tr>
<td>6</td>
<td>951</td>
<td>1197</td>
<td>246</td>
<td>0.1176</td>
</tr>
<tr>
<td>7</td>
<td>871</td>
<td>1210</td>
<td>339</td>
<td>0.1876</td>
</tr>
<tr>
<td>8</td>
<td>951</td>
<td>1362</td>
<td>411</td>
<td>0.1560</td>
</tr>
</tbody>
</table>

Table 3.9 Results: – Transverse Texture. Stress Quantities expressed in MPa.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\sigma_{22}^y$</th>
<th>$\sigma_{22}^x$</th>
<th>$\Delta \sigma$</th>
<th>$\bar{\varepsilon}_\text{max}^p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RD</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>885</td>
<td>1077</td>
<td>192</td>
<td>0.1393</td>
</tr>
<tr>
<td>2</td>
<td>984</td>
<td>1215</td>
<td>231</td>
<td>0.2229</td>
</tr>
<tr>
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<td>885</td>
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<tr>
<td>4</td>
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<td>331</td>
<td>0.2309</td>
</tr>
<tr>
<td>TD</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1064</td>
<td>1304</td>
<td>240</td>
<td>0.3445</td>
</tr>
<tr>
<td>6</td>
<td>1085</td>
<td>1359</td>
<td>274</td>
<td>0.3421</td>
</tr>
<tr>
<td>7</td>
<td>1064</td>
<td>1516</td>
<td>452</td>
<td>0.3995</td>
</tr>
<tr>
<td>8</td>
<td>1085</td>
<td>1582</td>
<td>497</td>
<td>0.4045</td>
</tr>
</tbody>
</table>
For loading in the rolling direction, the stress-strain responses for all three textured materials are both qualitatively and quantitatively similar for all combinations of relative CRSS ratios. In all of the cases for loading in the rolling direction, increases in $\tau_{\text{CRSS}}^{\text{pyr}(c+a)}$ only affect the saturated stress level of the material and not the yield strength, while increasing the value of $\tau_{\text{CRSS}}^{\text{pyr}(a)}$ to $2\tau_{\text{CRSS}}^{\text{prism}}$ results in an increase of yield strength of approximately 100 MPa. The true stress-strain response of the material for which the higher values for $\tau_{\text{CRSS}}^{\text{pyr}(c+a)}$ are used show a continued hardening up to 5% strain, while the simulations performed with the lower value of $\tau_{\text{CRSS}}^{\text{pyr}(c+a)}$ show a saturation in the response at a strain of 3.5%. The results also indicate that slip on the pyramidal $\langle c+a \rangle$ systems begins to contribute to macroscopic material behavior at approximately 2-2.5% strain. This is determined comparing the stress-strain curves of Case 1 versus Case 3 and/or Case 2 versus Case 4 and noting when they begin to diverge. Since the stress-strain responses are very similar for all three types of textures loaded in the rolling direction,
only the results for the basal textured material are given graphically. The results are given in Figure 3.20.

![Figure 3.20 Macroscopic true stress-strain response for basal texture loaded in the RD.](image)

As expected, uniaxial loading of the basal textured material in the transverse direction leads to the same stress-strain response as for loading in the rolling direction. However, the transverse and basal/transverse textured materials loaded in the transverse direction display significantly different stress-strain responses as compared to their behavior when loaded in the rolling direction. The stress-strain response for loading the transverse textured material in the transverse direction showed that the yield strength is not significantly affected by changes of either $\tau^{prr[a]}_{CRSS}$ or $\tau^{nr(c+a)}_{CRSS}$. This is somewhat of a surprise because it was expected that an increase of $\tau^{nr(c+a)}_{CRSS}$ would result in a higher yield.
stress because this is expected to be the dominant deformation mode due to the minimization of slip on systems with \( \langle \mathbf{a} \rangle \) type burgers vector. Instead a slight increase in yield strength (20 MPa) is observed for an increase of \( \tau_{\text{CRSS}, \langle \mathbf{a} \rangle} \). This indicates that macroscopic yield for loading in the transverse direction is not due to more pronounced slip on pyramidal \( \langle \mathbf{e}+\mathbf{a} \rangle \) systems. This also suggests that macroscopic yield is dictated by the relatively small number of grains that are able to yield on prismatic, basal and pyramidal \( \langle \mathbf{a} \rangle \) systems. The yield strength increases observed due to changes of \( \tau_{\text{CRSS}, \langle \mathbf{a} \rangle} \) are a result of further limiting of \( \langle \mathbf{a} \rangle \) slip in this small number of preferentially oriented grains. However, it is apparent that the pyramidal \( \langle \mathbf{e}+\mathbf{a} \rangle \) slip systems still play the dominant role in the post-yield stress-strain behavior. It warrants mentioning that the contribution of pyramidal \( \langle \mathbf{e}+\mathbf{a} \rangle \) slip to the macroscopic stress-strain response begins at lower strain levels (~1.5%) for the transverse textured material as compared to the basal textured material (~2-2.5%). This is directly related to the increased difficulty of slip on systems with \( \langle \mathbf{a} \rangle \) type burgers vectors for loading in this orientation. As a result of increased pyramidal \( \langle \mathbf{e}+\mathbf{a} \rangle \) slip activity at lower strains, the stress-strain responses for the transverse textured material loaded in the transverse direction are at or near the saturation point even for the cases in which the higher value of \( \tau_{\text{CRSS}, \langle \mathbf{e}+\mathbf{a} \rangle} \) is used which is not the case for loading in the rolling direction. The stress-strain curves for the transverse textured material loaded in the transverse direction are given below in Figure 3.19.
The basal/transverse textured material loaded in the transverse direction behaves qualitatively similar to the stress-strain response for loading in the rolling direction with some slight differences for the cases when the higher value of $\tau_{\text{CRSS}}^{\text{pr}(c+a)}$ is used. The main difference is that, similar to the cases for a transverse textured material loaded in the transverse direction, the stress-strain response saturates at higher strains for all combinations of relative CRSS ratios. While the saturation of the stress-strain response is very similar to the transverse textured material loaded in the transverse direction, the stress levels are significantly lower for the basal/transverse textured material. This is a result of the mixed nature of this type of texture which gives a stress-strain response intermediate to the basal and transverse textured materials’ behavior due to the presence of...
of elements of both types of textures. The mixed nature of the texture also explains the increased yield strength sensitivity to changes of $\tau_{CRSS}^{pyr(\phi)}$ as observed for basal textured materials as well as the contribution of pyramidal $\langle c+a \rangle$ slip at lower strain levels (~1.8%) as observed for transverse textured materials. The stress-strain curves for the basal/transverse textured material loaded in the transverse direction are given below in Figure 3.20.

![Stress-strain curves](image)

Figure 3.22 Macroscopic true stress-strain response for basal/transverse texture loaded in TD.
Peters et al. (1984) have carried out tensile tests on polycrystalline sheets of Ti-64 with the three types of textures considered in the simulations. In their experiments, a specimen with each type of texture is subjected to loading in both the rolling and transverse directions and they have determined Young’s Modulus (E) and 0.2% offset-defined yield strength ($\sigma_{0.2}$) for each combination of texture and loading direction. Although the current model consists entirely of primary $\alpha$-phase and has not been calibrated to fit these results, a qualitative comparison of the simulation results to their results is informative. The Case 2 and 6 simulations are used for the comparison; results are summarized in Table 3.11 and Figure 3.21-3.22.

<table>
<thead>
<tr>
<th>Texture</th>
<th>$E_{\text{exp}}$ (MPa)</th>
<th>$E_{\text{sim}}$ (MPa)</th>
<th>$\sigma_{0.2}^{\exp}$ (MPa)</th>
<th>$\sigma_{0.2}^{\text{sim}}$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B-RD</td>
<td>109,000</td>
<td>113,065</td>
<td>1120</td>
<td>954</td>
</tr>
<tr>
<td>B-TD</td>
<td>109,000</td>
<td>113,065</td>
<td>1120</td>
<td>951</td>
</tr>
<tr>
<td>T-RD</td>
<td>113,000</td>
<td>113,845</td>
<td>1105</td>
<td>984</td>
</tr>
<tr>
<td>T-TD</td>
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<td>128,481</td>
<td>1170</td>
<td>1085</td>
</tr>
<tr>
<td>B/T-RD</td>
<td>107,000</td>
<td>110,101</td>
<td>1120</td>
<td>967</td>
</tr>
<tr>
<td>B/T-TD</td>
<td>123,000</td>
<td>118,860</td>
<td>1170</td>
<td>1039</td>
</tr>
</tbody>
</table>

Table 3.11  Comparison of experimental and simulation results for Young’s Modulus and yield strength for various texture/loading direction combinations.
Figure 3.23 Macroscopic true stress-strain response for loading in RD (Case 2).

Figure 3.24 Macroscopic true stress-strain response for loading in TD (Case 6).
The simulation results seem to agree reasonably well, at least qualitatively, with the experimental observations. The elastic moduli as determined from the simulations are within 4% difference of the experimental measurements, and follow the appropriate increasing or decreasing trends according to the texture and loading direction quite well. The yield strength predicted by the simulations does not qualitatively match the experimental results as well as the modulus data, but nonetheless seem to exhibit reasonable agreement. The experiments show that a transverse (T) textured material loaded in the rolling direction (RD) has the lowest yield strength, whereas the highest yield strength reported is for a transverse or basal/transverse (B/T) textured material loaded in the transverse direction (TD). The simulations predict that the basal (B) textured material subjected to loading in either direction will have the lowest (although only slightly lower than T-RD and B/T-RD) yield stress, and the T-TD case will have the highest yield stress. In general, the simulation results follow the overall yield strength trends for the various combinations of texture and loading direction, and the relative differences between the yield strengths for the different cases remain within ±5% difference, i.e.,

\[
(B/T-TD:B-RD)_{\text{exp}} = 1170 \text{ MPa} : 1120 \text{ MPa} = 1.05
\]

\[
(B/T-TD:B-RD)_{\text{sim}} = 1039 \text{ MPa} : 954 \text{ MPa} = 1.09
\]

Figures 3.21 and 3.22 show that all three textured materials exhibit nearly the same response when loading in the RD, but when these materials are subjected to loads in the TD there is significant anisotropy. These results support the notion that the
anisotropy displayed in these materials is a function of the angle between the loading direction and the c-axes of the grains composing the polycrystal. When the loading direction is nearly perpendicular to the c-axis, the resolved shear stress for prism, basal and first-order pyramidal \( \langle a \rangle \) systems in a majority of the grains is high and the resultant yield stress will be lower. However, if the loading direction is parallel or nearly parallel to the c-axis, fewer grains in the polycrystal are able to deform by slip on systems with the \( \langle a \rangle \) type burgers vector because of the significantly lower values of resolved shear stress on these systems which results in a much higher macroscopic yield strength.

The stress-strain curves for each type of texture have also been plotted separately for loading in both the TD and RD in Figures 3.23-3.25. As expected, the basal textured material shows the most isotropic response within the TD-RD plane. The transverse textured material shows the most anisotropic response with respect to loading direction with the yield and saturated stress level being appreciably higher for loading in the TD. The basal/transverse textured material exhibits stress-strain behavior somewhere between the basal and transverse textured materials’ response, which is a reflection of the mixed nature of this type of texture.
Figure 3.25  Macroscopic true stress-strain response for basal texture (Cases 2 and 6).
Figure 3.26 Macroscopic true stress-strain response for transverse texture (Cases 2 and 6).

Figure 3.27 Macroscopic true stress-strain response for basal/transverse texture (Cases 2 and 6).
Figures 3.25-3.27 show the effective plastic strain distribution for Cases 2 and 6 of the relative CRSS ratios. Each Figure is arranged such that the contours on the left-hand side show the distributions for loading in the RD and the contours on the right-hand side show the distributions for loading in the TD.

![Figure 3.28](image)

**Figure 3.28** \( \bar{p} \) distributions for basal texture loaded in (a) RD (b) TD.

![Figure 3.29](image)

**Figure 3.29** \( \bar{p} \) distributions for transverse texture loaded in (a) RD (b) TD.
The basal textured material shows the most similar plastic strain distributions when loaded in either the transverse or rolling directions reflecting the in-plane (RD-TD plane) symmetry of this type of texture. The symmetry of the basal texture also leads to a relatively homogeneous distribution of plastic strain throughout the microstructure, as well as the lowest maximum effective plastic strain value (~12%) amongst all texture cases. The transverse and basal/transverse textured materials exhibit intense regions of plastic strain localization when loaded in the transverse direction as compared to loading in the rolling direction. This is indicative of the harder orientation of these microstructures as they consist of many grains being subjected to stresses parallel to their c-axes. The highest peak value of effective plastic strain occurs in the basal/transverse textured material loaded in the TD, and this is likely due to the mixed nature of the grain orientation in which grains with a basal orientation aligned for easy \{a\} glide are neighbors of grains with hard transverse orientations. The disparity in the availability of slip systems between neighboring grains can lead to intense strain localization during
deformation. The results of Section 3.3.2 and the current Section clearly show that the anisotropy of slip system strength, texture, loading sense, and loading direction all play a major role in influencing the effective plastic strain distributions as well as the location of regions of strain localization and their intensity. This highlights the need to include these features in the constitutive models for these materials in order to account for the highly heterogeneous nature of the deformation field.

Section 3.3.3 Influence of Phase Distribution

In this Section the dual-phase model for Ti-64 described in Sections 3.1.1 and 3.1.2 is used to investigate how the distribution of the secondary lamellar $\alpha + \beta$-phase has on material response. The primary $\alpha$-phase is known to be the mechanically softer phase at room temperature in which plastic deformation initiates. However, within the lamellar structures there are a small number soft deformation modes by which favorably oriented $\alpha + \beta$ grains may undergo micro-yielding simultaneously with the onset of plastic deformation in the primary $\alpha$-phase. This may lead to increased strain localization in regions near favorably oriented $\alpha + \beta$ grains.

The mechanical behavior of three different random phase distributions is investigated. Each distribution consists of approximately 60% primary $\alpha$ grains and 40% $\alpha + \beta$ lamellar regions, which is consistent with the material used in the previous experimental (Wallace, 1997; Swalla, 2003) and modeling (Morrisey, 2001; Goh, 2002) efforts in this project. The three phase distributions are shown in Figure 3.27, where the primary $\alpha$ grains appear gray and the $\alpha + \beta$ colonies are black. The relative CRSS ratios are held fixed in the simulations so that the variation in results can be interpreted in
terms of the interaction between phase distribution and texture. The material parameters used in these simulations are listed in Table 3.12 where it is understood that omitted parameters have the values as listed in Table 3.2.

![Figure 3.31 Random phase distributions used in simulations.](image)

Table 3.12 Material parameters used in dual-phase simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{\text{prism}}$</td>
<td>250 MPa</td>
</tr>
<tr>
<td>$D_{\text{basal}}$</td>
<td>250 MPa</td>
</tr>
<tr>
<td>$D_{\text{pyramidal}(a)}$</td>
<td>600 MPa</td>
</tr>
<tr>
<td>$D_{\text{pyramidal}(c+a)}$</td>
<td>950 MPa</td>
</tr>
<tr>
<td>$D^{(110)({111)}$</td>
<td>225 MPa</td>
</tr>
<tr>
<td>$d_{\text{colony}}$</td>
<td>30 μm</td>
</tr>
<tr>
<td>$d_{\alpha}$</td>
<td>1.5 μm</td>
</tr>
<tr>
<td>$d_{\beta}$</td>
<td>0.5 μm</td>
</tr>
<tr>
<td>$A$ (for prismatic slip in $\alpha$-phase only)</td>
<td>-0.1</td>
</tr>
</tbody>
</table>
For each phase distribution, three simulations have been performed; one each with basal, transverse, and basal/transverse textures. The simulations employ the usual random periodic boundary conditions, and are subjected to monotonic quasi-static strain-controlled loading in the transverse direction as been done in Sections 3.3.1 and 3.3.2. This loading direction is chosen since it has been previously shown in the texture study that loading in this direction elicits a more anisotropic response.

The results reveal that the macroscopic stress-strain response for a given texture is relatively insensitive to the distribution and arrangement of phases; therefore, for clarity of presentation the stress-strain curves for only one of the distributions is shown in Figure 3.28. Since an arbitrarily oriented lamellar grain can be appreciably harder than a primary $\alpha$ grain, an increase in the percentage of $\alpha + \beta$ colonies would lead to a harder mechanical response and vice versa. The stress-strain responses follow the same trends that were exhibited in the parametric study of texture for a material consisting of all $\alpha$-phase grains. The basal textured material yielded the softest response, and the transverse textured material exhibited the hardest response with the basal/transverse sample falling in between the two, but lying closer to the basal response.
Figure 3.32 Macroscopic true stress-strain curves for dual phase simulations (distribution 1).

Since the distribution of phases does not significantly affect the stress-strain response of the material, the importance of phase distribution and arrangement is its effect on the variation of the local effective plastic strain distributions and the location of regions of strain localization. The effective plastic strain distributions are shown in Figures 3.29–3.31. The results show that the effective plastic strain distributions in the case of the dual-phase material are markedly different from the distributions observed for the primary $\alpha$ microstructure studied in Section 3.3.2. The bands of intense strain localization for the basal and basal/transverse textured materials are more heterogeneously distributed in the dual-phase material due to the presence of harder lamellar phase. However, the transverse textured material shows an increase in the
number of high intensity plastic strain regions as compared to the primary $\alpha$ microstructure. This is most likely due to increased slip by the soft basal and BOR governed $(110)\{\overline{1}1\overline{1}\}$ deformation modes in the lamellar regions. Several of the $\alpha + \beta$ grains have accumulated significant levels of plastic strain (10-20%) which supports the proposition that these soft modes of deformation may play a more prominent role for this type of texture.

A common feature to all of the plastic strain distributions is that the location of maximum effective plastic strain always occurs at or near an $\alpha/\alpha + \beta$ phase boundary. This behavior is also in agreement with the results of Morrissey (2001) and previous experimental results. This is a by-product of the plastic anisotropy that exists between the two phases and the corresponding compatibility strains that develop during deformation. The arrangement of phases also has a significant effect on the continuity of the bands of plastic strain localization, as it is observed that the bands are impeded by the presence of $\alpha + \beta$ colonies. It should be noted that there are a couple of instances where the shear bands pass through the $\alpha + \beta$ regions, but very rarely do the bands pass through multiple lamellar colonies without a decrease in intensity. In most of these cases the band forms where there is a clear path of contiguous $\alpha$-phase on both sides of the lamellar grain which facilitates the shearing process. For the cases in which a band passes through multiple $\alpha + \beta$ colonies, it is likely that one or more of the lamellar grains are favorably aligned for activation of the soft deformation modes.
Figure 3.33 $\bar{e}^p$ distributions for basal texture loaded in TD: (a) distribution 1 (b) distribution 2 (c) distribution 3.
Figure 3.34 $\overline{\varepsilon}^p$ distributions for transverse texture loaded in TD: (a) distribution 1 (b) distribution 2 (c) distribution 3.
Figure 3.35 $\sigma^p$ distributions for basal/transverse texture loaded in TD: (a) distribution 1 (b) distribution 2 (c) distribution 3.
CHAPTER IV

CRYSTAL PLASTICITY STUDY OF CYCLIC DEFORMATION BEHAVIOR OF TI-6AL-4V

The motivation for developing the 3-D crystal plasticity model described in Chapter III was to be able to provide a more realistic description of the heterogeneous features of $\alpha/\beta$ Ti-Al alloys in order to better understand the role that microstructure plays during deformation. The works of Morrissey et al. (2003) and Goh et al. (2001) have used the planar triple slip 2-D idealization to model the high-cycle fatigue (HCF) and fretting fatigue behavior of Ti-6Al-4V, and their results have demonstrated that ratcheting of the cyclic plastic strain plays an important role in the fatigue of these materials. The amount of plastic strain ratcheting per cycle is relatively small, but may accumulate to significant levels over a large number of cycles thus leading to material failure via ductility exhaustion and/or other related mechanisms (Morrissey et al., 2003). These simulation results are consistent with the experimental observations of Morrissey et al. (1999a,b) in the case of uniaxial smooth specimen HCF tests and Kapoor (1997) for the case of fretting fatigue.

In this Chapter the crystal plasticity model described in Chapter III is used to simulate the cyclic deformation behavior (both uniaxial mean stress and fretting simulations) of Ti-6Al-4V with a duplex microstructure consisting of 60% primary $\alpha$ -
phase and 40% lamellar ($\alpha + \beta$)-phase. The intent of this work is to validate the previous results of Morrissey et al. (2003) and Goh et al. (2001) in regards to the dominant cyclic plastic strain behavior (i.e., ratcheting) with the new model, as well as investigating the influence of including a more realistic description of the microstructure and its effect on material behavior. The set of simulations completed in this Chapter is not as exhaustive and complete as those carried out individually by Morrissey (2001) and Goh (2002), and will instead focus on a smaller set of loading conditions to examine the differences in results that arise due to the more realistic description of the microstructure.

4.1 Model Calibration

Prior to performing the HCF and fretting simulations the model parameters are calibrated to the fit the stabilized cyclic stress-strain response for Ti-6Al-4V given by Kurath (1999). The temperature and strain rate have not been reported for the calibration data, and it is assumed that tests were performed at room temperature under quasistatic loading conditions. The model is calibrated to fit the stabilized cyclic stress-strain response, as the focus of this work is on the distribution and behavior of cyclic microplasticity under HCF loading conditions. The mesh for the calibration procedure is the same as that used in the parametric simulations in Chapter 3 (see Figure 3.10) and consists of 137 grains with 30 $\mu$m diameter with a random orientation distribution in the approximate phase proportions of 60% primary $\alpha$ and 40% lamellar ($\alpha + \beta$). Each grain is meshed with 48 generalized plane strain elements per grain; 36 4-noded reduced-integration quadrilateral elements (CPEG4R) for the grain interior and 12 3-noded
triangular elements (CPEG3) around the perimeter of the grain. The distribution of phases is taken to be that of the first distribution (referred to as distribution 1) given in Figure. 3.31 of Section 3.3.3. Random, doubly-periodic boundary conditions are employed along the edges of the statistical volume element as shown in Figure. 3.11. The generalized plane strain boundary conditions are applied such that the material is allowed to freely expand or contract uniformly in the out-of-plane direction. The calibration simulations are carried out for 3 fully reversed cycles under strain-controlled loading for a strain amplitude of 1% at a strain rate of 0.001 s\textsuperscript{-1}. After calibrating the model for the case of random texture, a series of simulations is carried out for different combinations of texture and loading direction which will provide macroscopic true stress-strain properties that will be used as input for the uniaxial mean stress and fretting simulations.

The complete list of model constants has not been optimized during the fitting process as many of the model parameters have simply been taken to correspond with the calibrated values determined by Goh (2002) for the planar triple slip crystal plasticity model for Ti-6Al-4V. The focus of the current optimization procedure is accurately determining the respective threshold and drag stress values for each slip system family to reflect the experimentally observed anisotropy of strengths for the different slip systems. The model calibration was carried out subjected to the following constraints. For a given microstructure, the slip system threshold stress is determined by the free slip length of that particular slip system. In the primary $\alpha$-phase the free slip length is dictated by the primary $\alpha$ grain size, while in the lamellar ($\alpha + \beta$)-phase the free flip length is dictated by one of three characteristic lengths, namely the secondary $\alpha$ lath thickness for the hcp systems, the $\beta$ lath thickness for the bcc systems, and the ($\alpha + \beta$) colony size for the
easy glide systems which can traverse the length of the colony because they either glide parallel to the $\alpha / \beta$ interface or are able to shear through the $\alpha / \beta$ interface due to the favorable alignment dictated by the BOR. The crystallographic details of these slip system constraints have been previously described in Chapter III. The characteristic length values used to determine the threshold stresses have been taken as average values from the experimentally characterized Ti-6Al-4V material used in the works of Morrissey (2000) and Swalla (2003) and are summarized in Table 4.1. It is noted here that to be strictly correct that the free slip length should be calculated as the projected free slip length for a given slip system based on the lath spacings and not the distance measured orthogonal to laths. However, the exact nature of the strengthening mechanism in the lath structures is still an open subject of debate in the literature, and the orthogonal spacing assumption is not viewed as a critical limiting feature of the current model in the light of this uncertainty.

Table 4.1 Characteristic length scales used to define slip system threshold stresses.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Length ($\mu$m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d^{\alpha_p}$</td>
<td>30</td>
</tr>
<tr>
<td>$d^{\alpha_3}$</td>
<td>1.5</td>
</tr>
<tr>
<td>$d^{\beta}$</td>
<td>0.5</td>
</tr>
<tr>
<td>$d^{colony}$</td>
<td>30</td>
</tr>
</tbody>
</table>

Now that the threshold stresses have been defined for the given microstructure, the initial critical resolved shear stresses for the primary $\alpha$-phase (i.e., $\tau_{CRSS}^\alpha = \kappa^\alpha + D^\alpha$ due to the high flow exponent) are determined subject to the additional constraints listed in Table 4.2, where $\tau_{CRSS}^{prism}$ is the parameter to be optimized.
Table 4.2  Constraints on slip system drag stresses in the primary $\alpha$-phase

<table>
<thead>
<tr>
<th>Ratio</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{\tau_{basal}}{\tau_{prism}}$</td>
<td>1</td>
</tr>
<tr>
<td>$\frac{\tau_{pyr(\alpha)}}{\tau_{prism}}$</td>
<td>2</td>
</tr>
<tr>
<td>$\frac{\tau_{pyr(\epsilon\omega \alpha)}}{\tau_{prism}}$</td>
<td>3</td>
</tr>
</tbody>
</table>

In this scheme, essentially the only fitting parameter is the drag stress for the prismatic systems in the primary $\alpha$-phase and the drag stresses for the other slip systems may be calculated via the constraints given in Table 4.2. It is mentioned here as a reminder that the drag stress values for the slip systems in the lamellar ($\alpha + \beta$)-phase are taken to be the same as the corresponding slip family drag stresses in the primary $\alpha$-phase for the hcp slip systems, while the drag stress for the bcc slip systems is defined to be $0.9\tau_{prism}$ to reflect the mechanically softer nature of this phase. In this fitting methodology, the initial CRSS’s for the lamellar slip systems are not defined as ratios of the prismatic $\alpha$ CRSS, but instead are a manifestation of lamellae and colony length scales (via the threshold stress) and the calibrated values of drag stress for the primary $\alpha$-phase. An illustrative example of determining the CRSS for each slip system for a selected value of $\tau_{prism}$ is given below.
Given: \( \tau_{\text{prism}}^{\text{CRSS}} = 300 \text{ MPa} \) \hfill (4.1)

Then using the Hall-Petch constant from Chapter III, \( k_y = 17.32 \text{ MPa} \cdot \text{mm}^{0.5} \), the threshold stress (neglecting non-Schmid terms for illustration purposes) for the primary \( \alpha \) slip systems is calculated as

\[
\kappa^\alpha_p = 17.32 \text{ MPa} \cdot \text{mm}^{0.5} \left( 0.03 \text{ mm} \right)^{-0.5} = 100 \text{ MPa}
\] \hfill (4.2)

The drag stresses for the different primary \( \alpha \) slip systems are then calculated using the constraints in Table 4.2 as

\[
\tau_{\text{prism}}^\alpha = \kappa^\alpha_p + D^\text{prism}
\]

\[
\Rightarrow D^\text{prism} = \tau_{\text{prism}}^\alpha - \kappa^\alpha_p = 300 \text{ MPa} - 100 \text{ MPa} = 200 \text{ MPa}
\] \hfill (4.3)

\[
\tau_{\text{basal}}^\alpha = \kappa^\alpha_p + D^\text{basal} = \tau_{\text{CRSS}}^\alpha
\]

\[
\Rightarrow D^\text{basal} = \tau_{\text{CRSS}}^\alpha - \kappa^\alpha_p = 300 \text{ MPa} - 100 \text{ MPa} = 200 \text{ MPa}
\] \hfill (4.4)

\[
\tau_{\text{pyr}(a)}^\alpha = \kappa^\alpha_p + D^\text{pyr}(a) = 2 \tau_{\text{prism}}^\alpha
\]

\[
\Rightarrow D^\text{pyr}(a) = 2 \tau_{\text{CRSS}}^\alpha - \kappa^\alpha_p = 600 \text{ MPa} - 100 \text{ MPa} = 500 \text{ MPa}
\] \hfill (4.5)
\[ \tau_{\text{CRSS}}^{\text{pyr}(c+a)} = \kappa^{\alpha_p} + D^{\text{pyr}(c+a)} = 3\tau_{\text{CRSS}}^{\text{prism}} \]  

\[ \Rightarrow D^{\text{pyr}(c+a)} = 3\tau_{\text{CRSS}}^{\text{prism}} - \kappa^{\alpha_p} = 900 \text{ MPa} - 100 \text{ MPa} = 800 \text{ MPa} \]  

From these values of slip system drag stresses the CRSS for the slip systems in the lamellar \((\alpha + \beta)\)-phase can then be calculated as

\[ \kappa^{\alpha_*} = 17.32 \text{ MPa} \cdot \text{mm}^{0.5} (0.0015 \text{ mm})^{-0.5} = 447 \text{ MPa} \]  

\[ \kappa^{\beta} = 17.32 \text{ MPa} \cdot \text{mm}^{0.5} (0.0005 \text{ mm})^{-0.5} = 775 \text{ MPa} \]  

\[ \tau_{\text{CRSS}}^{\alpha_*} = \kappa^{\alpha_*} + D^{\text{prism}} = 447 \text{ MPa} + 200 \text{ MPa} = 647 \text{ MPa} \]  

\[ \tau_{\text{CRSS}}^{\alpha_0} = \kappa^{\alpha_0} + D^{\text{basal}} = 447 \text{ MPa} + 200 \text{ MPa} = 647 \text{ MPa} \]  

\[ \tau_{\text{CRSS}}^{\text{pyr}(\alpha)} = \kappa^{\alpha_*} + D^{\text{pyr}(\alpha)} = 447 \text{ MPa} + 500 \text{ MPa} = 947 \text{ MPa} \]  

\[ \tau_{\text{CRSS}}^{[110]\{\overline{1}11\}} = \kappa^{\beta} + 0.9D^{\text{prism}} = 775 \text{ MPa} + 180 \text{ MPa} = 955 \text{ MPa} \]  

The calculations for the CRSS for the easy glide systems which are able to traverse the length of the lamellar colony are not given in the illustrative example to condense the presentation as the set of easy glide systems is made up of 3 basal, 1 prismatic and 2 \((110)\{\overline{1}11\}\) slip systems and at this juncture it would be belaboring the point. However, these quantities can be calculated in the same straight-forward manner. In the current
model only one of the BOR variants is considered for the lamellar structures and is given as

\[ (0001)[\overline{T2\overline{T0}}]_\alpha \parallel (101)[\overline{T1\overline{T1}}]_\beta \]  \hspace{1cm} (4.13)

From the BOR the explicit crystallography of the easy glide lamellar systems can be determined and is summarized in Table 4.3

<table>
<thead>
<tr>
<th>Table 4.3 Lamellar easy glide slip systems.</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0001)[\overline{T2\overline{T0}}]</td>
</tr>
<tr>
<td>(0001)[\overline{T210}]</td>
</tr>
<tr>
<td>(0001)[\overline{2T10}]</td>
</tr>
<tr>
<td>(10\overline{T0})[\overline{T2\overline{T0}}]</td>
</tr>
<tr>
<td>(101)[\overline{T1\overline{T1}}]</td>
</tr>
<tr>
<td>(101)[\overline{T11}]</td>
</tr>
</tbody>
</table>

Using the procedure described above, the model has been calibrated to fit the stabilized uniaxial cyclic stress-strain response given by Kurath (1999). The results are given in Figure 4.1
The calibrated model is now used to simulate the stabilized cyclic stress-strain response for the same loading and boundary conditions for a basal, transverse, and basal/transverse textured materials subjected to loading with respect to loading in both the transverse and rolling directions. The simulation results are given in Figures 4.2 and 4.3.
Figure 4.2  Simulated cyclic stress-strain response for loading in the rolling direction.

Figure 4.3  Simulated cyclic stress-strain response for loading in the transverse direction.
The simulated stress-strain responses given in Figures 4.2 and 4.3 are used to define the material properties of the various textured materials which are used to define the normalized loads/stresses (i.e., $\sigma_{\text{applied}} / \sigma_y$) used in the uniaxial mean stress and fretting simulations. Normalizing applied loads to critical limiting loads is undertaken to more accurately compare the effect that texture has on the cyclic plastic strain behavior. A list of the pertinent material parameters taken from the initial portion of the stress-strain curves is given in Tables 4.4 and 4.5. The list of parameters include the 0.2% offset stress, $\sigma_{0.2}$, the stress at a plastic strain of 0.001, $\sigma_y$, which in these simulations has been defined as the yield stress, and the yield strain $\varepsilon_y$.

Table 4.4 Summary of material parameters for various textured materials loaded in rolling direction.

<table>
<thead>
<tr>
<th></th>
<th>E (MPa)</th>
<th>$\sigma_{0.2}$ (MPa)</th>
<th>$\sigma_y$ (MPa)</th>
<th>$\varepsilon_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basal</td>
<td>112,838</td>
<td>744</td>
<td>682</td>
<td>0.00704</td>
</tr>
<tr>
<td>Transverse</td>
<td>113,498</td>
<td>823</td>
<td>760</td>
<td>0.00769</td>
</tr>
<tr>
<td>Basal / Transverse</td>
<td>109,893</td>
<td>791</td>
<td>722</td>
<td>0.00756</td>
</tr>
</tbody>
</table>

Table 4.5 Summary of material parameters for various textured materials loaded in transverse direction.

<table>
<thead>
<tr>
<th></th>
<th>E (MPa)</th>
<th>$\sigma_{0.2}$ (MPa)</th>
<th>$\sigma_y$ (MPa)</th>
<th>$\varepsilon_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basal</td>
<td>112,344</td>
<td>760</td>
<td>694</td>
<td>0.00717</td>
</tr>
<tr>
<td>Transverse</td>
<td>128,607</td>
<td>902</td>
<td>795</td>
<td>0.00719</td>
</tr>
<tr>
<td>Basal / Transverse</td>
<td>119,174</td>
<td>843</td>
<td>770</td>
<td>0.00746</td>
</tr>
</tbody>
</table>

The list of calibrated model parameters is given in Table 4.6. These are the parameters used in all of the uniaxial mean stress and fretting simulations.
Table 4.6  Calibrated model constants.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>162,400 MPa</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>92,000 MPa</td>
</tr>
<tr>
<td>$C_{13}$</td>
<td>69,000 MPa</td>
</tr>
<tr>
<td>$C_{33}$</td>
<td>180,700 MPa</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td>46,700 MPa</td>
</tr>
<tr>
<td>$\dot{\gamma}_0$</td>
<td>0.001</td>
</tr>
<tr>
<td>$m$</td>
<td>63</td>
</tr>
<tr>
<td>$\kappa_0$</td>
<td>0 MPa</td>
</tr>
<tr>
<td>$k_y$</td>
<td>17.32 MPa-mm$^{1/2}$</td>
</tr>
<tr>
<td>$D_{\text{prism}}$</td>
<td>175 MPa</td>
</tr>
<tr>
<td>$h$</td>
<td>500 MPa</td>
</tr>
<tr>
<td>$h_D$</td>
<td>100</td>
</tr>
<tr>
<td>$A$</td>
<td>-0.1</td>
</tr>
</tbody>
</table>

4.2 Uniaxial Mean Stress Simulations

Morrissey et al. (2000, 2001, 2003) have previously studied the cyclic plastic deformation behavior of Ti-6Al-4V in the HCF regime with the 2-D planar triple slip crystal plasticity model placing an emphasis on understanding the relationship between the remote loading conditions and the local distribution of microplasticity in unnotched specimens. In particular, this work focused on the effects that microstructural heterogeneity and variation of the $R$-ratio had on the cyclic plastic strain distributions. Morrissey et al. (2000, 2001, 2003) have shown that a transition in cyclic plastic strain behavior occurs at higher $R$-ratios (>0.7). Above this threshold, it is shown that bulk-dominated fatigue damage associated with the percolation of ratcheting cyclic plastic
strain in connected channels through the primary $\alpha$-phase is the dominant cyclic plastic strain behavior. It was also observed that large cumulative plastic strain gradients develop across phase boundaries indicating that this is likely the driving force for delamination of the $\alpha/\beta$ interface as the materialization of bulk damage in the HCF regime. Additionally, Morrissey et al. (2000, 2001, 2003) have looked at the influence of texture on the cyclic plastic strain behavior, albeit within the limitations of the 2-D planar triple slip assumption. It turns out that this is quite a limiting aspect of the planar triple slip crystal plasticity model as it is unable to capture the most important aspect of texture in these materials, which is angle between the c-axis of grains with respect to neighboring grains and the imposed deformation field. Not coincidentally, the cumulative effective plastic strain distributions do not vary significantly in morphology or magnitude with the changes in texture investigated in their study. It has clearly been shown in Chapter III of this thesis that true 3-D texture in addition to phase distribution can play a vital role in the morphology of the cumulative effective plastic strain distribution (as well as the magnitude) in Ti-6Al-4V. Therefore, the uniaxial mean stress tests conducted in this Section will focus on effect of variation of realistic textures for a single fixed distribution of phases.

The finite element mesh used for the uniaxial simulations consists of 280 grains subjected to random periodic boundary conditions in the usual phase proportions of approximately 60% primary $\alpha$ and 40% lamellar ($\alpha + \beta$). Each grain is meshed with 36 4-noded quadrilateral reduced integration generalized plane strain elements (CPEG4). The generalized plane strain conditions allow for unconstrained uniform extension/contraction in the plane strain direction, but do not allow rotation of the planes.
of plane strain with respect to each other. The finite element mesh and phase distribution used in these simulations are given in Figures 4.4.

Figure 4.4 Finite element mesh and phase distribution for uniaxial simulations.

The loading direction for the simulations is chosen to be the transverse direction since texture effects are more pronounced when the textured materials are loaded in this direction. Simulations are carried out at 2 different $R$-ratios ($R = 0.1$ and $R = 0.8$) with a fixed maximum stress for 10 complete cycles under load-controlled conditions. These stress ratios are chosen such that both regimes of stress ratio behavior as noted by Morrissey et al. (2003) are investigated. For each textured material, the maximum applied stress varies and is taken to be the yield stress as defined in Section 4.1 (i.e., the stress at $\varepsilon^p = 0.001$). The macroscopic hysteresis are given in Figures 4.5-4.10 for the initial ramp, the 1$^{st}$ cycle and the 10$^{th}$ cycle. The ratcheting increment given in the figure headings is calculated as the difference in the maximum strain from the 10$^{th}$ cycle as compared to the 1$^{st}$ cycle.
Figure 4.5 Stress-Strain Hysteresis for Basal Textured Material

\[ \sigma_{\text{max}} = 694 \text{ MPa}, \ R = 0.1, \ \Delta \varepsilon_{\text{ratch}}^{\rho} = 1.763 \times 10^{-4} \]

Figure 4.6 Stress-Strain Hysteresis for Basal Textured Material

\[ \sigma_{\text{max}} = 694 \text{ MPa}, \ R = 0.8, \ \Delta \varepsilon_{\text{ratch}}^{\rho} = 2.052 \times 10^{-4} \]
Figure 4.7 Stress-Strain Hysteresis for Transverse Textured Material
\( \sigma_{\text{max}} = 795 \text{ MPa} \), \( R = 0.1 \), \( \Delta \varepsilon_{\text{ratch}}^{\nu} = 1.312 \times 10^{-4} \)

Figure 4.8 Stress-Strain Hysteresis for Transverse Textured Material
\( \sigma_{\text{max}} = 795 \text{ MPa} \), \( R = 0.8 \), \( \Delta \varepsilon_{\text{ratch}}^{\nu} = 1.277 \times 10^{-4} \)
Figure 4.9  Stress-Strain Hysteresis for Basal / Transverse Textured Material

\[ \sigma_{\text{max}} = 770 \text{ MPa} , \ R = 0.1, \ \Delta \varepsilon_{\text{ratch}}^{\sigma} = 1.927 \times 10^{-4} \]

Figure 4.10  Stress-Strain Hysteresis for Basal / Transverse Textured Material

\[ \sigma_{\text{max}} = 770 \text{ MPa} , \ R = 0.8, \ \Delta \varepsilon_{\text{ratch}}^{\sigma} = 1.918 \times 10^{-4} \]
The macroscopic stress-strain hystereses indicate that a significant amount of plastic ratcheting occurs for all three textured materials at both stress ratios over 10 loading cycles. The amount of ratcheting (calculated as the difference between the 1st and 10th cycles) observed ranges from $\Delta \varepsilon_{ratch}^p = 1.277 \times 10^{-4}$ for the transverse textured material with $R = 0.8$ to $\Delta \varepsilon_{ratch}^p = 2.052 \times 10^{-4}$ for the basal textured material at $R = 0.8$. Somewhat surprisingly the amount of ratcheting strain is not very sensitive to the changes in the stress ratio except for the basal textured material. The transverse and basal / transverse textured materials show differences of $\Delta \varepsilon_{ratch}^p$ at the two different stress ratios of less than 2%. The ratcheting strain for these two textures actually decreases (although only slightly) with an increase in stress ratio, which is counter to what is expected to occur based on the results and observations of Morrissey et al. (2001, 2003) as the loading case of $R = 0.8$ is above the transition stress ratio ($R = 0.7$) observed by Morrissey. Although, it should be noted that Morrissey et al. (2001, 2003) varied the stress ratio as well as $\sigma_{max}$ such that the loading conditions agreed with values on the modified Goodman diagram for Ti-6Al-4V in the HCF regime (life of $10^7$ cycles) which indicates that the effect of the transition in behavior at higher stress ratios is likely related to the maximum applied stress as well. Nevertheless, it still seems that a larger plastic ratcheting strain would be observed for the higher $R$-ratio as the mean stress is much higher (~240-280 MPa) at a stress ratio of 0.8. The lack of change in $\Delta \varepsilon_{ratch}^p$ with change in stress ratio for the transverse and basal / transverse textured materials is not clearly understood at this point. Further investigation of additional sources of information, such as cumulative effective plastic strain distributions and plastic strain maps may provide an explanation of this discrepancy between observed and expected behavior. The basal
textured material does however show an increase in ratcheting strain of approximately 16% when cycled at the higher stress ratio, which is more in line with what is anticipated. The rate of ratcheting for each textured material on a cycle by cycle basis is shown in Figure 4.11.

![Figure 4.11 Plot of ratcheting increment versus loading cycle.](image)

Figure 4.11 indicates that the rate of ratcheting decreases rapidly over the first few loading cycles and reaches a near steady-state value around the 8th or 9th cycle.

Contour plots of the cumulative effective plastic strain, $\bar{\varepsilon}^p$, distribution of are given in Figures 4.12-4.14 for the three textured materials at both stress ratios. Snapshots of the plastic strain history are taken at three different points corresponding to the end of
the initial ramp loading, the end of the 5th cycle, and the end of the 10th cycle, respectively. The accumulation of plastic strain with increased cycling is apparent for each type of textured material, although it is more obvious for the basal textured material shown in Figure 4.12. It is also noted that there does not seem to be much of a difference in the cumulative effective plastic strain plots for loading at the different stress ratios indicating that the amount of ratcheting is nearly identical at both stress ratios considered.

As was the case for the monotonic simulations in Chapter III, the basal textured material shows a more even distribution of cumulative plastic strain as compared to the transverse and basal/transverse textured materials. The progression of the coalescence of the plastic strain can clearly be seen for this type of texture. At the end of the initial ramp several relatively unconnected regions of moderate cumulative effective plastic strain are formed, which gradually evolve into larger, slightly more intense, interconnected regions. This is the type of plastic strain behavior observed by Morrissey et al. (2001, 2003) at higher stress ratios. The transverse and basal/transverse textured materials however exhibit entirely different behavior. The lower availability of \(\{a\}\)-type slip systems for these orientations when loaded in the transverse direction leads to more localized regions of plastic strain as can be seen in Figure 4.13 and Figure 4.14. Unlike, the basal textured material, the evolution of plastic strain for these two textures does not progressively accumulate until contiguous bands of plastic strain span a large portion of the microstructure. Rather for these textures, after initial loading a small number of localized regions of plastic strain form, and upon continued cycling they grow in intensity without very much yielding occurring in new regions which inhibits the coalescence of previously formed plastic zones. This type of highly localized behavior explains why the maximum
cumulative effective plastic strain for the transverse and basal / transverse materials is an order of magnitude higher than that of the basal textured material. For macroscopic strains approximately equal to 0.72-78% (depending on the texture), the maximum cumulative effective plastic strains for the transverse and basal / transverse materials are 1.54% and 1.86%, respectively, whereas the peak cumulative effective plastic strain for the basal textured material is 0.4%. One feature common to all of the cumulative effective plastic strain contours is that the location of the maximum value of cumulative effective plastic strain always occurs at or near an \( \alpha / (\alpha + \beta) \) phase boundary. The large gradients in cumulative plastic strain that develop at the phase interfaces are a result of the significant differences in strengths of the different phases. This observation is also consistent with what Morrissey et al. (2001, 2003) have observed, where they have suggested that this sort of behavior is the likely mechanism responsible for the decohesion of phase boundaries.
Figure 4.12 Cumulative effective plastic strain plots for basal textured material

a) $R = 0.1$ \( (\overline{\varepsilon}_p^{\rho} = 4.027 \times 10^{-3}) \)

b) $R = 0.8$ \( (\overline{\varepsilon}_p^{\rho} = 3.967 \times 10^{-3}) \)
Figure 4.13 Cumulative effective plastic strain distributions for the transverse textured material a) $R = 0.1$ ($\bar{\varepsilon}_p^\max = 1.548 \times 10^{-2}$) 

b) $R = 0.8$ ($\bar{\varepsilon}_p^\max = 1.543 \times 10^{-2}$)
While it is possible to observe and quantify ratcheting in terms of the offset of a uniaxial stress-strain curve or by giving a sequence of cumulative plastic strain plots, in general engineering components are subjected to complex multiaxial load histories. In such cases, it is useful to know the nature of the cyclic plastic strain behavior pointwise within the body. Cyclic plastic strain behavior is generally separated into three regimes: elastic shakedown, reversed cyclic plasticity, and plastic ratcheting. Elastic shakedown is defined as the stress or strain level below which an initially yielded material is no longer deforming plastically due to the build-up and influence of internal stresses. Reversed
cyclic plasticity is said to occur when the material undergoes reversed plastic straining during cycling without a net accumulation of plastic strain. Plastic ratcheting, as it has been previously defined, is said to occur when a net directional plastic accumulates over a given cycle. In general, a material point will have both a cyclic and ratcheting component to its strain history. Accounting for this fact and that, in general, bodies are subjected to complicated multiaxial loading conditions Ambrico and Begley (2000) have defined effective measures of the ratcheting and cyclic portions of the plastic strain behavior. These measures are defined over one complete cycle of the load history as

\[
\left( \Delta \varepsilon_{ij}^p \right)_{\text{ratch}} = \varepsilon_{ij}^p \bigg|_{\text{end of the cycle}} - \varepsilon_{ij}^p \bigg|_{\text{start of the cycle}} \tag{4.14}
\]

\[
\left( \Delta \varepsilon_{ij}^p \right)_{\text{cyc}} = \left( \Delta \varepsilon_{ij}^p \right)_{\text{max}} \bigg|_{\text{over the cycle}} - \left( \Delta \varepsilon_{ij}^p \right)_{\text{ratch}} \tag{4.15}
\]

\[
\Delta \varepsilon_{\text{cyc, eff}}^p = \sqrt{2/3 \left( \Delta \varepsilon_{ij}^p \right)_{\text{cyc}} \left( \Delta \varepsilon_{ij}^p \right)_{\text{cyc}}} \tag{4.16}
\]

\[
\Delta \varepsilon_{\text{ratch, eff}}^p = \sqrt{2/3 \left( \Delta \varepsilon_{ij}^p \right)_{\text{ratch}} \left( \Delta \varepsilon_{ij}^p \right)_{\text{ratch}}} \tag{4.17}
\]

From these conditions, elastic shakedown is defined as the regions in which

\[
e_{ij}^p \neq 0 \quad \text{and} \quad (\Delta \varepsilon_{\text{cyc, eff}}^p \text{ and } \Delta \varepsilon_{\text{ratch, eff}}^p) \leq C_{\text{cut-off}} \varepsilon_y \tag{4.18}
\]
where $C_{cut-off}$ is a cut-off value that determines the transition between cyclic plastic strain behavior and elastic shakedown. For a fixed yield strain, $\varepsilon_y$, a small value of $C_{cut-off}$ leads to more regions of the material being predicted as having cyclic and/or ratcheting plastic strain behavior, whereas increasing $C_{cut-off}$ decreases the amount of predicted cyclic plastic zones and increases the size of the elastic shakedown region. Below this value, the reversed cyclic plasticity and ratcheting components of the strain history are assumed to have zero effective amplitude. Depending on the application and the details of the model, there may be several justified different levels of $C_{cut-off}$ that could be used.

Using the definitions presented by Ambrico and Begley (2000), it is possible to quantify the material behavior over the last cycle for every element in the finite element model such that it fits into one of five categories: 1) elastic (unyielded), 2) elastic shakedown, 3) reversed cyclic plasticity, 4) plastic ratcheting, and 5) combined cyclic plasticity and ratcheting. A region is said to be undergoing plastic ratcheting if

$$\frac{\Delta \varepsilon_{ratch, eff}}{\Delta \varepsilon_{cyc, eff}} > 10 \quad \text{and} \quad \Delta \varepsilon_{ratch, eff} > C_{cut-off} \varepsilon_y$$

(4.19)

Likewise a region is said to undergo cyclic plasticity if

$$\frac{\Delta \varepsilon_{ratch, eff}}{\Delta \varepsilon_{cyc, eff}} < 0.1 \quad \text{and} \quad \Delta \varepsilon_{cyc, eff} > C_{cut-off} \varepsilon_y$$

(4.20)

A region of combined cyclic plasticity and plastic ratcheting is defined as

$$10 \geq \frac{\Delta \varepsilon_{ratch, eff}}{\Delta \varepsilon_{cyc, eff}} \geq 0.1 \quad \text{and} \quad \Delta \varepsilon_{cyc, eff}, \Delta \varepsilon_{ratch, eff} > C_{cut-off} \varepsilon_y$$

(4.21)
Accordingly, elastic shakedown is defined as

$$
\varepsilon_y^p \neq 0 \quad \text{and} \quad \Delta \varepsilon_{cyc,\text{eff}}^p, \Delta \varepsilon_{\text{ratch, eff}}^p \leq C_{\text{cut-off}} \varepsilon_y
$$

(4.20)

Now that we have rigorously defined how to quantify (at least by one measure) the regions of the finite element mesh in terms of its cyclic plastic strain behavior, it is now possible to examine the distributions of each regime for the uniaxial mean stress simulations. Figure 4.15 shows the plastic strain map for the basal textured material loaded for a stress ratio of 0.1 for different values of $C_{\text{cut-off}}$. The plastic strain maps are constructed such that each marker in the map represents the behavior at the centroid (since reduced integration elements have been used) of a finite element. The yield strains used in the construction of the plastic strain maps correspond to those listed in Table 4.6 for the different textured materials loaded in the transverse direction. All plastic strain maps and effective ratcheting increment contours have been calculated over the 10th cycle. Notice that this particular plastic strain map only contains two regimes of cyclic plastic strain behavior, ratcheting and elastic shakedown, and that as $C_{\text{cut-off}}$ is increased that the regions of plastic ratcheting slowly diminish. In order to more clearly illustrate the differences in the plastic ratcheting behavior of the three textured materials, the lowest value of $C_{\text{cut-off}} = 0.0025 \varepsilon_y$, has been chosen for the plastic strain maps for the uniaxial simulations.
Figure 4.15 Plastic strain maps for basal textured material showing the sensitivity to $C_{cut-off}$, $R = 0.1$. 

a) $\varepsilon_{cut-off} = 0.0025\varepsilon_y$

b) $\varepsilon_{cut-off} = 0.00375\varepsilon_y$

c) $\varepsilon_{cut-off} = 0.005\varepsilon_y$
Figures 4.16-4.18 show contour plots of the effective plastic ratcheting strain increment, $\Delta \varepsilon^p_{\text{ratch, eff}}$, alongside the corresponding plastic strain map for each texture and stress ratio. For a given texture the effective plastic ratcheting contour plot is cropped such that the simulation with the lowest peak value is set to as the maximum value in both plots, with everything above that value appearing as red so that a better comparison can be made for loading at the two different stress ratios. As might be expected from the discussion of earlier results, the basal textured material exhibits distinctly different behavior than the transverse and basal / transverse textured materials. At the lower stress ratio for the basal textured material there is still a significant amount of ratcheting taking place during the 10th cycle, whereas at the larger stress ratio more of the material is in the elastic shakedown regime. The transverse and basal / transverse textured materials essentially show no difference in cyclic plastic strain behavior at the two different stress ratios. The regions of plastic ratcheting and elastic shakedown appear virtually identical for the different $R$ – ratios for these two textures, and the maximum values of the effective ratcheting plastic strain increment are within 2% difference for the transverse textured material and within 15% for the basal / transverse textured material. In the basal textured material, the maximum effective plastic ratcheting strain increment is approximately 36% lower for a stress ratio of 0.8. This again reinforces that the basal textured material tends to elastically shakedown faster at the higher stress ratio as compared to the other two texture types. This is a result of homogeneous nature of the plastic deformation for this type of texture due to the symmetry of the distribution of favorably oriented soft slip systems. It also warrants mentioning that the local nature of the cyclic plastic strain behavior as given in the plastic strain maps gives a more
insightful picture to the extent of plastic ratcheting as compared to quantifying ratcheting as the offset from the uniaxial stress-strain curve as shown in Figure 4.11. The peak values of the effective plastic strain ratcheting increment as given in the contour plots in Figures 4.16-4.18 are approximately 5-10 times higher than the plastic ratcheting increments measured from the uniaxial stress-strain curves over the 10th cycle. A summary of the maximum effective plastic ratcheting strain increments as calculated from the definition Ambriico and Begley (2000) and the plastic ratcheting increments as measured from the uniaxial stress-strain curve, each calculated over the 10th cycle is given in Table 4.7 for each simulation.

Table 4.7  Comparison of the plastic ratcheting strain increment measured from uniaxial stress-strain curves and the maximum effective plastic strain increment as defined by Ambriico and Begley (2000).

<table>
<thead>
<tr>
<th></th>
<th>$\Delta\varepsilon_{ratch}^p$</th>
<th>$(\Delta\varepsilon_{ratch, eff}^p)_{max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basal ($R = 0.1$)</td>
<td>1.303x10^{-5}</td>
<td>6.874x10^{-5}</td>
</tr>
<tr>
<td>Basal ($R = 0.8$)</td>
<td>8.044x10^{-6}</td>
<td>4.428x10^{-5}</td>
</tr>
<tr>
<td>Transverse ($R = 0.1$)</td>
<td>6.514x10^{-6}</td>
<td>6.766x10^{-5}</td>
</tr>
<tr>
<td>Transverse ($R = 0.8$)</td>
<td>6.079x10^{-6}</td>
<td>6.690x10^{-5}</td>
</tr>
<tr>
<td>Basal / Transverse ($R = 0.1$)</td>
<td>8.330x10^{-6}</td>
<td>1.044x10^{-4}</td>
</tr>
<tr>
<td>Basal / Transverse ($R = 0.8$)</td>
<td>9.901x10^{-6}</td>
<td>1.211x10^{-4}</td>
</tr>
</tbody>
</table>

Another interesting aspect that is brought out in the plastic strain maps and effective ratcheting strain increment contours is that contrary to what the cumulative effective plastic strain contours given earlier in Figures 4.12-4.14 suggest, continuous bands of plastic ratcheting do exist in the transverse and basal / transverse textured materials. The basal / transverse textured material has the most active ratcheting regions.
and the largest values of effective ratcheting increment over the 10\textsuperscript{th} cycle when compared to the other two materials. The basal / transverse plastic strain map is characterized by several long bands of plastic ratcheting regions nearly crossing the entire statistical volume element. It can also be clearly seen that for all of the textured materials at both stress ratios that the large majority of the active ratcheting regions lie in the primary $\alpha$-phase. Additionally, the location of the maximum effective plastic ratcheting increment lies at an $\alpha/(\alpha+\beta)$ phase interface for all of the simulations. Again, this is in total agreement with the work of Morrissey et al. (2001, 2003) in regard to decohesion at the $\alpha/(\alpha+\beta)$ phase interface due to extensive ratcheting.
Figure 4.16 Subsurface $\Delta \epsilon_{ratch, eff}^p$ contours (left) and plastic strain maps (right) for basal textured material for two stress ratios. In the plastic strain maps, blue regions represent plastic ratcheting and green regions represent elastic shakedown.
Figure 4.17  Subsurface $\Delta \varepsilon_{\text{ratch, eff}}^p$ contours (left) and plastic strain maps (right) for transverse textured material for two stress ratios. In the plastic strain maps, blue regions represent plastic ratcheting and green regions represent elastic shakedown.
Figure 4.18  Subsurface $\Delta \epsilon_{\text{ratch, eff}}^p$ contours (left) and plastic strain maps (right) for basal / transverse textured material for two stress ratios. In the plastic strain maps, blue regions represent plastic ratcheting and green regions represent elastic shakedown.

Now that the concept of plastic strain maps has been introduced and used to show how cyclic plastic strain behavior can be quantified locally in terms of the different regimes, an investigation of the cyclic plastic strain behavior during fretting fatigue will be undertaken.
4.3 Fretting Simulations

The process of attachment fretting fatigue occurs when two components in contact under the presence of a sustained normal force are subjected to additional bulk cyclic loading during which the majority of the contacts experience little or no relative displacement between mating components except for small regions near the edges of contact. Fretting fatigue is a boundary layer phenomenon in which most of the plastic deformation and damage accumulation occurs at depths on the order of tens of microns and encompasses regions of only a relatively few grains into the depth of the material. Previous works (Goh et al., 2001; Goh, 2002) have shown that conventional J2-type plasticity models are unable to capture the heterogeneous nature of the deformation field in the surface and subsurface regions during fretting fatigue, and that crystal plasticity models, with their ability to account for explicit microstructural features, can provide insight into the dominant deformation mechanisms and related processes that contribute to material damage. The use of physically-based microstructural models to investigate the phenomenon of attachment fatigue is a relatively new area of research (Goh et al., 2001; Goh, 2002; Morrissey et al., 2003).

The focus of this modeling effort is to use the newly developed 3-D crystal viscoplasticity model to discern the effects of 3-D slip geometry for each phase, realistic polycrystal texture, and slip system anisotropy on the associated deformation mechanisms and plastic strain distributions in the surface and subsurface regions during attachment fatigue. In particular, these simulations are designed and performed to
validate and expand upon the previously obtained results using the idealized 2-D planar triple slip model (Goh et al., 2001).

The fretting model used in this thesis employs the “ideal fretting model” studied in the Ph.D. thesis of Goh (2002). The model consists of a rigid cylinder with a 10 mm radius in contact with an elastic-plastic half-space. To reduce the complexity of the simulations and to avoid unnecessarily detail calculations in far-field regions, the elastic-plastic half-space material definition has been separated into three regions. In the subsurface region directly beneath the line of contact, the crystal plasticity model is used to capture the role of microstructure on the cyclic deformation behavior. In the area adjacent to the crystal plasticity zone, the material definition is given using a standard ABAQUS (2003) plasticity model for cyclically deformed metals using a nonlinear kinematic hardening rule. The constants in the nonlinear kinematic hardening rule are determined internally within ABAQUS (2003) upon providing data points from the stabilized cyclic stress-strain curves given in Figure 4.2 via the command “*PLASTIC, HARDENING = COMBINED, DATA TYPE = STABILIZED”. A different set of elastic-plastic properties is determined for each type of texture. It is noted that although an elastic-plastic macro-model is used in the region adjacent to the crystal plasticity region that the elements in this portion of the model do not yield. This aspect of the model was included merely to recreate the construction of the “ideal fretting model” as described in Goh (2002). The entire plastic zone is contained within the crystal plasticity portion of the model. The material definition of the elastic-plastic half-space is then completed by creating a mesh with elastic properties adjacent to the homogeneous plasticity material model which at its boundaries is then connected to a series of infinite
linear elastic elements (CINEP4). The mesh size in the crystal plasticity region of the half-space is 0.005 mm which provides sufficient resolution of the number of elements spanning the contact width as well as a sufficient resolution of the number of elements (at least 30) per grain. As in the previous uniaxial fatigue simulations the elastic-plastic regions of the mesh consist of 3- (CPEG3) and 4-noded (CPEG4R) reduced integration generalized plane strain elements. No constraints are placed on the out-of-plane deformation. The strains that develop due to the out-of-plane plastic deformation are negligible and are on the order of 0.0001. The load history consists of the application of a normal force per unit length, P, which is initially imposed and held constant throughout the duration of the simulation. A tangential force per unit length, Q, is then applied and is fully reversed from +Q to –Q for three complete cycles. No displacement boundary conditions are needed for the elastic-plastic half-space since infinite elements have been employed at the outer boundary. A standard ABAQUS friction model has been used in conjunction with the contact pair as in the work of Goh (2002) via the command “*FRICTION, LAGRANGE” with the coefficient of friction $\mu = 1.5$. The finite element model is shown in Figure 4.19. Two different realizations have been used for the phase distribution in the crystal plasticity portion of the model which are in the usual phase proportions of 60% primary $\alpha$ and 40% lamellar ($\alpha + \beta$). The first realization is from early work in this thesis and the region was kept to a minimum so as to limit the computational intensity of the calculations. As the simulation and post-processing techniques became more streamlined, expanding the area of the crystal plasticity zone became feasible. Realization #1 consists of 226 grains and realization #2 consists of 450 grains. The two microstructural realizations are shown in Figure 4.20.
Figure 4.19  Fretting finite element mesh.
To investigate the effects of texture a series of three different load cases have been analyzed for each type of texture. The three loading cases are listed in Table 4.8.

Case 1: $P/P_y = 1.0$ and $Q/P_y = 0.1$, Case 2: $P/P_y = 1.0$ and $Q/P_y = 0.15$, and Case 3: $P/P_y = 1.0$ and $Q/P_y = 0.2$ where $P_y$ is defined as the force per unit length required to initiate yielding in the subsurface region. After this initial set of simulations, a fourth case, Case
4, is undertaken to ascertain the effect on the deformation modes as a function of the angle between the normal load direction and the c-axes of the grains comprising the polycrystal. To study this effect, the transverse textured material is taken and rotated about the normal direction of the plane. Two additional textures called herein as transverse “45” and transverse “90” where the majority of the c-axes in the polycrystal are distributed about lines at 45º and roughly parallel to the normal load direction, respectively. These types of textures are illustrated in Figure 4.20.

<table>
<thead>
<tr>
<th>Texture</th>
<th>Case</th>
<th>$P_y$ (N/mm)</th>
<th>$P/P_y$</th>
<th>$Q/P_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basal</td>
<td>1</td>
<td>443</td>
<td>1.0</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>-</td>
<td>-0.15</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>-</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Transverse</td>
<td>1,4</td>
<td>547</td>
<td>1.0</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>-</td>
<td>0.15</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>-</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Basal / Transverse</td>
<td>1</td>
<td>510</td>
<td>1.0</td>
<td>0.1</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>-</td>
<td>0.15</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>-</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Transverse “45”</td>
<td>4</td>
<td>426</td>
<td>1.0</td>
<td>0.1</td>
</tr>
<tr>
<td>Transverse “90”</td>
<td>4</td>
<td>528</td>
<td>1.0</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 4.8 Fretting simulation loading cases.

Figure 4.21 Modified transverse textures simulated to study effect of angle between normal load direction and c-axes of grains.
Cases 1, 2 and 4 are carried out with the phase distribution of realization #1 and Case 3 is carried out with microstructure realization #2. This does not affect the interpretation of results as the interest is in the qualitative nature of the results due to changes in texture. 

$P_y$ is calculated using Hertzian contact theory under plane strain conditions with a value of Poisson’s ratio equal to 0.349 (Goh, 2002) for a material that obeys the von Mises yield criterion. These conditions are used to estimate the normal load required to initiate subsurface yielding based on a representative von Mises material with the same macroscopic uniaxial yield stress properties as the various textured materials loaded in the rolling direction (yield stress properties given in Table 4.4). This assumption is made in light of the fact that a critical load required to initiate subsurface yielding for a crystal plasticity material cannot be easily defined as the plastic deformation in such a material is heterogeneous and varies uniquely with different polycrystalline representations of the microstructure based on the orientation of the grains comprising the aggregate. While the veracity of the assumption used in predicting the critical load to initiate subsurface yielding may be called into question and may need to be modified in future work, the consistency of the methodology is maintained in the current work for each type of textured material and the qualitative trends of the results should not be affected.

$$P_y = \frac{\pi R^* (1.85\sigma_y)^2}{E^*}$$

(4.21)

$R^*$ is the reduced radius of contact, $\sigma_y$ is the tensile yield stress (as defined in Table 4.5), and $E^*$ is the effective elastic modulus. Since we are dealing with a rigid cylinder in
contact with a semi-infinite half-space, the reduced radius of contact is simply the radius
of curvature of the cylinder, 10 mm, and the effective elastic modulus is simply the
elastic modulus of the semi-infinite half-space which is given for the various textured
materials in Table 4.2. The forces per unit length required to initiate yielding for the
various textures are given in Table 4.8

The results of the fretting simulations are quantified with three different plots:
cumulative effective plastic strain distributions \( \bar{\varepsilon}^p = \int \sqrt{2/3 \varepsilon_y d\varepsilon_y} \) at the end of
the third cycle, plastic strain maps calculated over the third cycle, and plots of the effective
plastic ratcheting increment calculated over the third cycle, \( \Delta \varepsilon_{\text{ratch, eff}}^p \). To be consistent
with the work of Goh (2002) a value of \( C_{\text{cut-off}}^y = 0.005 \varepsilon_y \) has been used for construction
of the plastic strain maps and contour plots of \( \Delta \varepsilon_{\text{ratch, eff}}^p \) where the yield stresses for the
different textured materials is given in Table 4.5.

Figures 4.22-4.24 show the cumulative effective plastic strain distribution for
simulation Cases 1-3. The results are qualitatively very similar to the contour plots given
for the uniaxial simulations in the sense that the basal textured material has a peak
cumulative plastic strain value approximately five times lower than the transverse and
basal / transverse textured materials for load Cases 1 and 2 when the tangential load is
relatively low and does not cause significant deformation at the leading or trailing edge of
contact. However, for Case 3 in which the tangential load is large enough to cause
significant plastic strain accumulation at the surface of contact, the maximum values of
accumulated plastic strain for the basal textured material only differ roughly with the
other two textured materials roughly by a factor of two. It is also worth mentioning that
for the lowest value of the tangential load (Case 1) that the basal textured material is the only one of the three materials which shows much a peak cumulative effective plastic strain at the surface of contact. For Case 1, the transverse and basal / transverse textured materials both have a maximum cumulative effective strain in the subsurface region. This is likely due to a local misorientation of grains in the subsurface region in which one of the grains lies in a hard orientation. The overall features and nature of the plastic strain distributions for each type of texture are also very similar to the uniaxial mean stress simulations in that the distribution for the basal textured material is roughly distributed in a semi-circular orb-like shape directly beneath the rigid indenter, while the transverse and basal / transverse textured materials display a much more localized distribution of plastic strain that forms in narrow bands approximately the width of a grain. The effective cumulative plastic strain distributions also show that the same type of plastic strain gradients across the phase interface observed in the uniaxial case are also prevalent during fretting fatigue with peak values of subsurface cumulative effective plastic strain predominantly occurring at phase interfaces.

Comparing the cumulative effective plastic strain contours for Case 3 to those of Goh (2002) with the same loading conditions reveals that the planar triple slip results most closely match with the results for the basal textured material. The planar triple slip model predicts that the maximum cumulative effective plastic strain value to be $\bar{\varepsilon}_{\text{max}}^p = 6.52 \times 10^{-3}$ at the leading edge of contact, while the 3-D crystal plasticity model predicts a value of $\bar{\varepsilon}_{\text{max}}^p = 5.79 \times 10^{-2}$ also at the leading edge of contact. The discrepancy between the magnitudes of $\bar{\varepsilon}_{\text{max}}^p$ is likely an effect of incorporating realistic textures and 3-D slip system crystallography. In the planar triple slip model when each slip system
has the same set of constants defining the flow stress, a true hard orientation does not exist. For this type of idealized texture, there will always be a relatively high Schmid factor on at least two of the prismatic planes. A plot of the cumulative effective plastic strain distribution from Goh (2002) is given in Figure 4.25.
a) Basal Texture – $a = 222.5 \, \mu m$ ($\bar{\varepsilon}_p^{\mu \varepsilon} = 3.493 \times 10^{-3}$)

b) Transverse Texture 255 $\mu m$ ($\bar{\varepsilon}_p^{\mu \varepsilon} = 1.759 \times 10^{-2}$)

c) Basal / Transverse Texture – $a = 252.5 \, \mu m$ ($\bar{\varepsilon}_p^{\mu \varepsilon} = 1.095 \times 10^{-2}$)

Figure 4.22 Cumulative effective plastic strain distributions ($P/P_y = 1.0$, $Q/P_y = 0.1$).
a) Basal Texture – $a = 222.5$ $\mu$m ($\varepsilon_{\text{max}}^p = 0.896 \times 10^{-3}$)

b) Transverse Texture – $a = 257.5$ $\mu$m ($\varepsilon_{\text{max}}^p = 2.573 \times 10^{-2}$)

c) Basal / Transverse Texture – $a = 255$ $\mu$m ($\varepsilon_{\text{max}}^p = 4.269 \times 10^{-2}$)

Figure 4.23 Cumulative effective plastic strain distributions ($P/P_y = 1.0$, $Q/P_y = 0.15$).
a) Basal Texture – $a = 227.5 \, \mu m \ (\bar{\epsilon}_\text{max} = 5.79 \times 10^{-2})$

b) Transverse Texture – $a = 252.5 \, \mu m \ (\bar{\epsilon}_\text{max} = 8.11 \times 10^{-2})$

c) Basal / Transverse Texture – $a = 255 \, \mu m \ (\bar{\epsilon}_\text{max} = 6.214 \times 10^{-2})$

Figure 4.24 Cumulative effective plastic strain distributions($P/P_y = 1.0$, $Q/P_y = 0.2$).
Plastic strain maps corresponding to loading Cases 1-3 are given in Figures 4.26-4.28. For all load cases, except for loading Case 2 for the transverse textured material, the plastic strain maps indicate that plastic ratcheting of the plastic strain is the dominant cyclic plastic deformation mechanism which is in agreement with the previously obtained results of Goh (2002). It is not understood why for loading Case 2 that reversed cyclic plasticity dominates the cyclic plastic deformation behavior. Initially it was thought, that the higher tangential load for Case 2 as compared to Case 1 was the reason for this observed behavior. However, the results for Case 3 show that for the largest normalized tangential load simulated in this thesis that plastic ratcheting is the dominant deformation mechanism even at higher tangential loads. It is noted however that the transverse textured material still has a significant contribution to the cyclic plastic strain behavior from the ratcheting component as illustrated in Figure 4.31 in the contour plots of the effective plastic ratcheting increment. Again, the cyclic plastic strain behavior exhibited in the uniaxial mean stress simulations is closely followed in the fretting simulations. The majority of the subsurface region that has yielded in the basal textured material has
already reached the regime of elastic shakedown. This result is consistent for all of the loading cases considered. However, the transverse and basal / transverse textured materials still have significant portions of the subsurface region undergoing plastic ratcheting at the end of 3 complete tangential loading cycles. Much as in the case of uniaxial loading the regions of the subsurface undergoing plastic ratcheting form relatively long continuous bands, roughly the thickness of a grain, of plastic strain permeating throughout the microstructure.

Comparing the results of the plastic strain maps created from the 3-D crystal plasticity model for Case 3 (Figure 4.28) to the results of Goh (2002) (Figure 4.29) clearly shows the importance of incorporating realistic textures and the additional sources of anisotropy into constitutive models for these materials. The dependence of the plastic strain map on texture is clearly illustrated. The 2-D planar triple slip model predicts somewhat “globular” regions of plastic ratcheting, whereas the 3-D crystal plasticity model reveals a banded nature of the plastic ratcheting behavior. Additionally, the zone of subsurface yielding is much larger for the transverse and basal / transverse textured materials as compared to that predicted by the planar triple slip model. It is also noted that the planar triple slip model predicts a gap between the zones that have yielded near the leading and trailing edges of contact and the region of material that has yielded directly below the line of contact, whereas the 3-D model predicts a slightly more continuous transition from the leading and trailing edges of contact to the larger subsurface plastic zones.
Figure 4.26 Plastic strain maps (P/Py = 1.0, Q/Py = 0.1).
Figure 4.27 Plastic strain maps ($P/P_y = 1.0$, $Q/P_y = 0.15$).
a) Basal Texture  b) Transverse Texture

c) Basal / Transverse Texture

Figure 4.28 Plastic strain maps (P/Py = 1.0, Q/Py = 0.2).

Figure 4.29 Plastic strain map from Goh (2002) P/Py = 1.0 and Q/Py = 0.2.
The contours of effective plastic ratcheting increment shown in Figures 30-32 reemphasize that the bands of plastic ratcheting lie almost exclusively in the primary α-phase with a slight amount of shearing through (α + β) colonies. In general, the trend is observed that as the normalized tangential load increases so does the maximum value of $\Delta\varepsilon^p_{\text{ratch, eff}}$. The maximum value of $\Delta\varepsilon^p_{\text{ratch, eff}}$ occurs exclusively either at the surface near the edges of contact or at an $\alpha/(\alpha + \beta)$ phase boundary. Both of these locations are consistent with experimental observations that cracks often nucleate at the edges of contact and/or at phase boundaries resulting from the large plastic strain gradients that develop of the phase interface. In general the morphology of the regions of plastic ratcheting do not change much due to increases in the tangential force. The most pronounced effect of increases of the tangential load on the cyclic plastic strain behavior is an increase of the effective plastic ratcheting increment.
Figure 4.30 $\Delta \varepsilon_{ratch, eff}^P$ contours ($P/P_y = 1.0$, $Q/P_y = 0.1$).
Figure 4.31  $\Delta \varepsilon^p_{\text{ratch, eff}}$ contours (P/P_y = 1.0 , Q/P_y = 0.15).
Figure 4.32  \( \Delta \varepsilon^p \text{ratch, eff} \) contours (\( P/P_y = 1.0 \), \( Q/P_y = 0.2 \)).
Simulations investigating the modified transverse textures in which the nominal orientation of the c-axes of the grains comprising the polycrystal is varied with respect to the normal loading direction echo qualitatively similar results to the previously discussed fretting simulations. The results are given in Figures 3.33-3.35 for the cumulative effective plastic strain distributions, plastic strain maps, and effective plastic ratcheting strain increments, respectively. An additional insight that has been brought to light in the study of the modified transverse textures is that the bands of localized plastic strain seem to be related to the nominal orientation of the c-axes of the grains in the polycrystal. The maximum cumulative plastic strain values for all three modified transverse textures are quantitatively very similar, ranging from 0.0134 for the transverse “45” textured material to 0.0176 for the true transverse textured material. The plastic strain maps highlight the inherent texture dependence of results, but they do not display any remarkably distinguishable features inherent to any of these transverse-type textured materials. Each plastic strain map is consistent with the earlier results which show that ratcheting of the plastic strain is the dominant mode of cyclic plastic strain behavior. The plastic strain maps and contours of effective plastic ratcheting strain increment also show the by now familiar vein-like arrangement of bands of plastic strain ratcheting coalescing predominantly in the primary $\alpha$-phase. Also, as in the other simulations the peaks and/or intense regions of $\Delta \varepsilon_{\text{ratch, eff}}^p$ are located near the edges of contact as well as at or near $\alpha/(\alpha + \beta)$ phase boundaries.
a) Transverse Texture – $a = 255 \, \mu m$ ($\overline{\varepsilon}^p_{\max} = 1.759 \times 10^{-2}$)

b) Transverse “45” Texture – $a = 217.5 \, \mu m$ ($\overline{\varepsilon}^p_{\max} = 1.342 \times 10^{-2}$)

c) Transverse “90” Texture – $a = 242.5 \, \mu m$ ($\overline{\varepsilon}^p_{\max} = 1.579 \times 10^{-2}$)

Figure 4.33 Cumulative effective plastic strain distributions ($P/P_y = 1.0$, $Q/P_y = 0.1$).
a) Transverse Texture  
b) Transverse “45” Texture  
c) Transverse “90” Texture  

Figure 4.34 Plastic strain maps (P/P_y = 1.0 , Q/P_y = 0.1).
Figure 4.35 $\Delta \varepsilon_{\text{ratch, eff}}^P$ contours ($P/P_y = 1.0$, $Q/P_y = 0.1$).
A 3-D crystal viscoplasticity model has been developed that accounts for many of the heterogeneous microstructural features of Ti-6Al-4V. The model includes distinct 3-D slip geometry for each phase, anisotropic strengths of different slip system families, microstructural length scale dependent slip system strengths, dislocation core-spreading for prismatic dislocations in the primary \( \alpha \)-phase, and realistic texture effects.

It has been clearly shown that the combination of texture and slip system anisotropy play a key role in determining both the macroscopic and microscopic deformation behavior in low symmetry polycrystalline materials such as Ti-6Al-4V. Additionally, the crystal plasticity model has been used to study the process of attachment fatigue, a process in which the volume of material undergoing plastic deformation is on the same scale as prominent microstructural features. Naturally, the distribution and nature of the cyclic plastic strain is found to be heavily influenced by the local heterogeneity of the material at the microstructural level. The fretting fatigue simulations show that ratcheting of the plastic strain is the dominant mode of cyclic plastic strain behavior, and that the distribution of plastic strain is highly dependent on
the texture of the material as well as the phase distribution. The basal textured material, due to its symmetry and the inherent preferential alignment of grains for glide on prismatic and basal slip systems, exhibits distinctly different cyclic plastic strain behavior than the transverse and basal/transverse textured materials in both mean stress and fretting fatigue simulations. The plastic zone for the basal textured materials is more evenly distributed as compared to the transverse and basal / transverse textured materials. Additionally, the majority of the plastic strain for the basal textured material reaches the regime of elastic shakedown prior to the 3rd tangential loading cycle, whereas the transverse and basal / transverse textured materials still exhibit a large amount of cyclic plastic ratcheting over the 3rd loading cycle. Both phase distribution and texture are shown to serve as microstructural features that promote plastic strain localization; these must be accounted for in models for this material when local variations of the plastic deformation fields are important to the application of interest.

In addition to verifying prior 2-D polycrystal plasticity results of Goh et al. (2001) that plastic ratcheting is the dominant mode of cyclic plastic strain behavior during fretting fatigue, the simulations also confirm the results of the 2-D polycrystal plasticity study of Morrissey et al. (2003) regarding the distribution of plastic strain for a dual-phase material representation. As in Morrissey et al. (2003), it has been observed for the transverse and basal / transverse textured materials that the ratcheting strain coalesces to form vein-like structures lying predominantly in the primary $\alpha$-phase, and that large cumulative plastic strain gradients and effective plastic ratcheting strain increments form at the $\alpha / (\alpha + \beta)$ phase boundaries, serving as likely sites for interfacial fracture. However, for the basal textured material there is a distinct absence of these vein-like...
structures. Instead, for this type of texture in which the majority of the plastic zone has already reached elastic shakedown, only a few isolated grains are undergoing plastic ratcheting over the 3rd tangential loading cycle. As it has been discussed earlier, this is a result of a large number of grains being preferentially aligned for deformation on soft basal and prismatic slip systems. Even a majority of the lamellar grains for the basal textured material are oriented favorably for the soft basal deformation modes as it is a feature of the model that the basal slip systems are easy glide modes in the $(\alpha + \beta)$-phase. This provides further explanation for the observation that the plastic zone is more evenly distributed for the basal textured material as compared to the transverse and basal / transverse textured materials. For the lower normalized tangential loads, the difference in the maximum values of cumulative effective plastic strain and effective plastic ratcheting increments are more pronounced when comparing the basal to the transverse and basal / transverse textured materials. However, as the tangential load is increased and more intense plastic shearing occurs at the surface near the edges of contact the differences in the peak values of cumulative effective plastic strain and effective plastic ratcheting increment are reduced as the surface effects dominate the localized plastic strain behavior as opposed to the subsurface texture dependent differential yielding of preferentially aligned grains.

5.2 Recommendations for Future Work

The present work has clearly demonstrated that the heterogeneous nature of materials when viewed at the microstructural level is important to consider in problems
of small scale plastic deformation such as fretting fatigue. The focus of this thesis has
mainly centered on how the distribution and behavior of the cyclic plastic strain is
affected by the distribution of phases, anisotropy of slip system strengths, and realistic 3-
D textures for a relatively small subset of fretting loading conditions. The insight and
results obtained indicate that further research on the process of fretting fatigue using
physically-based micromechanical models is warranted. In light of what has been
learned in the current work, there are two main areas in which future research efforts
should focus: 1) improvement of the physics in the constitutive model and 2) refinement
of the fretting finite element model to more closely reflect experimental conditions.

5.2.1 Constitutive Modeling

The version of the crystal viscoplasticity model for duplex Ti-6Al-4V presented
in this thesis includes many more sources of microstructural heterogeneity than the 2-D
planar triple slip model that was previously used to study fretting fatigue of this material
(Goh et al., 2001). The importance of which has been summarized in Section 5.1. There
is, however, still room for refinement of the flow rule and corresponding internal state
variable (ISV) evolution equations to more completely represent the active deformation
mechanisms and the scale dependence of their collective behavior. A list of possible
flow rule and ISV evolution equation modifications is summarized below.

- Inclusion of temperature dependence.
- Incorporating the thermally activated dislocation locking/unlocking mechanism
  for prismatic glide in the primary $\alpha$-phase based on the model of Farenc et al.
  (1993).
• Include dislocation density and dependence of microstructural length scale parameters in the ISV evolution equations, and rewrite the flow rule in the form of the Orowan equation.

\[ \dot{\gamma} = \rho_m b v + \dot{\rho}_m b l \]  

(5.1)

where \( \rho_m \) is the mobile dislocation density, \( b \) is the burgers vector, \( v \) is the mean dislocation velocity, and \( l \) is the characteristic dislocation spacing.

• Incorporate a more thorough treatment of dislocation mechanisms responsible for deformation in the lamellar regions as more experimental evidence becomes available (cf. Savage et al., 2004).

• Determine if the slip system flow exponent as determined from macroscopic stress-strain data is reasonable by checking model polycrystal simulation predictions versus creep and/or stress relaxation tests.

5.2.2 Fretting Finite Element Modeling

The fretting finite element model employed in this thesis corresponds to the highly idealized 2-D problem of rigid cylindrical indenter in contact with a semi-infinite elastic-plastic half-space. Consequently, this work was mostly concerned with quantifying the cyclic plastic strain behavior in terms of general trends more so than providing a direct comparison to experimental fretting observations. In future work, a significant effort should be devoted to developing more detailed descriptions of the fretting fatigue boundary value problem that capture the conditions of fretting fatigue experiments. A list of items that should be considered for next generation finite element modeling of fretting fatigue is summarized below.

• Run simulations in which both contacted bodies are allowed to deform.

• Run a more complete set of fretting fatigue simulations spanning a wider range of loading conditions enabling the creation of fretting maps (Goh, 2002).
• Use electron back-scattered defraction (EBSD) data from virgin specimen to incorporate realistic starting textures of real materials, including extended regions of globular primary $\alpha$-phase with low misorientation.

• Track the evolution of texture in the surface and subsurface regions and compare with experimental observations (Swalla, 2003).

• Explore the possibility of performing 3-D (geometry) fretting simulations to compare with previous 2-D results.

• Explore application of hierarchical simulation methods such as discrete dislocations and variable resolution continuum crystal plasticity in fretting scenarios.

With the continued increase in computational power and the improved efficiency in the post-processing and analysis processes, the tractability of performing larger scale crystal plasticity fretting simulations incorporating the suggested changes should be possible in the near future.
REFERENCES


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